

Influence of the support on stabilizing local defects in strained monolayer oxide films

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Two-dimensional materials with a honeycomb lattice, such as graphene and hexagonal boron nitride, often contain local defects in which the hexagonal elements are replaced by four, five, seven, and eight-membered rings. An example is the Stone-Wales (S-W) defect, where a bond rotation causes four hexagons to be transformed into a cluster of two pentagons and two heptagons. A further series of similar defects incorporating divacancies results in larger structures of non-hexagonal elements. In this paper, we use scanning tunneling microscopy (STM) and density functional theory (DFT) modeling to investigate the structure and energetics of S-W and divacancy defects in a honeycomb (2×2) Ti₂O₃ monolayer grown on an Au(111) substrate. The epitaxial rumpled Ti₂O₃ monolayer is pseudomorphic and in a state of elastic compression. As a consequence, divacancy defects, which induce tension in freestanding films, relieve the compression in the epitaxial Ti₂O₃ monolayer and therefore have significantly lower energies when compared with their freestanding counterparts. We find that at the divacancy defect sites, there is a local reduction of the charge transfer between the film and the substrate, the rumpling is reduced, and the film has an increased separation from the substrate. Our results demonstrate the capacity of the substrate to significantly influence the energetics, and hence favor vacancy-type defects, in compressively strained 2D materials. This approach could be applied more broadly, for example to tensile monolayers, where vacancy-type defects would be rare and interstitial-type defects might be favored.

KEYWORDS: local structural defects, elastic strain, monolayers, two-dimensional materials, ultrathin oxide films, scanning tunneling microscopy (STM), density functional theory (DFT)

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Indoor organic photovoltaics with high efficiency and flexibility using ZnO/Ag/ZnO-based transparent electrodes

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Energy harvesting devices such as organic photovoltaics (OPVs), utilizing the energy from the indoor environment, have received great attention owing to the increase in the use of indoor electronic devices. These OPVs have such attractive features as low cost, flexibility, band gap tunability of organic materials, and eco-friendliness, as energy sources. In this study, we fabricated flexible indoor OPVs using ZnO/Ag/ZnO-based transparent conducting electrodes (TCEs). These TCEs provided electrical and optical properties (i.e., a transmittance of 92%, a sheet resistance of 4.8 Ω /sq, and a root-mean squared surface roughness value of 2.1 nm). The OPVs with these ZnO/Ag/ZnO-based TCEs also exhibited further enhanced light absorption and mechanical stability due to the micro-cavity effect and quasi-amorphous structural properties of the ZnO/Ag/ZnO electrode. OPVs fabricated with poly (3-hexylthiophene):indene-C60 bisadduct photoactive layer and the ZnO/Ag/ZnO (40/9/50 nm) electrode showed power-conversion efficiency values of over 12% under a 500 lux luminance of light-emitting diode lamp, which is 20% greater than that of the reference OPVs with typical ITO TCEs. Furthermore, the OPVs exhibited an excellent mechanical stability on flexible polyethylene terephthalate substrates with power-conversion efficiency values of over 10%.

Dangerous industrial wastewater treatment based on vacuum evaporation technology

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At present, some enterprises can not deal with the dangerous industrial wastewater in a cheap and easy way. In view of this situation, we proposed a new method to deal with the wastewater. The method aims to save energy greatly by using a self-designed Double-way Phase Change Heat Exchanger (DPCHE). The DPCHE has a single vacuum-compression pump as the power source. Due to the vacuum effect, the wastewater is evaporated into vapour under the low temperature and low pressure condition. Then the vapour is turned into an overheating steam under the high temperature and high pressure because of the compression. The overheating steam is recirculated in the DPCHE for heat transfer, so the heat is passed from the overheating steam to the wastewater, and overheating steam will condense into clean water. The influence factors (evaporation temperature and compression ratio) on power consumption was also analyzed and verified by the experiment. The experimental results showed that the decrease of the value of above factors can improve the system recovery rate and reduce the power consumption. A set of system design parameters were selected according to the analysis results as the reference for production design.

1882-A-1902

Thermodynamic model of the single-stage gradational lead screw vacuum pump used in the chemical engineering

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Compared with the constant lead screw (CLS) vacuum pump, the gradational lead screw (GLS) vacuum pump, widely used in the chemical engineering, has the advantage of heat dissipation and saving energy. A thermodynamic model can provide a well explanation on these phenomena. The single-stage GLS (SGLS) vacuum pump is suitable for mass production owing to the simple construction and easy manufacture. Taking the SGLS vacuum pump as the research object, this paper divides the pumping process into four successive stages and proposes a thermodynamic model to analysis quantitatively. The characteristic curves of thermodynamic parameters are drawn and explained in detail. Moreover, the power consumption under diverse operating conditions are plotted and illustrated. The performances with different design structures are contrasted and discussed. A comparison between the SGLS vacuum pump and CLS vacuum pump with the same pumping speed is presented at the end of this paper.

2014-A-1902

Formation of a nanophase wetting layer under non-equilibrium conditions and the growth of a transition metal on silicon

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The nanophase transition metal layer was found to wet a silicon substrate at a room substrate temperature and a low metal vapor temperature. As shown by Electron Energy Loss Spectroscopy data, this wetting is accomplished by adapting the metallic coating to the substrate. Atomic Force Microscopy data shows the nanophase topography of the coating, while IR and UV Optical Spectroscopy data show the metallization and nanostructuring the interface layer of the substrate. Auger Electron Spectroscopy data show the differences in the nanophase wetting layer from the bulk phases (metal and silicide) in electronic structure and composition. These differences are clearly manifested in the phase transition into these bulk phases with an increase in the thickness or the temperature of the coating. It is assumed that the adaptation itself occurs due to the formation of a nanophase or non-bulk cluster structure in the coating, as well as due to its reduced atomic density. In addition, it also occurs due to the nanostructuring of the interface layer of the substrate, which minimizes the energy of the system. It is discussed the application of given results for metal-semiconductor contact and for nanoplasmonics / nanospintronics.

2032-A-1902

Construction of inverse LEED states using results of repeated slab calculations

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Photoemission spectroscopy is a useful method for investigating electronic states of crystal surfaces. Photoemission is an excitation process of electrons by light from occupied states to unoccupied states above vacuum levels.

In evaluating matrix elements of photoemission we need wave functions of unoccupied states satisfying correct boundary conditions, called inverse LEED states.

We present a method of constructing inverse LEED states using results of repeated slab calculations.

Inverse LEED states contain only out-going Bloch states in crystal regions.

On the other hand, wave functions of repeated slab calculations contain both out-going and in-coming Bloch states.

We present a method of constructing waves functions containing only out-going Bloch states using wave functions of repeated slab calculations.

This method is applicable to the case of multiple Bloch states in crystal regions.

We apply the present method to the Bi (111) surface, for which a spin and angle resolved photoemission spectroscopy (SARPES) experiment was performed (K. Yaji et al., Nat. Commun. 8, 14588 (2017)).

Calculated results reproduce experimental results.

The difference from the previous calculations imposing out-going boundary conditions in vacuum regions (K. Kobayashi, Phys. Rev. B 95, 205436 (2017)) is small.

Repeated slab calculations are widely performed by density-functional methods using readily available simulation packages. Since the present method is simple and can make use of these packages, it extends the possibility of calculations of photoemission spectroscopy.

2039-A-1902

Reactions in cryogenic ice films. Enhanced dissociation of acids by configurational entropy of mobile protons in ice

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It has been conceived that chemical reactions are extremely difficult to occur in ice at very low temperature, where atoms and molecules are frozen in position with minimal thermal energy and entropy. Contrary to this general behavior, certain weak acids including fluoroacetic acids dissociate spontaneously and more efficiently in cryogenic ice than in aqueous solution at room temperature. The enhanced reactivity of weak acids is an unexpected consequence of proton transfer equilibrium in ice. The configurational entropy of highly mobile protons in ice shifts the acid dissociation equilibrium forward. Although this entropy is generated in the solid phase water, it is comparatively large in magnitude with the entropies of water vaporization and acid dissociation reactions in aqueous phase. Therefore, this thermodynamic driving force is quite effective for driving proton transfer reactions in the ice environment.

Probing exciton complexes and charge distribution in inkslab-like WSe₂ homojunction

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By virtue of the unique layer-dependent band structure and valley-selected optical/electronic properties, atomically-layered transition-metal dichalcogenides (TMDs) exhibit great potentials such as in valleytronics and quantum devices, and therefore have captured significant attentions. Precise control of the optical and electrical properties of TMDs is always the pursuing goal, not only for real applications but also for understanding fundamental physics of quasi-particles' (such as exciton's) many-body interactions; constructing advanced structures that allow playing with more degrees of freedom may hold the key.

Here, we introduce a triangular inkslab-like WSe₂ homojunction with a monolayer in the inner surrounded by a multilayer frame. Benefit from this interesting structure, the photoluminescence (PL) peaks redshift up to 50 meV and the charge density increases about 6 times from the centre to the edge region of the inner monolayer. We demonstrated that the Se-deficient multilayer frame provides the excessive free electrons for the generation of the electron density gradient inside the monolayer, which also results in the spatial variation and distribution gradient of a series of exciton complexes. Furthermore, we observed the strong rectifying characteristic and clear photovoltaic response across the homojunction by measuring and mapping the photocurrent of the devices. Our result provides another route for efficient modulation of the exciton-complex emissions of TMDs, which is exceptionally desirable for the layer- & charge-engineered photonic and optoelectronic devices.

Damping Property of YSZ Coatings Prepared by Flame Spraying/EB-PVD

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With the continuous advancement of aviation technology, the vibration damage of key structural components (compressor blades, turbine blades, etc.) in aeroengines has become more prominent. Applying damping coatings to the vibrating structure is an effective means of suppressing vibration and reducing vibration damage. Due to its poor environmental stability, traditional organic polymer damping coatings have been unable to cope with the increasingly harsh working conditions of advanced aeroengines, which promotes the development of hard coating damping technology. Hard coating is a kind of coating materials made of metal, ceramics or both. The hard coating has sufficient strength and toughness, and has the characteristics of no dependence on amplitude or frequency. It is less dependent on temperature and has higher damping characteristics compared to the organic polymer material. Based on the above advantages, hard coating has a broader prospect than traditional polymer damping coating.

YSZ(ZrO₂-8%Y₂O₃) coating samples were prepared by flame spraying method and electron beam physical vapor deposition (EB-PVD). The surface morphology, chemical composition and phase structure of the coating samples were analyzed by scanning electron microscopy (SEM), energy dispersive spectrometer (EDS) and X-ray diffraction (XRD), respectively. The damping property of coating samples were characterized by dynamic thermomechanical analyzer (DMA).

Manganese-Doped Tin Oxide for Highly Flexible and Transparent Multilayer Electrodes with Index-Matching Layers

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Transparent electrodes for flexible devices are limited by the brittleness of the transparent conductive oxide layer. To address this issue, we fabricated transparent Mn (2.59 wt.%) -doped tin oxide (MTO)/Ag/MTO films with refractive index-matching layers (IMLs) on a polyethylene terephthalate (PET) substrate. To reduce refractive index-mismatching, polydimethylsiloxane (PDMS) and MTO layers were inserted between the MTO/Ag/MTO multilayer film and the PET substrate. MTO and Ag were deposited by RF/DC magnetron sputtering at room temperature, whereas spin-coating was used to deposit PDMS at various dilution ratios in hexane. In this study, pattern visibility was examined by comparing the differences in the color and reflectance of oxide/metal/oxide multilayers before and after adding the PDMS and MTO IMLs. In addition, the effects of the PDMS dilution ratio on the electrical and optical characteristics were also investigated. The MTO/Ag/MTO/PDMS/MTO multilayer films showed high transmittance (>86% at 550 nm) except at the dilution ratio of 1:50. As the PDMS dilution ratio increased from 1:50 to 1:200, the reflectance difference (ΔR) increased from 0.08% to 0.35% and the color difference (Δb^*) increased from 0.31 to 1.23. The maximum resistance changes of the multilayer films were 0.126% and 0.124% after outer and inner bending, respectively, for 10,000 cycles with a radius of curvature of 4 nm. Owing to their improved pattern visibility properties and bending properties, the developed multilayer films with IMLs will be applicable to a wide variety of flexible devices.

Performance investigation of the perovskite solar cell with vacuum sputtered vanadium oxide anode interface modified layer

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In recent years, organic solar cells have attracted many scholars and experts to invest in research, especially the increased efficiency of perovskite solar cells (PSCs) is beyond the others. In this study, a vanadium oxide (VOx) film was deposited on ITO glass substrate by radio frequency magnetron sputtering system as an interface modification layer of PSCs. The interface modification layer was inserted between the ITO anode and the PEDOT:PSS hole transport layer of the PSCs to avoid PEDOT:PSS with acidic etched ITO, which could reduce interface defects. The ultraviolet photoelectron spectroscopy (UPS) was used to measure the work function (4.62 eV) and the valence band maxima (4.96 eV) of the VOx film and the optical energy bandgap of the VOx measured and evaluated using transmittance spectrum was 2.82 eV. Consequently, the energy level of the PSCs with VOx interface modification layer could be more match, which could improve the transmission efficiency of the photo-generated carriers. The PSCs with VOx interface modification layer were fabricated and investigated. Compared with the performance of the PSCs without VOx interface modification layer, the short-circuit current density and power conversion efficiency of the PSCs with VOx interface modification layer were increased from 21.15 mA/cm² to 29.66 mA/cm² and 11.04% to 16.77%, respectively. Consequently, the VOx film was quite suitable as an interface modification layer for PSCs to improve the performance of PSCs.

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2059-A-1902

molecular dynamics simulation of erosion failure mechanism of thermal barrier coatings

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At present the main development direction of aero engines is to increase the inlet temperature of the engine turbine and the thrust-weight ratio of engines. In order to meet the higher performance requirements of advanced aero-engines, thermal barrier coatings (TBCs) have been widely used and developed as a viable technology to reduce the operating temperature of hot-end components. However, the working environment of the aero-engine is complicated, Particles in the air will corrode the thermal barrier coatings and eventually lead to the coating peeling failure. In order to overcome the coating damage caused by particle erosion, it must be explained from the microscopic failure mechanism.

Yttrium oxide stabilized zirconia(YSZ) crystals were constructed by Material Studio software, and models of erosion particles of different mass were established. The impact simulation calculation was carried out by LAMMPS software. NiCrAl bonding layer was prepared by Atmospheric Plasma Spraying(APS), and YSZ coating was prepared by electron beam physical vapor deposition (EB-PVD). Using supersonic flame currents to conduct particle erosion experiments. The etched substrate was characterized locally by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The surface morphology and microstructure of the etched substrate were obtained. The experimental results were compared with the simulation results.

oxygen reduction reaction activity for surface-strain-controlled Pt(111) model shell surfaces

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Oxygen reduction reaction (ORR) is a key reaction of polymer-electrolyte fuel cells (PEFC): ORR activity enhancement mechanisms for Pt-based alloy (Pt-M) catalysts directly likes to developments of highly-efficient cathode catalysts for the PEFC. To clarify ORR enhancement mechanisms, well-defined model catalyst approaches are effective. In this study, the relation between ORR activity and surface nano-structures are investigated for the Pt/M (M=early transition metals, e.g., Zr, Mo) model catalysts. The UHV-APD-EC apparatus is described elsewhere [1,2]. Pt and M were alternately deposited onto a clean Pt(111) substrate by the APDs in UHV. Structural analysis for the prepared Pt/M model catalyst samples are conducted by in-plane XRD, cross-sectional STEM, etc. Electrochemical evaluations were conducted in N₂-purged and O₂-saturated 0.1M HClO₄. Surface strain estimated by in-plane XRD showed that tensile strain worked on Pt(111) shell surfaces on the investigated Pt-M(111) alloy layers. The ORR activities of the samples were several times higher than clean Pt(111) surface, indicating that not only compressive- but also tensile-strained Pt(111) shell on the Pt-M(111) alloy layers contribute to the ORR activity enhancements.

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Improved efficiency of CNT-PEDOT:PSS/n-Si heterojunction solar cell by optimization of CNT content

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The formation of p-n junction in a traditional silicon solar cell needs high temperature process. Recently, polymer/n-Si hybrid solar cells feature the low cost advantage for their simple and low temperature processing therefore it is worthy for further study. In this study, we replace PEDOT:PSS with CNT-PEDOT:PSS composite to fabricate the CNT-PEDOT:PSS/n-Si heterojunction solar cell. PEDOT:PSS is commonly used as a p-type semiconductor or hole transport layer in the organic solar cell because its high transparency and good conductivity. Adding CNT into PEDOT:PSS hopes to optimize the characteristics of PEDOT:PS, so that the efficiency of CNT-PEDOT:PSS/n-Si heterojunction solar cell can be further improved.

CNT-PEDOT:PSS films were fabricated with mixed of PEDOT:PSS and CNT aqueous solutions by spin coating. In order to optimize the conductivity of CNT-PEDOT:PSS, we first optimized the content of DMSO in PEDOT:PSS, and then followed a systematic study in varying CNT content. The optical and electrical properties of CNT-PEDOT:PSS films were characterized by UV-VIS spectrometry and four point probe, respectively. Finally, the power conversion efficiency (PCE) of CNT-PEDOT:PSS/n-Si heterojunction solar cell was performed under AM1.5 illumination with a solar simulator.

The results show that CNT-PEDOT:PSS composite could effectively enhance the PCE of CNT-PEDOT:PSS/n-Si heterojunction solar cell. The highest PCE of 7.1% is achieved for CNT-PEDOT:PSS/n-Si solar cell with 3% CNT in composite. This value is 47% higher than the PCE of PEDOT:PSS/n-Si solar cell.

New sputtering technology based on strongly non-equilibrium process

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Strongly non-equilibrium processes used at an atomic level in a new sputtering technology of thin films and coatings are: (1) heating to high temperatures without slow substrate heating, (2) high pressures (>1000 GPa) used in the coating formation, and (3) extremely fast cooling (> 10¹⁰ K/s) of the created coating material. The principle of this technology is explained. The utilization of this technology for creation of advanced coatings with new unique properties is demonstrated in sputtering of the following coatings: (1) alloy coatings with high-temperature beta-phase sputtered at low temperatures close to room temperature [1], (2) overstoichiometric nitrides which exhibit high hardness due to the presence of the singly bonded pernitride structural unit [2,3], and (3) superhard flexible Ti coatings with high hardness (up to 20 GPa) several times higher than that of the bulk Ti metal [4]. The technology may be used for depositions not only on large areas such as sheets but also on parts of complex shapes, and hence it has a high application potential.

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Note for the program committee (not to appear in the abstract): We would much appreciate if our contribution could be included into the super area 10 Advanced processing. We did not find a way to indicate that super area in the selection of the topic.

optimization of geometry for sputter-ion pump by a multi-physics coupling simulation

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The sputter-ion pump (SIP) is widely used to get clean vacuum environment as well as Extreme high vacuum condition. The advantages such as no noise, no vibration, and no oil pollution has helped SIP to win a huge popularity in application fields, like X-ray photoelectron spectroscopy[1], medical instruments[2] and Micro-Electro-Mechanical Systems fabrication[3]. The authors perform simulations of pumping performance at the low magnetic field using Multi-physics coupling method and Monte Carlo method to optimize the structure of a SIP. Firstly, Penning discharge is simulated by Multi-physics coupling method. The incident angle and energy of ions are obtained as initial conditions of sputtering yield calculation. Secondly, the sputtering yield on the cathode are obtained from the Monte Carlo simulation. Finally, we calculate the effective pumping speed for various structures. And the pumping speed is the evaluation criteria for structural optimization. We have carried out the experimental verification and achieved a good agreement. We hope the method will provide an instructive guidance for the future SIP design and development.

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Research on Transport Characteristics of Charged Particles in Sputtering Ion Pump

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Sputter ion pump, also known as Penning pump, is widely used in ultra-high vacuum systems due to its non-polluting and vibration-free characteristics[1]. In this research, the finite element method[2] was used to simulate the single-cylinder discharge model of the sputter ion pump, and the electron density distribution and electron temperature distribution were obtained. By tracking the incident ions, the average angle and the average energy of incident ion on the surface of the cathode plate are obtained, and then the sputtering yield and the theoretical pumping speed are obtained. The study found that the angle of incident ions has a huge impact on the pumping speed, while the incident energy has little effect on the pumping speed. Therefore, by optimizing the geometry and electromagnetic field distribution, increasing the angle of incidence ions will have a positive impact on the pumping speed of the sputter ion pump.

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Bonding state analysis of zirconium-oxygen-coated tungsten (100) surface at 1500K

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We investigated a zirconium-oxide-coated-tungsten (100) surface, which has been widely used as electron emitting surface of Schottky emitters. To extract the electrons, the emitter is heated up to approximately 1800K. The work function of the (100) surface is selectively lowered by the coating of Zr and O, and surface diffusion of the atoms are very fast on the tungsten surface at the operation temperature. These characters are favorable for high brightness and stability of the electron source, that is, the high brightness is originated from the low work function, and the stability is based on the quick surface recovery. The mechanism behind these characters, however, are not cleared. This is because the characters appear at more than 1400K, but it is difficult to analyze the surface at high temperature.

In this report, we improved our sample heating system and investigated the zirconium-oxide-coated-tungsten (100) surface by using X-ray photoemission spectroscopy at more than 1500K. The stable heating system enable us to obtain highly reliable spectra, and we can discuss the detail bonding state of the atoms on the surface at high temperature. We found that a large amount of oxygen is stably maintained on the surface even at the high temperature. Moreover, zirconium and tungsten are partially oxidized, and stoichiometry of those oxides are clearly different from the stable oxide in the bulk. From these results, we suppose that the partial oxidation are the origin of the low work function and fast surface diffusion on the tungsten surface.

Bi₂O₃ films prepared by rf reactive magnetron sputtering

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The Bi₂O₃ films have been deposited onto quartz substrate by rf reactive magnetron sputtering. The deposited Bi₂O₃ films have been annealed at different temperatures. The phase transition of the films is characterized by x-ray diffraction and Raman scattering. The film structure is characterized by SEM. The as-deposited Bi₂O₃ film shows the δ -phase dominated amorphous structure. This δ -phase dominated amorphous structure transforms completely to β -phase and α -phase after annealing at 300 °C and 500 °C respectively. The film annealed at 400 °C shows very strong α -phase with small portion of β -phase. The films annealed at 400 °C also shows a nanorod structure, which may have a potential application in the photocatalytic area.

Aesthetic multilayered thin film coatings on Japanese traditional paper ‘Washi’

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Japanese traditional paper ‘Washi’, which is hand-made from natural fibers of the wood pulps and therefore has the coarse fiber-formed surface, has been coated with the 7-layered TiO₂/SiO₂ thin films with thicknesses of TiO₂:240 nm /SiO₂:110 nm for red-colored reflection, TiO₂:190 nm /SiO₂:85 nm for green-colored reflection, and TiO₂:175 nm /SiO₂:70 nm for blue-colored reflection by magnetron sputtering to enhance its decorativeness by using the dispersion of the interference reflection due to its coarse surface. The black-dyed Washis coated with the 7-layered TiO₂/SiO₂ thin films showed red, green, or blue-colored interference-reflections as designed. Due to the dispersion of the viewing angle and to the unevenness of the film thickness, the reflections with areal-dispersion of the color were shown. The optical microscopy images of the Washis coated with the 7-layered TiO₂/SiO₂ thin films also showed red, green, or blue-color reflections from the surface organized by the coarse fibers, showing the dispersion of the reflection colors in 1-10 μm ranges. This results in the fine-areal dispersion in the reflection colors. Whereas the non-black-dyed Washis coated with the 7-layered TiO₂/SiO₂ thin films showed weaker reflections of red, green, and blue colors compared to the black-dyed Washis coated with the 7-layered TiO₂/SiO₂ thin films, by the optical microscopy observation, the dispersion of the interference reflection colors was confirmed. The fine-areal dispersion of the reflection color enhances the attractiveness of the Washi and widens its aesthetic applications.

A model of coordination self-assembly of Fe-terephthalate on Cu(100) surface

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Surface confined metal-organic networks (SMON) have been attracting much attention in recent years, since they represent a unique type of two-dimensional materials that have new magnetic, electronic and catalytic properties [1]. SMON structure is determined by a subtle balance between molecule-molecule interactions, metal-molecule interactions, and molecule-surface interactions. In this regard, the structure and properties of SMON are much richer comparing to 3D MOFs. On the other hand, for the same reason, the structure and physicochemical properties of SMON are extremely difficult to control. It requires a detailed understanding of the mechanisms and driving forces of the SMON self-assembly.

Here we report a detailed lattice gas model of adsorption layer of terephthalic acid and Fe on Cu(100) surface under ultra-high vacuum conditions, taking into account multiple interactions in the adlayer: hydrogen bonds, surface mediated interactions and carboxylate-Fe coordination bonds. We have calculated the ground state phase diagram of the adlayer. At non-zero temperatures the model was investigated with Monte Carlo method as implemented in the SUSMOST code [2]. We have explored the effect of metal-ligand partial pressures ratio and temperature on the structure of adsorption layer. Based on the published STM results [3] we have determined the minimal set of the interactions that reproduces all the experimentally observed phases.

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A lattice model of 1,3,5-trispyridylbenzene/copper adsorption layer on Au(111) surface: phase diagram and Monte Carlo simulation

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Molecular self-assembly is a promising approach to create functional nanostructures. Recently, much attention has been given to self-assembly in adsorption layers consisting of organic molecules coordinated by metal atoms on solid surfaces [1,2]. To find the most effective strategy for designing surface confined metal-organic frameworks with the desired structural, electronic, and magnetic properties it is necessary to understand in details the mechanisms and driving forces of the self-assembly.

We developed a detailed lattice model of self-assembling monolayer of 1,3,5-trispyridylbenzene (TPB) molecules and Cu atoms on Au(111) surface under ultra-high vacuum conditions, taking into account two types of TPB-Cu coordination interactions: bi- and tridentate. Series of "flower" type ordered structures appear in the adlayer at zero temperature as a result of the competitive bidentate and tridentate interactions. It is demonstrated that our model can describe the whole class of the adsorption systems differing by the metal atom. We performed a statistical simulation of the model using the Monte Carlo method at room temperature in SuSMoST code [3]. We were able to reproduce the experimentally observed phase behavior of the adsorption layer [2]. The developed model can be further applied to predict self-assembling layers of "Y-shaped" molecules and transition metal atoms on a metal surface.

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Characteristics of AlN epilayers grown by mixed-source hydride vapor phase epitaxy

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Epilayers of AlN and AlGa_N alloys with high Al composition have been employed in high-frequency, high-voltage switching devices as well as solid-state ultraviolet (UV) optoelectronics performance for III-nitride devices [1, 2]. In this study, AlN epilayers using a mixed source (Al+Ga) with 95 % atomic fraction of Al by a mixed-source hydride vapor phase epitaxy (HVPE) method was grown directly on sapphire substrates without a buffer layer at around 1120 °C. The grown epilayer consists of AlN alloy at the upper region and AlGa_N alloy in the nucleation region just above the sapphire substrate. The upper part of the epilayer gradually transformed from AlGa_N into AlN alloy owing to a decrease in the Ga content of the AlGa_N alloy grown on the sapphire substrate with increasing growth thickness. During the growth of epilayer grown directly on the sapphire substrate, the role of Ga in the mixed source (Al+Ga) and the growth mechanism of the epilayer with varying Ga contents depending on the growth thickness were investigated. We found that Ga in the mixed source (Al+Ga) only acted as an activation material rather than directly contributing to the growth of the epilayers. The mixed-source HVPE method appears suitable for the growth of thick AlN epilayers.

Properties of AlGaIn/GaN epilayers grown by HVPE method

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In this study, we prepared two epilayers, namely an AlGaIn/GaN DH and a thick GaN:Si layer on a sapphire substrate grown by a previously developed method based on mixed-source HVPE. The mixed-source HVPE consists of a source zone with an RF heating coil, which is used to control high temperatures and to easily regulate the change in temperature; a multi-graphite boat filled with the mixed source, to insulate against high temperatures and for the control of growth rate through the adjustment of the quantity of the mixed source; and a growth zone with three furnaces. These two epilayers were used to fabricate a vertical blue LED without a traditional substrate. Additionally, the thick GaN:Si layer was grown like a bulk material to minimize the effect of dislocations formed during the epilayer growth. The dislocation density in the thick GaN:Si layer was investigated at four positions in the bare chip by using field-emission scanning electron microscopy (FE-SEM), high-resolution X-ray diffraction (HR-XRD), and transmission electron microscopy (TEM). Furthermore, the bulk-like thick GaN:Si layer served as both a buffer layer and a new substrate for the vertical blue LED. It appeared that the AlGaIn/GaN DH, which was grown on the thick GaN:Si epilayers with low TD density, far away from bottom of the bare chip, minimized the interference by TDs owing to the thick buffer layer. By growing the AlGaIn/GaN DH and the GaN:Si layer as both the buffer layer and the new substrate using the multi-graphite boat and mixed-source HVPE method, we succeeded in fabricating the vertical blue LED.

Mixed-source hydride vapor phase epitaxy method for the growth of AlN nanowires

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AlN NWs with AlGa_N heterostructures, such as AlGa_N/AlN quantum wells or quantum dots, attain high internal quantum efficiency even at room temperature leading to significant advances in single photon sources, electrically pumped nanolasers, photovoltaic devices, optical sensors and deep ultraviolet LEDs [1, 2]. In this study, the AlN nanowires (NWs) were grown on sapphire, quartz, Si (111), and 6H-SiC substrates by the mixed-source hydride vapor phase epitaxy (HVPE) method. The simplified reactor was designed to minimize the reaction between quartz and AlCl₃ vapor species with a high partial pressure at 1150 °C and to reduce the response distance between the vapor species and source gases by overlapping the source zone edge just above the first substrate in the growth zone. AlN NWs grew directly on the sapphire substrate, and on AlN epilayers on the quartz, Si (111), and 6H-SiC substrates, respectively, using the mixed-source (Al+Ga). The characteristics of AlN NWs grown on the four substrates were investigated by energy dispersive X-ray spectrometry and field emission scanning electron microscopy. These results suggest that the mixed-source HVPE method performed in a simplified reactor designed in series without any separation between the source zone and growth zone is suitable for the growth of AlN NWs and epilayers on various substrates.

Antimicrobial nanocellulose-based materials functionalized in supercritical carbon dioxide

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Supercritical carbon dioxide is a non-toxic green solvent demonstrating great interest in the biomedical field. The high diffusion coefficient, low critical parameters and easy solvent recovery make it a great alternative to conventional solvents. In this context, bio-based cellulose nanofibrils (CNFs) aerogels with various morphologies were functionalized in supercritical CO₂ to yield antimicrobial wound dressings.

To study the influence of the structure on the loading/release efficiency and final antibacterial activity, three types of CNFs-based materials were prepared from different processes and compared. Highly porous aerogels were obtained from supercritical drying. Cryogels with sheet-like structures were prepared from directional freeze-drying. Finally, vacuum filtration and drying of CNFs suspension formed non-porous membranes.

Synthetic and natural antimicrobial molecules were grafted or impregnated on the nanocellulose matrices in a pressurized chamber under mild supercritical conditions. X-ray photoelectron spectroscopy, fluorescence spectroscopy and solid-state NMR analysis were performed to confirm the presence of active compounds. Drug release profiles with time were obtained from UV-visible spectroscopy analysis of the released drug in a buffer solution and showed that the structure plays an important role on the released amounts, which varied from 5 to 85 mg/g of material.

Finally, the impregnated nanocellulose-based materials were tested against three microorganisms representative of the wound microflora: two bacteria (*Escherichia coli* and *Staphylococcus epidermidis*) and a yeast (*Candida albicans*). The promising results showed zones of bacterial inhibition in solid nutrient media, bacterial concentration decrease in liquid growth media as well as contact active properties.

Dielectric tunable Bi₂O₃-MgO-Nb₂O₅ thin films

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Cubic pyrochlore Bi_{1.5}MgNb_{1.5}O₇ (BMN) thin films were prepared onto Pt-coated sapphire substrates by rf magnetron sputtering deposition from stoichiometric targets. The effects of growth condition (such as substrate temperature, total pressure, O₂/ (O₂+Ar) ratio) on structures and dielectric properties of BMN thin films are studied. Finally, we have prepared the BMN thin films with dielectric constant of 179, dielectric loss of 0.007, and dielectric tunability of 50% at 1.5 MV/cm. The Bi_{1.5}Mg_xNb_{2.5-x}O_{8.5-1.5x} (x=0.7-1.3) materials with different Mg contents are investigated to study the dielectric tunable mechanism of BMN materials, which indicated that the Mg²⁺ ions occupied the B-site first and then entered A-site after the B-site were fully occupied. The dielectric tunability of BMN thin films increased with Mg²⁺ concentration when x<1, whereas it did not exhibit further increase in the thin films with excess Mg²⁺ content. However, the dielectric loss of BMN thin films changed little with the studied compositions, which remained in a low level of ~0.006 at 1 MHz.

2096-A-1902

multi-parameter analysis on pumping performance of gas-liquid jet vacuum pump by numerical method

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Gas-liquid jet vacuum pump is a low vacuum equipment, in which water is used as working fluid and ejected through the nozzle to obtain a vacuum environment. The mixing process of gas and liquid flow in gas-liquid jet vacuum pump will reduce the pumping efficiency due to the loss of momentum and energy. The influence of different structural parameters of gas-liquid jet pump on the performance was studied by computational fluid dynamics (CFD) method. Based on ANSYS Workbench platform and Design Explorer, the synergistic effects on the performance of gas-liquid jet pump was analyzed by multi-parameter approach. The good agreement between simulation results and experimental data is shown that the numerical simulation modeling can be used to predict flow structure and pumping feature of gas-liquid jet pump. The simulation results shows that three structural parameters, nozzle exit position (NXP), throat area ratio and length-throat diameter ratio, all have influence on the performance of gas-liquid jet pump. A steady and higher pumping performance would be obtained as the NXP is 1.5~2 times as big as nozzle diameter, the value of throat area ratio and length-throat diameter ratio is 4~6.25 and 6~12 separately. The sensitivity analysis of the design variables to the objective function is shown that the throat area ratio has a more significant influence on the suction gas flow, and plays a major role in the influence on gas-liquid jet pump pumping performance.

The effect of the throat structure on critical back pressure in the steam ejector

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The steam ejector refrigeration system has attracted researchers' attention for its simple structure, environmental protection and good economy. The steam ejector is the key component affects the system pumping performance. The critical back pressure plays an important role in judging the fluid flow state and improving the ejector working stability which is rarely studied before. The CFD method is used to analyze the flow characteristics and state region internal the ejector. The effects of the throat diameter and length on the critical back pressure and the pumping performance are comprehensively discussed. A small steam ejector refrigeration experimental system is established to verify the CFD model. The numerical results indicate that the critical back pressure increases with the throat length. The ability to resist the back pressure of the outlet is enhanced and the system works more steadily. The increase of throat diameter leads to the decrease of critical back pressure and the ability to resist back pressure. Furthermore, the stable flow state is easy to be broken and the system working stability is seriously affected. Considering the whole throat structure, the optimal analysis method is adopted to obtain an ideal structure which make the ejector works stably and has high efficiency.

Study the influence of operating parameters on the ejector in the absorption-ejector combined refrigeration system

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The absorption-ejector combined refrigeration system not only improves the single-effect absorption refrigeration efficiency but also reduces the heat source temperature and improves energy utilization. The ejector is the main component which affects the energy efficiency and economy of the combined system. In this working, the numerical simulation and the experimental method are used to analyze the flow structure inside of the ejector by changing the operating parameters. The main influence factors- back pressure, the saturation temperature of the primary and secondary have been simulated for improving the efficiency and stability of the system, which is proposed by analyzing the single operation parameter under the fixed geometric structure. The results show that the higher the saturation temperature of the primary fluid is, the more obvious the choke in the diffuser is and the higher critical back pressure is. However, the ejector pumping efficiency first increases and then decreases. The higher the saturation temperature of the secondary fluid is; the larger pumping efficiency is. The variations of the back pressure are opposite to the secondary fluid. The COE method is also adopted to study the optimization of the operating parameters. The analysis results indicate that there are a larger expansion ratio and a smaller compression ratio in a certain parameters range which maximize the ejector efficiency and minimize the energy consumption of the whole system.

Novel surface treatment technology on the back channel of amorphous oxide semiconductor thin film transistors

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Despite the fact that the amorphous oxide transistors reveal high electrical and stability performances, the rapid degradations such as negative V_{th} shift and disappearance of on/off characters essentially encountered in the oxide thin film transistors (TFTs) with the high indium composition and quasi two-dimensional thin channels, especially low process temperature for the flexible application accelerates the deterioration due to the numerous surface broken bonding in the quasi-2D oxide films and the uselessness of oxidation treatments. Strategically, we firstly proposed the use of non-centrosymmetric gas as more reactive oxidizer gas at room temperature for highly robust and fast field-effect mobility properties in the quasi-2D oxide transistors. From XPS analysis, we found that novel gas stably reconstructs the surface chemical bonding by capturing charged electrons and oxygen. Interestingly, we tactically create new process design for the fabrication of self-aligned co-planar quasi-2D transistors with metal/semiconductor homojunction aiming scale-down and replacing conventional hydrogen ion and UV/EUV irradiation. This idea is designed from the troublesome aging effect and the impact of new treatment at the same time. The co-planar top gate quasi-2D a-IZO transistors exhibited outstanding device performances with a field-effect mobility of $> 10\text{cm}^2/\text{Vs}$ at a maximum process temperature of 150 oC.

Zinc and cobalt azolate frameworks from acid-catalyzed synthesis for CO₂ adsorption and separation

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In present work, the zinc and cobalt azolate frameworks with a diamond-type (dia-) crystal structure have been synthesized by an acid-catalyzed route successfully. Two organic ligands, imidazole (im) and benzimidazole (bim), were respectively mixed with zinc or cobalt oxides in an acidic aqueous solution, forming zinc (dia-Zn(im)₂ and dia-Zn(bim)₂) or cobalt (dia-Co(im)₂ and dia-Co(bim)₂) azolate frameworks. The crystal structures and morphologies of these zinc/cobalt azolate frameworks were characterized with X-ray diffraction (XRD) and field-emission scanning electron microscopy (FE-SEM), respectively. Existences of intermolecular bonds between organic ligands and metal cations were confirmed with Fourier transform infrared spectroscopy (FTIR). High thermostabilities of zinc/cobalt azolate frameworks were demonstrated using a thermogravimetric analyzer (TGA) with a flushing nitrogen gas. The nitrogen isotherms of these zinc/cobalt azolate frameworks were classified as Type III (non-porous) with low Brunauer–Emmett–Teller (BET)/Langmuir surface areas compared with IUPAC (International Union of Pure and Applied Chemistry) standard isotherms. In addition, the near-edge structure/extended X-ray absorption fine structure (XANES/EXAFS) spectra verified that the valences of zinc and cobalt atoms are Zn(II)/Co(II). Carbon dioxide uptakes of zinc/cobalt azolate frameworks distributed from 1.0 to 4.5 wt% at 0 °C and 30 bar. The CO₂ selectivities of zinc/cobalt azolate frameworks located in the range of 0.08-3.57. Both Langmuir and Freundlich adsorption isotherm models were well-fitted with the CO₂ adsorption isotherms of zinc/cobalt azolate frameworks with good agreements.

Change of Catalytic Performance of metal-doped SnO₂ Nanoparticles: Size Dependence

Hangil Lee

To determine the size-dependent catalytic activity variation of transition-metal-doped SnO₂ nanoparticles (TM@SnO₂ NPs; TM = Cr or Fe), we used the annealing method at three distinct temperatures (300, 600, and 900 °C). Moreover, we identified the correlation between the size of the NPs and their catalytic activities because the NP size is associated with the formation of the defect structure (surface area). We analyzed the structure of the synthesized TM@SnO₂ NPs by using transmission electron microscopy (TEM) and scanning transmission X-ray microscopy (STXM). We analyzed changes in their catalytic properties using the oxidation of thiophenol via high-resolution photoemission spectroscopy (HRPES), methylene blue degradation via ultraviolet–visible (UV–Vis) spectrometry, and the radical formation of benzoic acid via a 300-W Xe arc lamp with a 320 nm cut-off filter (for visible light irradiation). Both types of test samples (denoted as Cr@SnO₂-900C and Fe@SnO₂-900C) obtained by 900°C annealing show improved crystallinity, but the catalyst characteristics worsen. Our results showed that the catalyst characteristics are closely related to the defect structure. In other words, if the size is smaller, the amount of defect becomes larger. Therefore, if the catalytic properties change through annealing, the size of metal oxide (MO) NPs must be selected for practical applications.

A New TPMC Algorithm for Pumping Mechanism of Turbomolecular Pump

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In order to further reveal the pumping mechanism of turbomolecular pump, a new algorithm based on test particle Monte Carlo method was proposed in this paper. The real three-dimensional topology of rotor and stator blade rows were modelled. The analytical equations of 6 planes for each blade, they are the front blades, the rear blades, the blade root, the casing, the upstream of blades and the downstream of blades, were established in the Cartesian coordinate system. Combined with the random motion equation of gas molecules, the time-of-flight from one plane to the other five were formulated. Taking the minimum time-of-flight as the criterion, the position and path of each gas molecule within a rotor–stator blade row were tracked and counted by the written program according to the new algorithm. The transmission probability, maximum pressure ratio and the maximum speed factor of the rotor–stator blade were obtained. The simulating results have a good agreement with the previous known experimental data, thus it confirms the feasibility of the presented new algorithm. The uniqueness of this algorithm lies in its ability to provide an accurate description of a gas molecular motion and to count the probability distribution in six planes. The new algorithm could further reveal the pumping mechanism of turbomolecular pump and provide a theoretical basis for the accurate design and improvement of the turbine blade.

2111-A-1902

Determination of the hydrogen permeation characteristics of various polymers for hydrogen vehicle systems

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Polymers and their composites are currently used for hydrogen storage tanks, seals, and pipes in hydrogen fuel cell vehicles, because they have the advantage of weight reduction, and therefore can be used for storage of large volume. However, they are vulnerable to hydrogen permeation, and susceptible to the formation of microcracks when exposed to various mechanical and thermal cycles. Therefore, in order to evaluate the safety and assess material suitability for hydrogen storage, it is very important to measure the hydrogen permeation of the polymers. In this work, we have developed the hydrogen permeation testing equipment based on the differential-pressure method, and studied the hydrogen permeation through various polymer materials.

Delamination behavior in compression bending test of organic semiconductor device

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In the present study, experimental study was conducted on delamination caused in the compression bending test of organic semiconductor devices, and the effect of layer structure, bending strain, and bending frequency on delaminating occurrence and progression was investigated and discussed. In order to improve the flexibility of the flexible OLED, the authors have mainly conducted a tensile test and investigated the delamination behavior due to crack susceptibility and compressive strain of constituent materials of organic semiconductor elements. In this study, specimens such as PEN substrate/Alq/MgAg, PEN substrate/PEDOT/Alq/MgAg were prepared using wet process and vacuum process and subjected to compression bending test. As a result, the number of stripes due to delamination showed a constant value or a decreasing tendency when the compressive strain was 1% or more, and it was found that the maximum width of the stripes tended to increase although the minimum width of the stripes was not greatly changed. This is considered to be due to the fact that the width of the fringes initially generated increases with the increase in compressive strain and merges with the adjacent stripes. Furthermore, it has been suggested that the adhesion of the film could be semi-quantitatively evaluated by the compression bending test, in the case of the same layer configuration, since it is presumed that delamination did not occur until the high compressive stress as the number of stripes increased, from the basic equation of buckling.

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In situ X-ray spectroscopy in energy science

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Global climate warming and environment pollution have spurred scientists to develop new high-efficient and environmental-friendly energy technologies. Sunlight is a clean, renewable and abundant energy source on the earth. Its conversion to hydrogen has been considered an ideal solution to counter the depletion and environmental problems of fossil fuels. Hydrogen is an ideal fuel for fuel cell applications. Hydrogen has to be produced from renewable and carbon-free resources using nature energies such as sunlight if one thinks of clean energy and environmental issues. In this regard, a photoelectrochemical cell consisting of semiconductor photoelectrodes that can harvest light and use this energy directly for splitting water is a more promising way for hydrogen generation. Photocatalysis utilizes the energy delivered by light and enables chemical reactions that otherwise cannot take place. When used to power thermodynamically uphill reactions, photocatalysis offers a solution to large-scale solar energy storage. Despite over four decades of intense research, however, photocatalysis remains either too expensive or too inefficient or both. Poor understanding of the mechanisms behind the low performance is a key reason that limits the progress of this important field. To address this critical challenge, and to complement existing efforts focused on discovering new materials for photocatalysis, we present here a series of experiments designed to elucidate the working principles of photocatalysis.

direct comparison between subnanometer hydration structures on hydrophilic and hydrophobic surfaces via three-dimensional scanning force microscopy

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Investigating interfacial water ordering on solid surfaces (hydration layers) with different hydrophobicities is fundamentally important for better understanding of solid-liquid interfacial phenomena. In previous AFM studies, some groups reported that the oscillation force profiles related to hydration layers at hydrophobic HOPG-water interface (0.3-0.4 nm) are larger than that typically measured at hydrophilic mica-water interface (0.2-0.3 nm). However, Gillian et al. reported no oscillation at hydrophobic-water interfaces using a hydrophilic or a hydrophobic tip. Schlesinger et al. presented that oscillatory force curves at hydrophobic-water interfaces were detected in some measurements but not in others. In these studies, they cannot rule out the possible effects of the tip on the force curve measurements because only a single type of solid-water interface (hydrophilic-water or hydrophobic-water) is prepared for these measurements. Here, we prepared hydrophilic mica substrates with some areas covered by mildly hydrophobic graphene layers, and studied the resulting hydration layers using three-dimensional (3D) force measurements based on frequency-modulation atomic force microscopy. Hydration layers of 0.3-0.6 nm were detected on bare graphene regions; these layers were considerably larger than the spacing measured on mica (0.2-0.3 nm). On the graphene-covered regions, we also observed formation of special ordered structures of adsorbates over time, on which, surprisingly, no prominent hydration layers were detected. Based on these findings, we present one possible scenario to describe the formation process of the ordered interfacial structures and the enhanced oscillation period in the force profiles. This work also demonstrates the capability and significance of 3D force measurements in probing hydration behaviors on a heterogeneous substrate with a lateral resolution smaller than several nanometers.

Development & characterization of indigenously designed helium leak artifacts

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With the advancement in nanotechnology, nano-leaks have become very important in the field of high-tech research and development. In this regard, fabrication and optimization of standard helium permeation leak artifact, a type of nano-leak, has been a field of interest for the researchers in the field of vacuum metrology. Some applications of these artifacts include calibration of helium leak detectors, residual gas analyzers, and mass spectrometers etc.

The current paper summarizes a long-term study of the indigenously developed standard helium permeation leak artifacts with different filled pressures in the helium reservoirs and variable wall thicknesses of glass (Quartz & Pyrex) leak elements. The study was aimed at producing a leak rate in the range of 10^{-8} mbar l/s, which was achieved successfully. Furthermore, it was observed that as compared to Quartz, the Pyrex (Type 7740) leak rate is more stable and durable with low depletion rate in about 07 years. The leak rate dependency on leak element's wall thickness, filled pressure & temperature has also been analyzed. The average recorded value for the temperature coefficient is $2\% \text{ } ^\circ\text{C}^{-1}$ which lies well in the range reported in literature.

Keywords: Leak element, Permeation leak, Tracer gas, Temperature effect

Oscillatory rarefied gas flow in a vertically driven comb-type assembly

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Oscillatory gas flows are common in comb-type micro-electromechanical system where computation of the damping forces in the narrow gaps between moving elements is of major importance either in low (e.g. accelerometers) or in high (e.g. resonators) frequencies. Damping forces are usually computed with continuum-based models, which are valid however, only when the mean free path and intermolecular collision frequency are much smaller than the characteristic channel size and the wall oscillation frequency. When these restrictions are not satisfied, the flow inside a comb-type assembly must be modeled by kinetic theory. Here, the oscillatory rarefied gas flow in a comb-type structure driven by the vertical motion of the moving element is investigated, based on the linearized unsteady Shakhov kinetic model equation. Due to the element vibration, complex flow patterns are formed in the direction perpendicular and parallel to its motion. Computational results are presented for the normal and shear stresses of the moving walls in terms of the oscillation frequency, the gas rarefaction and the comb geometry. It is found that both stresses have a non-monotonic behavior in terms of the gas rarefaction parameter. Also, there are certain oscillation and gas rarefaction parameters where the stresses are minimized resulting to a reduction of the damping forces. Finally, it is seen that the deduced stresses strongly depend on the comb geometry only in low frequencies. Overall, the proposed methodology and the computed results support the design and optimization of comb-type micro devices depending upon the specific application and the associated operating conditions.

Work-function engineering in ultra-scaled 2D-TFET devices: an atomistic DFT-NEGF study.

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Two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) have recently been included in the International Roadmap for Devices and Systems (IDRS) as promising channel materials for next-generation sub-10nm technology nodes [1,2]. In this contribution, we investigate the electrical characteristics of an ultra-scaled tunnel FET (TFET) device, where the channel is a heterojunction based on 2D semiconducting MoTe₂ and SnS₂ monolayers [3]. We characterize the electronic structure and the transport properties of the 2D-TFET device by means of density functional theory (DFT) combined with the non-equilibrium Green's function (NEGF) method [4] and with advanced electrostatic solvers, as implemented in the QuantumATK software [5]. We show how the electrical response of the device to electrostatic gates can be tuned by using an asymmetric contact scheme. The latter is analogous to that proposed for graphene-based photodetectors [6], where metals with different work functions have been used to contact the 2D channel. Our large-scale DFT-NEGF device simulations demonstrate that the electrical characteristics of ultra-scaled 2D devices can be engineered by an appropriate choice of the metallic electrodes, and highlight the importance of atomistic device simulations for the optimization of the electrical characteristics of future devices based on non-conventional semiconductors.

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Title: Coupling of plasma power and electron temperature in RF plasmas

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Abnormal behavior of electron temperature (T_e) was observed in inductively coupled plasmas [1]. In the low RF power or plasma density region, T_e decreased, while it remarkably increased in the high RF power region. From the kinetic model analysis, the apparently abnormal trend in T_e can be understood by the contrasting effects of stepwise ionization and gas heating. Our experiments and improved modeling show that T_e has a much stronger relationship with plasma power than we initially expected, and the gas heating effect should be considered. [1] Appl. Phys. Lett. 110, 014106 (2017). E-mail: LHC@kriss.re.kr

Model calculation of competitive formation and etching of compound layer on target surface in reactive sputtering

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It is well recognized that in reactive sputtering the total reactive gas kinetics result from the formation and etching of the compound layer on the target surface. The time to reach a steady-state affects the stability of the reactive sputtering process. In this study, the kinetics on the compound layer formation and etching on the target surface were discussed based on the two-type model calculations of Ti-O₂ reactive sputtering: the time-dependent oxidation or etching for a fixed O₂ flow rate and that for a step-change of O₂ flow rate. In the time-dependent oxidation or etching for a fixed O₂ flow rate, under given conditions, after approximately 15 s of elapsed-time, the amount consumed to form the oxide on the target surpassed that sputtered from the target, resulting in the avalanche-like increase in target coverage and in the decrease in the sputtered Ti amount and, at 28 s, the target surface reactions reached a steady-state.

In the O₂ consumptions calculation for the sequential step-increase in O₂ flow rate from 0.5 to 10 sccm with a step of 0.5 sccm, at 6.5 sccm, the avalanche-like target surface oxidation occurred. At this point, a small excess of the target oxidation to etching induced the avalanche-like change and made a time-delay longer as a result of competitive target oxide formation and etching. The time needed to reach a steady-state at the avalanche-like transition point, which results from the competitive target oxidation and etching, affects the time-dependent whole reactive process change.

Light induced deposition of polypyrrole on semiconductor surfaces

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Thin organic films of various polymers can be used as an active charge carrier layer or as resists in production of various electronic devices such as FETs, LEDs and others, as well as for various surface modifications (1). The easiest way of film preparation is deposition onto the substrate by processes such as spin coating, creating a physically adhering film. In contrast to this, it is also possible to attach thin films chemically by surface reactions, such as "grafting" on reactive surface sites (2).

Hereby we present the results of the investigation of thin polypyrrole films deposited onto different doped silicon samples, functionalized with a Pyrrole containing self-assembled monolayer. Upon illumination of the samples with white light in a solution of pyrrole and silver nitrate in acetonitrile, charge carriers are generated in the crystal, leading to an electropolymerisation of pyrrole on the surface (3).

Films deposited in this way were investigated using SPM, ellipsometry, XPS and cyclic voltammetry with regard to the influence of illumination time and intensity, as well as the composition of the reaction solution.

The photoelectropolymerisation of polypyrrole on semiconductor surfaces creates smooth, regular films, chemically attached to the substrate. This can be useful in device manufacturing or for the creation of organic semiconductors.

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Optical transitions of MAPbCl₃-xBr_x

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Organic-inorganic hybrid perovskite (Methyl-ammonium-lead-trihalides : MAPbX₃, X=Cl, Br and I) materials are vastly investigated last one decade due to the application of highly efficient solar cell and other optoelectronic devices. We have measured photoluminescence of MAPbCl₃-xBr_x (x=0, 0.5, 1, 1.5, 2) in high magnetic fields. We found several optical transitions from each samples believed to be trap mediated monomolecular and band to band bimolecular transitions. In the presence of magnetic fields, these transitions show red- and blue-shifts depend on samples. We believe that these anomalous transitions are related with the spin states of Rashba splitting in the conduction and the valence bands. Normally, it is said that the Rashba effect in the valence band is small and can be ignored in comparison to the conduction band splitting. However, we found a clue that the valence band effect cannot be ignored. The valence band of the sample structures consists of Pb 6s and Cl 3p (or Br 4p) levels. Our preliminary experimental data showed that the Rashba effect was enhanced as the ionic radius changes from Cl to Br. In this proposal, in order to verify the enhanced Rashba effect in the valence band, we will present detailed experimental results of the polarized optical transmission and photoluminescence measurements of MAPbCl₃-xBr_x crystal samples in high magnetic fields.

Structural and Chemical Reactivity Studies of Tungsten Oxide One-Dimensional Nanostructure

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In this contribution we present studies of physico-chemical properties of self-organized tungsten oxide nanostructure prepared on Cu(110) surface. Tungsten oxide belongs among reducible oxides and it is an important material in the fields of heterogeneous catalysis and gas sensing. Electron diffraction (RHEED, LEED) and scanning tunneling microscopy (STM) were used for investigation of the sample structure and morphology. Oxidation state of tungsten and other chemical properties were studied by means of photoelectron spectroscopy (XPS, SRPES). Formation of a self-organized one dimensional tungsten oxide structures parallel to Cu [1-10] crystallographic direction was observed. The STM images showed tungsten oxide nanorods on the substrate surface. Momentum-dependent modulation of the valence band electron structure shown by ARPES measurement also reflected one-dimensionality of the system.

The structure was studied further by Density Functional Theory calculations using the generalized-gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional. We modelled the wires formed by one and two lines of tungsten oxide developing the one-dimensional structures. Comparing the calculations with the experimental results permitted to estimate structure of nanosized tungsten oxide.

Reactivity of this nanosized system was investigated by a low temperature methanol adsorption and decomposition. The methanol adsorption was carried out at the sample temperature below 120 K. Partial methanol dehydrogenation was observed immediately after adsorption. Subsequent series of flash heating at increasing temperature led to gradual decomposition and desorption of methanol and its complete disappearance at 350 K. Formation of methoxy group and other products was observed during the process.

Vanadium based two-dimensional materials

Two-dimensional (2D) transition metal oxides and dichalcogenides have garnered much interest due to distinctive physical properties from their bulk counterparts.¹ Herein, we report the V₂O₅ nanosheets for an effective selector devices and VSe₂ nanosheet as a candidate of intrinsic ferromagnetic 2D materials. V₂O₅ nanosheets synthesized by facile chemical vapor deposition show highly stable and low threshold voltages, which have not been previously reported on the threshold switching properties. The electrons occupying trap sites in poly-crystalline V₂O₅ nanosheet contribute to the perfectly symmetric threshold switching feature at the bias polarity and low threshold voltages in V₂O₅, confirmed by high-resolution transmission electron microscopy measurements. Furthermore, we find an additional PdO interlayer in V₂O₅ nanodevices connected with a Pd/Au electrode after thermal annealing treatment. The PdO interlayer decreases the threshold voltages, and the Ion/Ioff ratio increases because of the increased trap density of V₂O₅. These studies provide insight into V₂O₅ switching characteristics, which can support low power consumption in non-volatile memory devices. For VSe₂ nanosheet, we report for the first time the atomistic real-space observation of van der Waals layered structure of VSe₂ by using HAADF-STEM images. Furthermore, simply by controlling the carrier gas flow rate, a morphological variation of surface area and thickness of VSe₂ nanosheets was observed. The room temperature ferromagnetic feature of single VSe₂ nanosheet was also revealed by magnetic force microscopy measurements. Our findings will play a significant role in the research of intrinsic 2D ferromagnetic materials.

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Thermoelectric Titanium Dioxide doped with Niobium Thin Films for TCO Applications

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Transparent conducting oxides (TCOs) are on high demand for touch-screen and solar cell applications and the design of a TCO material with thermoelectric properties is a promising technology, making it possible to produce electrical energy through the harvesting of heat from the environment. In general, in order to achieve the required transparency the film thickness must be ~ 100 nm, while to enhance the thermoelectric "Figure of Merit" (ZT), the films must have a high Seebeck coefficient, high electrical conductivity and low thermal conductivity. This relation is challenging and requires very fine tuning of the production parameters. As an alternative to the conventionally used ITO, TiO₂ has been extensively investigated due to its interesting optical and electronic properties and good stability in the adverse environment. A cationic doping of TiO₂ has been documented to improve its electrical conductivity, which will increase the thermoelectric power factor (PF) and ZT of the film. In this work, transparent TiO₂:Nb thin films were obtained by d.c. magnetron sputtering with low electrical resistivity (10^{-2} ohm·cm), good thermal conductivity (2 W/m/K) and a high absolute Seebeck coefficient (-2×10^{-4} V/K) corresponding to a PF of $\sim 10^{-4}$ W/K²/m and ZT of ~ 0.1 . Several process parameters were adjusted, such as reactive gas (O₂) partial pressure and deposition time and temperature, which affect the morphology and crystalline structure of the thin films. Hence, tuning the properties of the produced TiO₂:Nb thin films enables their suitability for applications thermal energy harvesters in devices in order to render them more sustainable.

Low-energy electron point projection microscopy/diffraction study of suspended graphene

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Graphene has received much attention owing to its outstanding electrical and mechanical properties. It is considered to be a model system of two-dimensional (2D) materials. Suspended graphene is also a good supporting substrate for observation of nano-objects and molecules in electron microscopy. We have constructed a low-energy electron point projection microscopic/diffractive instrument and used it to characterize suspended graphene samples [1]. We use highly coherent electron beams emitted from a single-atom tip for the measurements. This method allows imaging of individual adsorbates on graphene at the nanometer scale and characterizing graphene layers and graphene lattice orientations. Most importantly, ripples on graphene membranes of amplitude 1 Å are sufficiently strong to cause noticeable intensity variations in high-order diffraction patterns [1,2]. Thus, very weak ripples associated with strain caused by adsorbates on the graphene surface can be directly visualized and studied. This method suggests that convergent electron beam diffraction based on highly coherent electron sources are useful in characterizing 2D materials and van der Waals heterostructures with nanometer or sub-nanometer resolution [3], including the layer thickness, the lattice orientation, lattice periodicity, adsorbates, encapsulated structures, defects, ripples, etc. Further improvement of the experimental method and development of theoretical reconstruction methods may allow reconstruction of three-dimensional atomic structures of suspended 2D materials.

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Comparative study of online leak detection techniques for large vacuum system

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In an ideal condition, a vacuum chamber should maintain the achieved vacuum pressure forever after switching off the pumps. In practice, it is impossible to build a completely leak-tight vacuum system under an operational condition with many other integrated components. Thus leak detection is an important step in the production of vacuum to guarantee that the required pressure and gas composition conditions for continuing the experiments onward. There are several methods available starting from soap bubble test, tracer gas (helium) based mass spectrometer detection to ultrasonic leak detector for vacuum leak detection in different industrial applications. The smooth operation of large vacuum system requires a kind of online tool which keeps watching on leak integrity of all circuits and can give the indication of a leak for various types of gases without disturbing the pumping process.

This work aimed towards primary leak detection (for small leak rates below 10^{-8} mbar l/s.) in large vacuum systems (i.e. used in accelerators, fusion plasma, and space simulation) by use of mass spectrometry, gas analysis and advanced simulation technique with consideration of different phenomena and volume of vacuum systems. A standard residual gas analyser (RGA) has been used as a potential instrument for online leak detection to avoid practical limitations of other techniques. For this purpose, an established co-relation of partial pressure ratio (Nitrogen and Oxygen ratio in air 4:1) has been used and experimentally validated for a given leak rate between leak detector and RGA during online leak detection. This method is capable to give an instant detection of a leak in a specific large vacuum system. In addition, a comparative study with simulation result has been carried out to realize the advantage, disadvantage, and limitation for different leak detection techniques and their application.

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Algorithm improvement for pumping characteristics of compound molecular pump

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The Monte Carlo method is used to calculate the transport probability of single stage blade, and the model of reflection coefficient of gas molecules and solid wall is introduced to evaluate the influence of different reflection conditions on the pumping characteristics of single stage blade. The integral mean value method is used to calculate the transmission probability of blades, and the calculation accuracy of the turbine stage pumping characteristics is improved. The Monte Carlo method is used to calculate the transmission probability of three-dimensional single-stage blade, and the accuracy of two-dimensional model transmission probability calculation is evaluated by comparing it with the integral median method.

towards schottky defined p-type gasb quantum dot transport devices

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P-type III-V semiconductors promise a high degree of spin control and long coherence times due to strong spin-orbit interaction and a reduced coupling of hole spins to nuclear spins [1]. That makes them promising material systems for double quantum dot (DQD) transport devices, which are interesting systems to study fundamental spin physics and are considered candidates for the realization of spin qubit applications [1,2].

Nanowire based devices yield the possibility for enhanced gate control and easier device fabrication in comparison to planar III-V heterostructures [1]. First realizations of p-type nanowire embedded DQDs in InSb [1] and quantum dots (QD) in GaSb [3] have already been demonstrated. Because GaSb exhibits the highest hole mobility within the III-V family [4], we aim at fabricating and characterizing p-type GaSb nanowire DQD devices for future spin transport studies in this project.

We show how Schottky contacts to GaSb nanowires can be used to define quantum dots within the enclosed nanowire segment between source and drain contacts. By introducing additional sidegates, we electrostatically form a DQD and present initial finite bias spectroscopy measurements on what we believe to be the first p-type GaSb nanowire DQD device. Finally, we suggest how device stability can be improved by advanced gate structures.

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The susceptibility of (3,1) chiral graphene nanoribbons to oxidation via air or oxygen exposure

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Graphene nanoribbons (GNRs) have been the subject of intensive research effort in recent years. Unlike pristine graphene, their width/edge dependent bandgaps allow for potential applications as semiconductors in electronics. The synthesis of chiral graphene nanoribbons, which offer a combination of both armchair and zig-zag type edges, also further enhances the tuneability of GNR electronic properties. It has recently been demonstrated that such nanoribbons may be formed via on-surface synthesis on metallic substrates, such as Cu(111) [1,2], Ag(111) [2] and Au(111) [2]. However, any applications of these nanoribbons may be limited in nature by their stability when exposed to air.

In this study, we have examined the durability of on-surface synthesised (3,1)-cGNRs on Au(111) when exposed to either the atmosphere or pure oxygen at low pressures. We find that, even after a room temperature exposure to oxygen in only the 10^{-5} mbar regime, the chiral nanoribbons undergo significant structural changes due to oxidation. Using high-resolution scanning tunnelling microscopy, combined with theoretical calculations, we attempt to identify the resulting structural defects and suggest the possible reaction pathways that lead to their formation. Some correlation between the presence of the defective regions and changes to the electronic structure of the nanoribbons is also evident from scanning tunnelling spectroscopy measurements.

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The influence of crystal structure in the development of magnetic nanosized mixed iron oxides by cation-exchange

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The extensive field of application of magnetic nanoparticles (NPs) makes them a wide, popular and attractive class of materials, with different compositions and morphologies being proposed to improve the NPs' magnetic features. In regards to this, cation exchange (CE) could represent a promising approach to obtain complex, modulated magnetic nanostructures, but its application to this class of materials has been sporadic and not always consistent. To this aim we studied the effect of a post-synthetic CE approach on same-sized magnetite and wüstite NPs by performing in-depth morphological, structural, spatially resolved chemical and magnetic behavior analyses, finally obtaining bi-magnetic core/shell NPs with mixed Fe/Mn and Fe/Co ferrite shells that still maintained the initial shape and size. The combination of such diverse techniques evidenced unanimously that the crystal structure of the two starting phases (non-defective for magnetite, defective for wüstite) was the only variable among the NPs populations that affected the CE and was responsible for the higher percentage of doping cation (Co or Mn) present in the post-CE wüstite NPs. Besides, the evolution of the magnetic features could be attributed to the combination of three separate factors: the formation of well-defined shells, the introduction of different magnetic cations and the presence of different crystal structures in the cores. These results give a new insight on the mechanisms that command CE of nanosized magnetic oxides, while providing a clearer picture over the possible capabilities of CE approach to develop novel, complex magnetic nanostructures.

Radioactive Emissive Phenomena on Contacting Surfaces

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It was shown [1] that physical nature of mechanically stimulated X-rays emission is result of initial thermo (hyper) electrons [2] of contacting surfaces action with atoms of another ones. The mean measured X-rays intensity for friction pairs: "grinder-steel", "silicon-silicon" was 14.01 mcSv/h., and the ground intensity was 13.05 mcSv/h. Theory of friction [3] describes the number of the unfamiliar phenomena at friction: gases exchange, hydrogen diffusion into bodies of friction pair, hydrogen isotopes generation, dissolution, desorption. Fig.1. shows the hydrogen isotope tritium appearing into cutting instrument.

Fig.1 Tritium atom concentration CT at/m³ in cut before and after cutting on depth 0,5 mic.

The tritium advantage for experiments is its radioactivity ("beta"-emission) with half-life period 13.5 years, and the experimental data: X-rays and "beta"-emission before/after cutting: 0.11/0.13 [mcSv/h] and 0.10/0.19 [1/(cm²*min)]. The common hydrogen gas advantage is its lightness and its rise possibility into gas media. The mentioned tritium advantages were used in the experimental installation, Fig.2

Fig.2 Installation for tritium appearing control: 1-drive, 2- friction pair, 3- volume, 4-valve, 5- bottom dosimeter, 6- upper dosimeter

The "beta"-emission control shows the tritium atoms appearing with upper 6 and bottom 5 dosimeters usage. The mean figures are: 1.99/0.97 [1/(cm²*min)] that proves the hydrogen isotopes generation idea.

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Tailoring physico-chemical properties of conducting polymer interface for sensing and biosensing

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Conducting polymers, with unique ion/electron transfer capability, reversible doping/dedoping and controllable chemical and electrochemical properties, have received many attention as advanced interfaces in electronic and bioelectronic devices. Recent advancement is focus on fine-tailoring the conducting polymer interfaces with addition functionality and controlled morphology with enhanced performance beyond its intrinsic properties.

Here, we demonstrate the tailoring of physico-chemical properties of poly (3,4-ethylenedioxythiophene) (PEDOT) with high density carboxyl functionality and tailored nano-structure, and its application in dopamine sensing and lactate biosensing with enhanced selectivity and sensitivity.

For dopamine sensing, we developed a high-density negatively-charged carboxyl functionalized PEDOT interface using a low-cost organic acid citrate as dopant. Citrate contains a high content of carboxyl functionality and small size allowing well distribution of the citrate dopant within the PEDOT with a high surface carboxyl density upto 26 $\mu\text{M}/\text{cm}^2$. The carboxyl confined PEDOT interface with nano-globular structure showed increased electrode kinetics and increased discrimination of dopamine from interferences (ascorbic acid and uric acid).

For lactate biosensing, we further developed a nano-fibrillar carboxyl PEDOT interface that can detect dihydronicotinamide adenine dinucleotide (NADH) at low potential at ~ 0.43 V. Based on the post-immobilisation of NAD-dependent lactate dehydrogenase via carboxyl coupling, lactate biosensor was developed with good analytical performance and low operation potential to reduce interferences.

These results demonstrated tailoring of physico-chemical properties of PEDOT interface with improved sensing performance, thus could potentially applied for next generation bioelectronic devices such as wearable and flexible sensors and biosensors.

Characterization of the (In,Pb)/Si(111) systems

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The discovery of self-assembled 3D nanostructures based on quantum size effects on Pb/Si(111) and In/Si(111) surfaces has begun a new trend of study of metal-semiconductor systems. Indium and lead, as foreign metal adsorbates, so-called surfactant, passivate the silicon surface and reduce the number of active sites through saturation of surface dangling bonds. It leads to a very low surface diffusion barrier and results in an increase of the mobility of new adsorbent atoms on the surface. Therefore, in the field of controlled formation of self-assembled metallic nanostructures the choice of a type and initial ordering of the surfactant is extremely important.

In this work, the (In,Pb)-Si(111) systems were characterized in dependence of the initial Pb reconstruction on Si(111) surface. The aim of the study was to gain knowledge of long range orders and thermal stability of ultrathin layers of metals. For In/Si(111)-alpha ($\sqrt{3}\times\sqrt{3}$)-Pb system In atoms inverse with the Pb surfactant at 470 K resulting in formation of disordered mixed (In,Pb) overlayers. Moreover, Pb atoms located on the topmost layer desorb easily until the critical coverage is reached when the ordered structures appear. Unreconstructed mixed (In,Pb) layers were also observed for In/Si(111)-beta ($\sqrt{3}\times\sqrt{3}$)-Pb system at RT. Increasing the temperature of the samples over 470 K yields an arrangement of the adsorbate and surfactant atoms to 2D alloyed structures with various periodicity.

Maximising the resolving power of the scanning tunneling microscope

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The usual way to present images from a scanning tunneling microscope (STM) is to take multiple images of the same area, to then manually select the one that appears to be of the highest quality, and then to discard the other almost identical images. This is in contrast to most other disciplines where the signal to noise ratio (SNR) of a data set is improved by taking repeated measurements and averaging them. Data averaging can be routinely performed for 1D spectra, where their alignment is straightforward. However, for serial-acquired 2D STM images the nature and variety of image distortions can severely complicate accurate registration. Here, we demonstrate how a significant improvement in the resolving power of the STM can be achieved through automated distortion correction and multi-frame averaging (MFA) and we demonstrate the broad utility of this approach with three examples. First, we show a sixfold enhancement of the SNR of the Si(111)-(7 × 7) reconstruction. Next, we demonstrate that images with sub-picometre height precision can be routinely obtained and show this for a monolayer of Ti₂O₃ on Au(111). Last, we demonstrate the automated classification of the two chiral variants of the surface unit cells of the (4 × 4) reconstructed SrTiO₃(111) surface. Our new approach to STM imaging will allow a wealth of structural and electronic information from surfaces to be extracted that was previously buried in noise.

Effects of deposition temperature on microstructure and properties of multicomponent Ti-Nb-Zr-Ta nitride coatings

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Multicomponent refractory metal nitrides have drawn great attention as advanced coating materials in the past decade. Their applications include diffusion barrier layers[1], hard wear-resistant coatings[2], and corrosion-resistant coatings[3]. In this work, a series of Ti-Nb-Zr-Ta nitride coatings with thickness above 1 μm was deposited using reactive magnetron sputtering with four segmented targets. A fixed nitrogen flow ratio $[RN=N_2/(Ar+N_2)]$ of 3% and floating bias were applied. Deposition temperatures varied from room temperature to 700 °C. Microstructure of coatings were characterized by electron microscopy, atomic force microscopy, compositional analysis, and X-ray diffraction. Coatings deposited below 400 °C all showed a single solid solution FCC phase. A (002) preferred orientation of FCC was observed in coating deposited at 400 °C and higher. At the highest temperature of 700 °C, a phase segregation was observed with a mix different FCC. Effect of deposition temperature in the film and morphology on the electrical and mechanical properties were studied with four-point probe and nanoindentation respectively. The resistivities of all TiNbZrTaN coatings were between 184 $\mu\Omega\text{ cm}$ to 211 $\mu\Omega\text{ cm}$, slightly affected by deposition temperature.

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Anti-reflection coating with glancing angle deposition on InGaAsP/InGaAs double-junction solar cells

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Due to the increasing demands on clean and renewable energy, high efficiency solar cells have been widely studied using various structures with quantum dots, heterojunctions, intermediate bands, and multi-junctions. Among them, the multi-junction solar cells based on III-V compound semiconductor showed the highest photoelectric conversion efficiency (PCE) of 46%. To get such high PCE, an optimization of anti-reflection coatings (ARC) is necessary for each layer of solar cells. In general, refractive indices of transparent materials are very limited while effective ARC with multilayer needs various refractive indices. Using glancing angle deposition method, however, the refractive indices and nano-structures of thin film can be easily controlled which only requires tilted angle of vapor flux during the deposition process.

In this work ARCs with glancing angle deposition method using MgF₂ and ZnS on InGaAsP/InGaP double-junction solar cells were optimally designed and fabricated. To form anti-reflection layer, the optical properties of MgF₂ and ZnS films deposited at the tilted angle of vapor flux were investigated. Cross-section images of ARC were obtained by scanning electron microscope. Figure 1 shows the simulation result of optimized ARC with four layers. The current-voltage characteristics were measured by using solar simulator (Oriel Sol1A) and I-V measurement system (Keithley 2638A). By optimized ARC, PCE of InGaAsP/InGaP double-junction solar cells was improved to 16.1% from 12.4% due to the increase of the current density as shown in Fig.2.

Growth of thin Pt films on 4H-SiC(0001) and graphene/4H-SiC surfaces

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Silicon carbide is a semiconductor characterised by a wide band gap, high electric breakdown field, high-saturation electron velocity and tolerance to high-temperature and radioactive field. The fundamental structural unit in SiC is a covalently bonded tetrahedron of four C atoms with a single Si atom at the centre. In each layer the silicon (or carbon) atoms have a close-packed hexagonal arrangement. By repeating 2D layer along the c-axis it is possible to form many specific polytypes of SiC crystal (the most popular are 3C, 4H and 6H). This unique crystallographic structure allows to obtain the graphene layers on top of the SiC by the high temperature thermal decomposition process.

Graphene is the most promising electronic material discovered in the past decade. This material exhibits a number of interesting properties such as high electron mobility at room temperature, remarkable optical transparency, high thermal conductivity, exceptional mechanical properties and unique electronic band structure. Therefore graphene has a huge range of potential applications which includes flexible electronics, optoelectronics, bio-sensing, nanocomposites, and energy storage devices (supercapacitors).

In this work, the results of growth of thin Pt films on 4H-SiC(0001) and 4H-SiC(0001)-graphene surfaces are presented and compared. The properties of as deposited films – chemical composition and surface structure – were studied using X-ray Photoelectron Spectroscopy and Low Energy Electron Diffraction. More detailed analysis of determined binding energies and performed comparison of new surface reconstructions observed allow to characterise physical properties of selected systems.

Electronic structure of disordered Ni-Mn-Sn

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The class of off-stoichiometric Heusler alloys that exhibit Magnetic Field Induced Reverse Phase transition (MFIRPT) has gained adequate scientific attention due to large magnetocaloric effects and giant magneto-resistance [1], which lead to potential applications like magnetic refrigeration and magnetic sensors. The off-stoichiometric Ni-Mn-Sn undergo MFIRPT from high temperature austenite phase to low temperature martensitic phase (MP). The change in Gibbs free energy is positive, which implies that the MP is unstable. The changes in electronic states might be responsible for the unstable martensite which in turn causes MFIRPT. Thus, the electronic structure via the valance band of Ni₂Mn_{1.4}Sn_{0.6} as a function of temperature has been studied by high resolution ultra-violet photoelectron spectroscopy and density functional theory (DFT).

The shape of valance band (VB) changes as a function of temperature because redistribution of the Ni 3d, Mn1 3d (Mn at Mn site) and Mn2 3d (Mn at Sn site) states occurs due to structural phase transition to lower symmetry. In the martensitic phase the VB density of states (DOS) near Fermi level decreases as a function of temperature. These two reasons could induce instability in the martensitic phase leading to MFIRPT on application of magnetic field. The origin of martensitic transition and the nature of magnetic coupling is also obtained using DFT [2] which further helps in understanding MFIRPT.

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Adhesion and friction at nanoscale: A correlation study

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Obtaining a general correlation between adhesion and friction at smaller length scales is fundamentally important. However, there were experimental limitations for such a study in terms of configuring a nanoscale sliding contact with well-defined geometrical and chemical cues. We experimentally investigated the correlation between nanoscale adhesion and friction at a sliding contact consisting of an indenter sliding on well-defined nano scale cylindrical, mushroom-shaped, and hierarchical patterned surfaces. The structures were fabricated in polystyrene (PS) and poly(methyl methacrylate) (PMMA) using an intricate combination of capillary force lithography and nano-drawing procedures. The study was performed by friction force microscopy, using a borosilicate ball tip of 10 μm diameter. Results showed that parameters such as curvature, surface energy, hierarchy, and density of the patterns which control the real contact area between the indenter and the patterns, influenced both the adhesion and friction. Further, lateral contact stiffness dominantly determined friction characteristics. Interestingly, in contrast to the literature, cylindrical and mushroom-shaped patterns having equal real contact area exhibited similar adhesion characteristics but very different friction characteristics. Finally, we report a master curve in the graph of adhesion versus friction that encompasses the data for two orders of magnitude of adhesion. Such a correlation between adhesion and friction at nanoscale, will help identify simple pattern parameters that can be tuned to control adhesion and friction.

Metal-deficient "polysulfide" surfaces of metal sulfides: spectroscopic and DFT studies

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Previously, we found using HAXPES, XAFS, DFT+U that the near-surface regions of metal sulfides, which are depleted in metals due to the preferential release of cations upon the reaction with atmosphere and aqueous media, are composed of several layers of various composition and structure. Here, we studied outer surface layers of several metal sulfides applying DFT+U and low-temperature XPS of the samples etched in aqueous solutions and fast-frozen to LN temperature to preserve volatile interfacial species. DFT simulation revealed surprising stability of surface defects involving cation vacancies and S-S bonding. In particular, S₃, S₅ and S₃+S₂ groups were established to be highly favorable at Fe-deficient chalcopyrite, CuFeS₂, (012) and (110) surfaces; disulfide anions were instable, in contrast to "disulfide" underlayers, and the Fermi level shifted below the valence band edge. Typically, S_{2p} spectra showed intense signals with the binding energy slightly less than that of elemental sulfur, which decreased with decreasing the total excess of S, while monosulfide bands increased, and "disulfide" remained minor. The signals arise from bridging S atoms in polysulfide anions unbound to metals or/and adsorbed S evaporated in vacuum upon warming-up to room temperature, leaving S₅ and S₃ anions predicted by DFT. The very stable "polysulfide" surfaces seem to arrest decomposition of sulfides to elemental sulfur, triggering the formation of metal-deficient structures in the early stages of oxidation. The surfaces can have special physical properties; particularly, we found a correlation between the polysulfide content and NIR surface localized plasmon resonance at CuxS nanoparticles.

Prediction of composition and properties of sputtered multi-component coatings by an interactive raytracing software

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To achieve a specific film thickness distribution and well-defined material composition by magnetron sputtering, especially for complex kinematics and multiple sources, is a non-trivial task. To predict these parameters a so-called virtual machine (VM) was designed. The correlation of the model with a lab sized sputter plant will be discussed within this talk.

For preprocessing a 3D-model with well-defined components such as targets, substrates and obstacles, for example shutters or screening arrangements, with associated kinematics and sampling positions as well as basic process parameters, like substrate temperature, racetrack geometry and operating power of the sputter sources is required. Film thickness and chemical composition are computed by line-of-sight deposition which takes into account the decay of the flux density of particles through gas phase scattering. The simulated data has been compared to large area thickness distribution measurements assessed from optical transmission data. The simulated chemical composition of a single sampling position is plotted for multiple materials over several time steps. This stack of chemical compositions is equal to an EDX line scan carried out on a metallographic cross section, from the coating interface to the substrate to the surface. Multiple composition stacks are then equal to an element mapping of the cross section. Finally, examples of the above mentioned comparisons are given.

Investigation on the metal filament formation process of the atomic switch

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The atomic switch is one of the most promising alternatives to current non-volatile memory. Previous studies have revealed the formation and dissipation of a metal filament in atomic switches, however, the chemical species of the metal filament is not clear up to now. The chemical species can be determined by spectroscopic techniques, but it is generally difficult to measure the buried nano structures by spectroscopy.

Here, we focus on the point contact spectroscopy (PCS) to study the chemical species of the metal filament formed in the metal sulfide of the atomic switch. Since the PCS measures the electric current through the conductor, it can study the metal filament itself. In this study, we report the PCS study on the metal filament for the metal sulfide atomic switch. The PCS revealed the formation of the Ag filament in the case of the Ag/Ag₂S/Pt atomic switch. We applied this technique to the other atomic switches, including Ag/Cu₂S/Pt, Cu/Ag₂S/Pt, Cu/Cu₂S/Pt. The systematic study revealed that the source of metal filament was both metal electrode and metal sulfide. We also studied the high-resistive state with the transition voltage spectroscopy (TVS), which provided the information about the energy difference between conduction orbital and Fermi level of the metal electrodes. The TVS revealed that stoichiometric Ag₂S was present between metal electrodes at the high-resistive state in the case of the Ag/Ag₂S/Pt atomic switch.

3d quantum dot superlattice formation - real time x ray scattering study

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Semiconductor quantum dot (QD) superlattices are very promising since the materials embedded with repeatedly ordered QDs found its potential applications as highly efficient solar cells, memories, sensor devices etc. It is evident that the ability to monitor the formation of 3D correlated QDs in-situ and in real time opens an efficient route to optimize fabrication process. Herein, we employed a laboratory-based in-situ grazing-incidence small-angle X-ray scattering (GISAXS) technique to track the formation of Ge QDs in an amorphous Al₂O₃ matrix. [1]

Ge/Al₂O₃ (1 nm/3 nm) multilayers with 20 periods were sputter deposited on a Si substrate. Real-time tracking of the deposition was performed by a fast acquisition of repeatedly taken consecutive GISAXS frames with an integration time of 5 s at the incidence angle of 0.3°. [2]

The strong Bragg spot obtained at $q_y = 0.0 \text{ nm}^{-1}$ confirms the expected ML period of 4 nm. The symmetrically arranged maxima along q_y suggest the presence of 3D correlated Ge QDs in Al₂O₃ matrix. Using numerical simulations, the parameters of ABA stacking based on 3D paracrystal model with base-centered tetragonal lattice of QDs were estimated. Based on the intensity modulations we can elucidate the very early stages of Ge QDs formation. The kinetics of QDs formation, the temporal evaluation of lateral and vertical correlation lengths in 3D QDs system etc. were discussed. We acknowledge support of APVV SK-CN-RD-18-0006.

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2195-A-1902

High performance of phototransistors based on ZnGa₂O₄ epilayer grown by MOCVD

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A deep-ultraviolet (DUV) photodetectors with good responsivity and response time based on an annealed ZnGa₂O₄ epitaxial film grown on (0001) sapphire by metal organic chemical vapor deposition have been investigated in our previous study [1]. However, it still has some room for improvements of these characteristics. To meet with the conception, we alter the device's structure from metal-semiconductor-metal (MSM) finger-type PDs to the thin-film phototransistors. As the results, a ZnGa₂O₄-based phototransistor shows a large responsivity as high to 82260 (A/W) under 230 nm light illumination. The rising time is as fast to 0.18 (sec). Due to transistor behaviors, the photodetector achieves a large photocurrent and optical response successfully. It indicates a better performance of ZnGa₂O₄ DUV phototransistor.

2197-A-1902

A New Laser Interferometric Oil Manometer with High Resolution

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The laser interferometric oil manometer (LIOM), developed at VNIIM, Russia, in 2011, is the national pressure standard in the range 0.1-1000 Pa. The uncertainty of pressure measurements in the lower part of the range is mainly determined by the resolution of the interferometer, which is a half of laser wavelength (1.4 mPa).

Now a new LIOM with high resolution is being developed in VNIIM. This manometer is equipped with the phase modulation interferometer. One of the interferometer mirrors is mounted on a piezo driver, which is controlled by a sawtooth voltage. The voltage amplitude is that the path difference changes periodically and linearly in time by one wavelength. The modulating voltage is synchronized with a pulse generator having a frequency 128 times higher than the modulating voltage. The fractional part of the fringe is determined by the number of pulses counted from the start of the modulation period till the beginning of the next fringe.

It is assumed that the resolution of the new LIOM will be about one hundredth of the laser wavelength.

Microstructures and perpendicular magnetic properties of Co-rich Co-Pt multilayer films

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Materials having high magnetocrystalline anisotropy constant (K_u) are generally desirable for high density magnetic recording applications due to their thermal stability even with smaller grain size. The K_u of hcp Co₃Pt alloy films is as high as $2 \times 10^7 \text{ erg/cm}^3$, and the temperature required for obtaining high perpendicular magnetic properties is relatively low at 300 °C. Therefore, Co₃Pt alloy films have significant potential to be utilized in ultra-high density ($>1 \text{ Tb/in}^2$) magnetic recording media.

In this study, Co₈₀Pt₂₀ films were deposited onto Ru/Ag bilayer films. The perpendicular magnetic anisotropy was achieved by depositing a Co₈₀Pt₂₀ film onto Ru/Ag bilayer films using an argon working pressure of 3 mTorr to sputter the Ru layer at ambient temperature. Its perpendicular coercivity and perpendicular squareness are 3980 Oe and 0.76, respectively. When the working pressure increases to above 10 mTorr, the perpendicular magnetic anisotropy of the films deteriorates greatly. However, both perpendicular coercivity and perpendicular squareness of the films can be increased to 4530 Oe and 0.82 respectively if the Co₈₀Pt₂₀ film is deposited on a higher texture Ru(0002)/Ag(111) bilayer that has been annealed at 300 °C. When this Co₈₀Pt₂₀/Ru/Ag multilayer film is subsequently post-annealed at 300 °C, the perpendicular coercivity and perpendicular squareness of the films are further increased to 5040 Oe and 0.87 respectively, which reveal its significant potential as perpendicular magnetic recording media for ultra-high density recording.

Microstructures and optoelectronic properties of NiO films deposited by HiPIMS

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Within a few p-type transparent conductive oxides (TCOs), NiO with wide bandgap is a promising candidate. Due to its resource availability, low production cost and non-toxicity, NiO film can be employed in various fields. In order to clarify the p-type conductivity mechanism of NiO, a series of work has been reported. Nandy et al. reported that the p-type conductivity of NiO maybe derive from the conversion of Ni²⁺ to Ni³⁺ under oxygen-rich conditions [1]. In this process, Ni vacancies and holes are associated, resulting in an increment in carrier concentration and film's conductivity.

Recently, the high power impulse magnetron sputtering (HiPIMS) technology developed on the basis of conventional magnetron sputtering has attracted people's attention because of its extremely high target ionization rate. The high target ionization rate of this technology is beneficial to increase Ni³⁺ content level during the film's formation, thereby improving the probability of the generation of Ni vacancies, which in turn enhances the film's p-type conductivity. In the current work, the influence of oxygen flow ratio on the microstructural and optoelectronic properties of NiO films deposited by HiPIMS technology was studied. The results show that, compared with DC magnetron sputtering, NiO films deposited by HiPIMS technology possess better electrical properties. In addition, the films resistivity significantly reduces with increasing the oxygen flow ratio.

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2202-A-1902

site acceptance test of the first batch of vacuum chambers for high energy beam transport

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A new accelerator facility (FAIR) is currently being built at GSI Helmholtz Centre for Heavy Ion Research in Darmstadt, Germany. The FAIR accelerator facility will consist of various beam lines which accommodate different functions and experiments with various particle beams (ions, proton and anti-protons). The High Energy Beam Transport (HEBT) provides the transfer of these particle beams to and from the synchrotron, storage rings, Super FRS (Fragment Separator) and some experimental areas. This work presents an overview of results of the site acceptance test of the first batch of HEBT vacuum chambers, which consist of vacuum chambers for various dipole magnets. The chambers under test were predominantly bending chambers of varying degree, length and some branching chambers.

X-ray absorption fine structure studies on surface limited redox replacement(SLRR) for Pt monolayer formation on Au single crystal surface

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Because the large surface tension, it is easy for Pt to aggregate to three dimensional particles and flat monolayer structure is hardly obtained. The Surface limited redox replacement (SLRR) provides the flat Pt surface by using a replacement reaction with Cu underpotentially deposited(UPD) on Au surface[1]. In order to clarify the atomic scale deposition mechanism we have carried out polarization dependent fluorescence XAFS method combined with XPS, AFM and cyclic voltammetry[2,3]

We proposed that Pt deposition via SLRR of Cu UPD monolayer leads to formation/deposition of Pt-surface species mainly consisting of Pt(II) chloride with a square planar local structure [PtCl₄] parallel to the Au surface (60%) which has a strong interaction of the Pt-complex with the Au substrate. The rest (40%) was one-monolayer Pt metal cluster. This result provides a new understanding into the mechanism and stoichiometry of the SLRR reaction, which has a wide application for synthesis of monolayer catalysts.

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Towards in-situ size control of aerotaxy nanowire growth

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Nanowires are promising candidates for next-generation optoelectronic devices since they show strong light trapping at a lower material consumption than bulk-like devices. A substrate-free, high growth-rate approach has been achieved by the aerotaxy technique. To control the size of the aerotaxy nanowire, we propose an in-situ method to monitor the size of nanowire through a non-destructive optical process in the growth reactor. In this method, a beam of light is sent through the growth chamber and the transmission spectrum is collected. By comparing measured optical spectra with simulation results, we can extract the nanowire dimensions. In the simulations, we employed the finite element method, the discretized dipole method and the Mie scattering theory to solve the Maxwell equations. Firstly, the gold catalyst can be ignored in the simulations when the semiconductor nanowire is an order of magnitude larger than the gold catalyst and the diameter is small compared to the incident wavelength. Secondly, We can apply the fast Mie scattering analysis of an infinitely long cylinder to simulate the finite nanowires when the following conditions are fulfilled: (1) the length of the nanowires is larger than or comparable to the incident wavelength (2) the length of the nanowires is much larger than the nanowire diameter (3) the angle between the incident light and the nanowire long axis is larger than 70 degrees. In addition to this, in finite nanowire calculations, we can use the symmetry of the problem to reduce the calculation time by two orders of magnitude.

Electron-stimulated desorption as quality control for annealing procedures

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Heavy ion-induced desorption impairs the vacuum in ion accelerators. Lost ions stimulate desorption by hitting the beam tube. The gas load into the vacuum results in a large pressure increase. This leads to vacuum instabilities and reduced beam lifetime.

Future heavy ion accelerators like FAIR, SPIRAL2 or HIAF will deliver beam currents which are orders of magnitude larger than the intensity of existing facilities. So common solutions like collimators, which catch up the beam losses under controlled conditions, and increased pumping speed will not be sufficient for this high intensities. It is necessary to find low desorbing materials and procedures to reduce the amount of desorbed gas per incident particle, the so-called desorption yield.

Special thermal annealing is the most promising procedure to pretreat critical accelerator components for lower desorption. Results from Thermal Desorption Spectroscopy (TDS) indicate a reduction of the desorption yield by more than two orders of magnitude.

The desorption of different accelerator-relevant materials were investigated by electron-stimulated desorption (ESD) before and after the annealing procedure. The analysis was done in-situ without breaking the vacuum between the desorption measurements and the annealing. For ESD electrons with an energy of a few keV were used. Electron-stimulated desorption offers a simple tool to test the quality of the annealing process without the need of access to the ion beam.

Investigation of the thermally generated Au/Ag nanoislands for SERS and LSPR applications

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Gold and silver nanoparticles are widely used as signal amplification elements in various electrochemical and optical sensor applications. Although these NPs can be synthesized in several ways, perhaps one of the simplest methods is the thermal annealing of pre-deposited thin films on glass. With this method, the parameters of the annealing process (time, temperature) and the pre-deposited thin film thickness influence and define the resulting size and distribution of the NPs on the surface.

Localized surface plasmon resonance (LSPR) is a very sensitive optical phenomenon and can be utilized for a large variety of sensing purposes. Surface-enhanced Raman spectroscopy (SERS) is an analytical method which can significantly increase the yield of Raman scattering of target molecules adsorbed on the surface of metallic nanoparticles. The sensitivity of LSPR and SERS based devices are strongly depending on the used material and also on the size and geometry of the metallic nanoparticles. By controlling these parameters the plasmon absorption band can be tuned and the sensitivity can be optimized.

In this work, the performance of Au/Ag nanoislands was investigated for SERS and LSPR applications. The nanoislands were generated by thermally annealing thin layers of silver and gold, which were previously sputtered onto glass surfaces. Both pure metallic (silver and gold nanoparticles – AuNP and AgNP) and composite systems (silver-gold core-shell structures – Ag-Au core-shell) were evaluated based on their plasmonic and SERS sensitivity.

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Patterning on photosensitive layers for photonic applications

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. Light-sensitive amorphous chalcogenide glasses, as well as some acrylate polymers are well known as optical memory materials applicable for amplitude-phase optical recording. An unique property of these materials consists in the light-stimulated changes of structure, optical, electrical, mechanical parameters, which result in situ changes of refractive index, optical transmission, as well volume, i.e. surface patterning without wet or dry etching.

In the last two decades, the development of light-sensitive chalcogenide glasses systems as well as of polymers got a new stimulus due to the introduction of nanolayered composites from chalcogenide glasses, as well as nanocomposites, including ones with plasmon effects.

In this work, the results of light-induced volume and structural changes in chalcogenides and organic materials are presented. 1D and 2D surface structures were created on the surface of the samples by two interfering laser beams. The holographic recording process and photo-polymerization effect could be enhanced by the localized plasmon field of the created gold nanostructures. The optical and structural changes were detected by optical spectrophotometer and Raman spectroscopy, while the volume change was estimated with atomic force microscope. Besides it, AFM was used to perform point-spectroscopy measurements to establish the mechanical properties of modified samples. The elastic properties of the irradiated areas were compared to the reference material by obtaining and evaluating AFM force-curves. All these gave us information about the possible mechanism of recording processes and selection of upgraded materials for optical recording of photonic elements.

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Effective Fuel Based on Tribology Physics

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The presented technology [1] being realized in vacuum, is based on milling process and may be realized in regions isolated of oil sources also as of petrol manufacturers. The nano-structured fuel is 2-3 times cheaper than diesel fuel and approaches to low cost of coal fuel, although the calorific value is approaching to diesel fuel. The main aim of the technology is ecology pure fuel manufacturing that uses renewable resources, like coal, wood, peat, e.g. Last time a large number of companies search sources of renewable fuel [2]. The described nano structured fuel technology is based on fundamental aspects of "dry friction theory" [3, 4] and shows its high heat ability, that is shown on Fig.1

Fig.1 The weight heat ability (J/kg) different fuels: 1-petrol, 2-diesel fuel, 3-mineral coal, 4- ethylene, 5- nano-structured fuel-suspension[1]

We consider hydrogen atoms as a by-product of milling procedure, because of atmosphere hydrogen atoms solution into the solid particles of fuel. According the theory, sorbed water molecules dissociate in the first coverage monolayer into H₂ and OH parts, then hydrogen atoms dissolve into solid parts being milled: coal pieces, grains, wood rasping in form of a hydrogen-enriched fuel component with high heat ability.

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2215-A-1902

Desorption of frozen CO-clusters

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Beam loss in heavy ion accelerators causes stimulated desorption of gas molecules from the vacuum chamber walls. The resulting degradation of the dynamic vacuum can put a stable accelerator operation at risk. The use of cryogenic superconducting magnets in modern accelerators introduces cold surfaces to the inside of the vacuum chamber. A high sticking probability of gases on cold surfaces can cause residual gas to accumulate to a significant surface coverage over time, presenting a potential reservoir for desorbed gas.

Experiments were conducted to investigate the desorption yields of frozen gas as a function of layer thickness. CO, a prominent gas within ion-induced desorption, was frozen onto a gold-coated copper-target, at a temperature of 7.5 K. Desorption measurements were conducted by measuring the pressure-increase during irradiation with 4.8 MeV/u Au ions. Between each irradiation the layer thickness was increased. A steep increase of the desorption yield for the first 50 monolayers is followed by an asymptotic saturation. This effect could be observed in independent experiments on frozen CO irradiated with various ions of different energies and charge states.

This contribution describes an experimental setup which uses a time-of-flight mass spectrometer in addition to investigate the desorption of CO-clusters. It consists of an electrically isolated, cryogenic target which is mounted perpendicularly to a TOF-mass spectrometer. This setup enables the repetition of the experiment described above, with the addition of a cluster size distribution as a function of layer-thickness. A maximum cluster size is suspected to limit the desorption yield.

2220-A-1902

In Situ Q-plus AFM/STM characterization of the TiO₂ (001)-(1 × 4) Surface

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Anatase TiO₂ has been extensively studied in recent years due to its excellent catalytic performance. In theoretical calculations, the anatase TiO₂ (001) surface is considered to be the most reactive one in different polymorphs, but its surface structure is still under debate to date. In this study, we prepared an anatase TiO₂(001) single crystal film and characterized its surface structure using Q-plus AFM/STM at low temperature. The Q-plus AFM images gave quite different features than STM. Our results proved that the ridge structure of anatase TiO₂ (001) was a good combination of both the ad-oxygen model (AOM) and the ad-molecule model (ADM). The mixed structure of oxidative AOM and reductive ADM effectively released the surface stress to lower the surface energy and play an important role in the catalytic reactivity of this surface since the surface electronic structure is determined by the surface atoms.

Plasma Atomic Layer Etching of Silicon Dioxide Layers in Different Plasma Operation Modes

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In the highly integrated structure due to the miniaturization of semiconductor devices, patterning method is becoming more important. However, the conventional etching method (Reactive ion etch) has many problems such as profile, selectivity, micro loading, and thin film damage. Atomic layer etching (ALE) is a technique that overcomes the technical limitations of Conventional etching. The purpose of this study is to select the plasma reactor suitable for the ALE process and to confirm the plasma operation mode. We also want to find a way to overcome the slow process speed, which is the technical limit of self-limited etching.

Etch rate were compared using the same pressure, gas, and power to verify that ALE is suitable for micro-film control. Although the concept of basic unit is different, ALE has lower etch rate than Reactive ion etching process, which is suitable for process control in thin film.

ALE process characteristics were analyzed by changing the plasma operation mode. CCP mode (Bias power 5W), E mode (source power 10W) and H mode (source power 55W) were measured at the fluorination step, and the fluorocarbon deposition rate was the lowest at 2.7 Å / cycle in the E mode. This is because the location of the plasma generation is far from the wafer. In Etching step, SiO₂ layer etching did not occur in ICP mode (source power 35W), but similar etch rates were obtained at 4Å/cycle in CCP mode (Bias power 20W) and Mixed mode (Source power 10W + Bias power 5W). The voltage of CCP mode measured by the VI probe differs more than twice, but the reason why the etch rate is similar is because the ion density is similar. Mixed mode can generate high-density plasma with ICP source, and can achieve same plasma density with low bias power. However, CCP mode showed higher roughness value than mixed mode in thin film damage test using AFM.

Therefore, we expect that ICP type ALE process will be able to realize low damage & low etch rate & high speed ALE characteristics compared with existing CCP mode.

Reduced dimensionality effects in two-dimensional electronic silicon

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The gas-phase dosing of dopant precursor molecules, such as phosphine (PH₃), onto atomically-clean and flat silicon (001) surfaces provides a means to fabricate sharply defined, two-dimensional doping profiles in silicon [1], with out-of-plane confinements of order 1 nm. In conjunction with atomic-scale hydrogen desorption lithography, this technique provides the ability to fabricate nano-scale wires [2], quantum dots [3] and single atom transistors [4]. Notwithstanding these exciting advancements, the electronic properties of the 2D layers are not yet fully understood, particularly in relation to the roles played by quantum confinement and valley interference effects.

Here, we present the first soft x-ray angle-resolved photoelectron spectroscopy (SX-ARPES) experiments on high-density (metallic), shallow delta-layers buried 2 – 3 nm below the Si(001) surface. In contrast to previous work [5], SX-ARPES allows us to directly access the buried dopant layers without interference of surface band bending effects and over a much wider region of k-space [6]. We discuss our results in relation to valley-interference effects [5], theoretical predictions [7] and practical implications for future stacked two-dimensional device architectures.

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2D electron gas at the surfaces of III-V semiconductor crystals

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2D electron gas (2DEG) formed at the surfaces of semiconductors has attracted great attention mostly for its technological importance and interesting relevant physical phenomena (i.e. high density of electrons [1], large mobility [2], two-dimensional superconductivity [3], quantum Hall effect [4]). Within the presented work investigations of the 2DEG hosted at the (001) surfaces of InAs crystals have been performed, using angle-resolved photoemission spectroscopy (ARPES). This 2DEG arises due to the surface electric field and subsequent band bending confining the conduction electrons in thin subsurface layer [5]. These electrons are free to move parallel to the surface but are localized perpendicular to it. Comparative work on clean and sulfur-doped InAs has been done. Crystals surfaces have been prepared to be In-rich and passivated with atomic sulfur. Changing surface reconstructions have been investigated with a low-energy electron diffraction (LEED) technique after the annealing to increasingly higher temperatures. 1×1,

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2229-A-1902

Nanostructure Ga₂O₃/SiO₂ by the magnetron sputtering

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Ultrahigh vacuum radio frequency magnetron sputtering is one of the qualified physical vapor deposition methods i.e. a molecular beam epitaxial method and a pulsed laser deposition method. Gallium oxide based layered thin films and solid solution films are deposited by the ultrahigh vacuum radio frequency magnetron sputtering. Deposition parameters are substrate crystallinity, substrate temperatures and sputtering gas compositions. Basic properties are characterized by the optical measurements and high-resolution photoelectron spectroscopy. Single layer Ga₂O₃ on the MgO substrate is discussed on the crystallinity and optical stoichiometry. Solid solution Ga_{2-x}Cu_xO₃ layer are investigated on the optical absorption characteristics. Nanostructured Ga₂O₃ and SiO₂ films are characterized with high-resolution photoelectron spectroscopy. The sputter depth profile of Si2p, Ga3d, Ga2p, O1s spectra with low accelerating voltages and with neutralizing beam indicates the formation of nanostructured oxide films. The Ga3d and Ga2p spectra are found to be most suitable for the layers with thicknesses less than about 20 angstroms. Nanostructured Si/SiO₂ quantum well films are prepared referring to the Ga₂O₃/SiO₂ film preparations.

Gas-Cluster Ion Beam Sputter Depth-Profile Study of Interface Mixing in Solution-Processed Organic Light-Emitting Diodes

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We investigated interfacial mixing of solution-processed organic light-emitting devices (OLEDs) and its impact on device performance. X-ray and ultraviolet photoelectron spectroscopy and argon gas cluster ion beam sputtering are used to investigate the distribution of chemical species near the interface. We revealed that extensive interfacial mixing is found in solution-processed OLEDs regardless of crosslinking[1], and thermal annealing done after solution process is main reason of interfacial mixing[2]. It is found that there is a partially mixed interface in the solution-processed devices prior to the annealing, which seems to promote effective interdiffusion during the annealing. In addition, the extensive interfacial mixing after the thermal annealing appears to enhance the efficiency of OLEDs.

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Unraveling the Structural and Electronic Properties of Graphene/Ge(110)

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The direct growth of graphene on a semiconducting substrate opens a new avenue for future graphene-based applications [1]. Understanding the structural and electronic properties of the graphene on a semiconducting surface is key for realizing such structures; however, these properties are poorly understood thus far. Here, we provide insight into the structural and electronic properties of graphene grown directly on a Ge(110) substrate [2]. Our scanning tunneling microscopy study reveals that overlaying graphene on Ge(110) promotes the formation of a new Ge surface reconstruction, i.e., a (6 × 2) superstructure, which has been never observed for a bare Ge(110) surface. The electronic properties of the system exhibit the characteristics of both graphene and Ge. The differential conductance spectrum from a scanning tunneling spectroscopy study bears a parabolic structure, corresponding to a reduction in the graphene Fermi velocity, exhibiting additional peaks stemming from the p-orbitals of Ge. The density functional theory calculations confirm the existence of surface states due to the p-orbitals of Ge.

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Development of cryogenic deuterium pellet injectors and experimental results for EAST Tokamak

Plasma fueling with pellet injection and pellet pacing for edge localized mode (ELM) control are important techniques to achieve high performance operation for EAST tokamak. At present two pellet injectors for fueling and ELM pacing have been developed for EAST, respectively. The injector for fueling can inject pellets of 2 mm diameter and 2 mm length at 100~300 m/s velocity at 10 Hz with reliability over 95%. The injector for ELM control is capable to inject 1.5 mm diameter and 1.2-1.8 mm length pellets at frequency up to 50 Hz with velocities 200~250 m/s.

The injector for fueling has served experimental campaigns many times up to now and good results have been obtained. Recently, multiple pellets have been injected into type-III ELMy H mode in a upper signal null (USN) divertor configuration from LFS and a string of high frequency small ELMs were induced. In addition, deuterium pellets have also been injected in H-mode with ELM suppression by RMP. But a string of small ELMs often were induced during this time. Meanwhile, plasma confinement became better, which could be observed through plasma energy increasing. As for the injector designed for ELM control, its reliability is more than 85% when the launching frequency is 50 Hz, which means this system can be used for ELM mitigation on EAST in the future. At present, the 50 Hz pellet injection system has been installed and used in physical experiments preliminary on EAST.

non-destructive chemical depth profiling for thin film and buried interface by high-energy synchrotron radiation xps and xas

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Non-destructive depth profile analysis with better depth resolution is required for characterization of nano-materials. Sputter etching is commonly used for conventional way of depth profiling. However, it makes damages because of atomic mixing and surface roughening. X-ray photoelectron spectroscopy (XPS) is typically non-destructive analysis, however, XPS with fixed excitation energy source cannot provide depth profile without additional technique. On the other hand, analyzing depth of XPS can be varied with energy tunable excitation source, such as synchrotron-radiation (SR), since escape depth of photoelectrons depends on their kinetic energy. We can obtain XPS spectra from different analyzing depth by varying excitation energy. This technique can provide depth profile non-destructively. We also examined a method to perform depth profiling with X-ray absorption spectroscopy (XAS) by changing electron energies for detection ranging from 5 to 50 eV using electron spectrometer (partial electron yield detection). In the present study, Ge (2~4 nm) and Au (1~10 nm) thin films on Si(100) have been analyzed. The measurements have been performed at KEK-PF, Tsukuba using 1.8~3.7 keV X-ray. XPS spectra clearly show the interface under the deposited films can be observed even for the 4 nm Ge sample. Chemical state changes at the interface by the two substrates are also clearly observed. From XAS analysis, obvious correlation between Si/Au ratios and the electron energies are observed. These results suggest that SR-XPS and XAS are powerful technique for non-destructive chemical depth profiling of surface and buried interface.

STM/STS study on local electronic states of H:Si(110)-(1x1) surface

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The Si(110) surface has attracted growing attention and interest because of high hole mobility among low index silicon planes as well as of anisotropic surface properties arising from its rectangular symmetry. Although a clean Si(110) surface reconstructs into a complex “16x2” structure, a bulk-truncated (1x1) structure can be obtained by passivating surface dangling bonds with hydrogen (H) atoms, whose phonons and electronic states exhibit one-dimensional character [1–3]. In this study, we have performed scanning tunneling microscopy/spectroscopy measurements on H-terminated Si(110)-(1x1) surface. We found that the contrast of STM image drastically changes depending on the polarity of bias voltage: In the filled state image, zigzag chains running along [1 -10] direction are clearly observed, whereas the empty state image shows straight lines with small corrugations. Such polarity dependence has not been reported in the previous experimental/theoretical studies [3–6]. Our STS measurements in atomic resolution elucidate that the filled states near Fermi level mainly localize at the outermost H-atoms, while the empty states localize around Si-Si bonds in the first layer. The results are also supported from our theoretical calculations.

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Thermal effect on laser-assisted field evaporation from Si(110) surface: A time-dependent first-principles theory combined with molecular dynamics simulation

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Laser-assisted atom probe tomography (La-APT) is a powerful technique for analysis of three-dimensional structure of semiconductors and insulators. Although La-APT showed remarkable successes in many fields, the microscopic mechanism of laser-assisted field evaporation (LAFE), which is a key phenomenon utilized in La-APT, is still unclear. Electronic excitations and temperature increase are key quantities to understand the mechanism of evaporation. Previously, LAFE from Si cluster was investigated using a time-dependent density functional theory (TDDFT) simulation [1]. However, they focused only on the electronic excitation caused by laser illumination and did not take account of thermal effect on evaporation dynamics.

Therefore, we explore and clarify the finite electron- and lattice-temperature effects on LAFE from Si surface by TDDFT combined with molecular dynamics simulations in the present study.

We found that surface dangling bond states assist thermal excitation under finite electron-temperature conditions, leading to electron transfer from surface to bulk and ionization of surface atoms under dc fields. The finite electron-temperature effect on evaporation is, however, not appreciable. In contrast, the finite lattice-temperature effect promotes atomic motion in the directions of both parallel and perpendicular to the surface, which naturally enhances evaporation under dc and laser fields. Since this result is consistent with La-APT experiments, the present first-principles simulations provided the theoretical evidence of the thermal effect on LAFE.

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study on pumping performance of multi-stage vacuum pump rotors of different stages

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Multi-stage vacuum dry pumps are widely used in industries such as the semiconductor industry. In order to improve the pumping performance of multi-stage vacuum dry pumps, the research institutes and vacuum pump manufacturers have carried out extensive and in-depth research on the multi-stage vacuum pump pumping principle and upgrade design. However, the existing research mainly focuses on the optimization of the structure of a certain rotor, and the test method of the vacuum dry pump is only for the whole pump product. The systematic study of the multi-stage vacuum dry pump and the difference of different rotors are still in the initial stage. This paper aims to further explore the difference in pumping performance of different rotors of multi-stage vacuum dry pumps, and obtain the pumping performance test and evaluation methods of different rotors of multi-stage vacuum dry pumps under real operating conditions. In this paper, the theoretical analysis of the pumping performance of multi-stage vacuum dry pump with different blade Roots rotors has been carried out. The internal flow field and pumping speed of different leaf type Roots rotors were compared by Fluent numerical simulation. A new test method was proposed for single-stage or combined-stage test of different rotor pumping performances in multi-stage vacuum dry pumps. At the same time, an experimental vacuum pump with adjustable rotors was developed for different rotor designs. It provides a simple and feasible solution and provides a theoretical basis and reference means for the development of multi-stage vacuum dry pumps.

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investigations on internal temperature field analysis and control mechanism of screw vacuum pump

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Dry screw vacuum pumps have been widely used in petroleum and petrochemical, aerospace, semiconductor, surface science and other industries. However, in some severe process environments, the dry screw vacuum pump produces a higher exhaust gas temperature during the operation of the compressed gas, resulting in the extracted medium decomposing highly toxic and corrosive substances at high temperatures, which increase the security risks in actual process. To get good temperature control effect, this paper designed a variety of pump body structures to achieve adjustable temperature inside the pump chamber. According to the basic principles of fluid mechanics and thermodynamics, the internal mechanism of dry screw vacuum pump under different working processes was analyzed. With the FLUENT simulation software, dynamic grid technology was used to simulate the internal temperature field, rotor and pump chamber thermal deformation of dry screw vacuum pump with different structures. In addition, the rationality and feasibility of the internal temperature structure design of the adjustable pump chamber were verified by experiments. Combined with theoretical analysis and experimental investigation, the optimal pump structure for adjusting the internal temperature of the pump chamber is obtained. Under the demand of special working conditions, this paper provides theoretical research value for the development of new products of dry screw vacuum pump.

comparative study on the influence of different screw rotors on the pumping performance of screw vacuum pump

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Dry screw vacuum pump (DSVP) is a dry vacuum pump with broad application prospects and huge market potential. At present, DSVP has been successfully applied in many industries such as semiconductor, medicine, food, chemical and so on. The screw rotor is the most critical pumping component in DSVP, which directly determines the pump's performance and service life. This paper aims to investigate the effect of screw rotor structure on the operation of DSVP performance parameters under different pressure zones. Based on FLUENT using dynamic mesh technology for finite element analysis, the internal flow field and pumping speed of the screw rotor process with different expansion modes are compared. The theoretical analysis of the pumping performance of the equal pitch and variable pitch screw rotor has been carried out. At the same time, a dry pump test bench was set up to test the DSVP pumping performance of different rotor types under different inlet and outlet pressures to verify the correctness of the theory. It is found that the equal pitch set at the suction and exhaust sides under low pressure and high pressure is beneficial to increase the pumping speed and the ultimate pressure of the pump, and the variable pitch is set in the intermediate pressure region to help reduce the power consumption of the pump. This paper lays the foundation for the exclusive design of DSVP under various working conditions.

inas nanowire devices for thermionic and hot-carrier energy conversion

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The concept of hot carrier photovoltaics (HCPV) is based on collecting hot carriers that are photo-generated above the band edge before they have time to relax via phonon emission, in an attempt to minimize energy lost as heat. III-V nanowires (NWs) are of great interest for such applications for several reasons such as: extended hot carrier relaxation time [1]; the ability to grow lattice mismatched heterostructures [2] and the possibility to control where light is absorbed by designing photonic or plasmonic elements.

The principle of a NW-based HCPV has been realized [3] based on InAs NWs with a small segment of InP that results in a potential barrier for electrons in the conduction band. When light is focused on one side of the barrier, the lattice temperature is raised locally, altering the Fermi Distribution on that side, allowing thermalized electrons to diffuse over the barrier.

In this work InAs NWs with single barrier structures are studied with the aim of evaluating the heat conversion efficiency and maximum power output as a function of barrier shape. In order to apply a controlled local thermal bias, top heaters are fabricated on top of the device leads, similar to recent work on quantum dots [4]. The current status of the project will be presented.

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Application of Direct-Current Glow Discharge Cleaning in 2 T strong magnetic field for fuel retention removal in EAST superconducting tokamak

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In Experimental Advanced Superconducting Tokamak (EAST), DC-GDC is successfully operated under strong magnetic field of up to 2 T in 2018, which is successful application of DC-GDC under strong magnetic field for the first time in the world. Four anodes and 4 independent DC power supplies are used together. GDC plasmas are started easily in helium pressure of 0.5 – 4 Pa under 2 T without any breakdown problem, and breakdown pressure is lower than that without magnetic field. GDC current is probably maintained between anode and surrounding components which are along the magnetic field lines, therefore the strong magnetic field could improve the GDC plasma confinement in radial direction rather than block the formation of GDC current. GDC plasma with a total current of (1-6)×4 A in 2 T are approximately uniform in toroidal direction, while it's concentrated almost on GDC anode position in poloidal direction, due to strong confinement of toroidal magnetic field. Deuterium particles are strongly released by helium DC-GDC plasmas with a maximum surface current density of 0.4 A/m². The removal rate of retained deuterium is weakly dependent on magnetic field in the range of 1 – 2 T, but it's almost linear to GDC current. The removal rate of deuterium is (0.2 – 11.2)×10¹⁹ D/s, which is much higher than that of RF discharge cleanings in EAST. The application of DC-GDC under strong magnetic field provides an efficient and feasible method for tritium removal in future fusion devices, such as ITER.

Biocompatibility and mechanical property evaluation of Zr-Ti-Si thin film metallic glasses grown by a hybrid high power impulse and radio frequency magnetron sputtering system

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The amorphous thin film metallic glasses (TFMGs) have been studied widely due to their unique properties such as good corrosion resistance and high hardness. In this study, five Zr-Ti-Si thin film metallic glasses (TFMGs) with different Si concentrations were fabricated by a hybrid high power impulse and radio frequency magnetron sputtering system. The amorphous phase of TFMG was determined by the X-ray diffractometer (XRD) and transmission electron microscopy (TEM). The nanoindentation test was used to evaluate the mechanical and adhesion properties of coatings. The corrosion resistance of TFMGs were evaluated by the electrochemical test in Hank's solution. The MG-63 cell line (human osteosarcoma) was used to investigate the cell-material interaction and biocompatibility of coatings. We can conclude that very fine and dense featureless microstructure was discovered for amorphous Zr-Ti-Si TFMGs. The hardness and elastic modulus of Zr-Ti-Si TFMGs increased with increasing Si content. Very good corrosion resistance and biocompatibility was found for all Zr-Ti-Si TFMGs indicating their great potential for biomedical application.

Growth of epitaxial silicon carbide films by metal-organic chemical vapor deposition and their optical properties

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In this paper, we successfully prepared the thin film of cubic SiC on Si(001) substrates by metal-organic chemical vapor deposition (MO-CVD) method using a single source precursor at various growth parameter such as temperatures and times. As a single source precursor, we used a 2,5-Bis(silyl)-1,4-disilacyclohexane without carrier gas. This precursor is also optimized for synthesis of cubic SiC because silicon and carbon atoms are designed to have the same amount. After MO-CVD process, SiC/Si(001) thin films were measured by reflection high energy electron diffraction (RHEED) pattern under the UHV condition to confirm the certain crystallinity. For further optical study, we measured X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Since the single crystalline SiC thin film has attracted much attention due to its excellent electrical and mechanical properties, our research that minimizes the growth process of the thin film will have sufficient advantages for application in the future.

detailed lattice models: filling the gap between dft calculations and experimental surface science

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Self-assembly of molecular monolayers on solid surfaces has a great potential for mass production of nanodevices and new materials. The development of experimental techniques, such as atomic-resolution microscopy, made it possible to see a huge amount of ordered structures formed by adsorbed molecules. Nowadays, the attention of researchers is focused on the development of processes for controllable self-assembly of nanostructures with desired properties. It requires special theoretical tools that allow to predict in-silico the self-assembly and properties of the monolayers. The time scale of self-assembly processes often significantly exceeds the typical time integration step in classical molecular dynamics. Thus, it is very difficult to obtain a representative sample even with the advanced sampling techniques.

To simulate complex adsorption systems, we propose the Surface Science Modeling and Simulation Toolkit (SuSMoST). It includes a number of utilities and implementations of algorithms that allow to predict or explain the structure and properties of adsorbed monolayers based on the data known from the experiments and DFT calculations, such as geometry of the adsorption complexes, binding energies and energies of intermolecular interactions. As an example, we present a detailed study of the hard disk model using the methods of statistical physics: Monte Carlo, transfer matrix and the renormalization of tensor networks.

2260-A-1902

Actual status of the High Energy Beam Transfer (HEBT) for the FAIR accelerator

Lukas urban, Phe Man Suherman

FAIR will be one of the largest and most complex accelerator facilities in the world. The FAIR accelerator facility will have the unique ability to provide particle beams of all the chemical elements (or their ions), as well as antiprotons. The particles will be accelerated to almost the speed of light in the FAIR accelerator facility and made available for scientific experiments. FAIR will generate particle beams of a previously unparalleled intensity and quality. At the heart of the facility is an underground ring accelerator with a circumference of 1,100 meters. There are also additional experimental rings and experimental stations. The existing accelerator facility of the GSI Helmholtzzentrum für Schwerionenforschung will serve as the injector for the new FAIR facility. The High Energy Beam Transfer (HEBT) lines will connect all these different machines, such as Rings and Experiments, together. The HEBT system will be operated at room temperature at an ultimate pressure of less than 10^{-7} mbar. Some of the vacuum chambers will be required to operate at ultimate pressure of less than 10^{-10} mbar and therefore require an in-situ bake out cycle.

High-temperature fiber optical feedthroughs and applications

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Based on the rapidly enhanced complexity of industrial processes in vacuum, the requirements concerning in-system diagnostics are more and more demanding. On the one hand, the process parameters have to be diagnosed, characterized and controlled by a measurement and monitoring system in vacuum. On the other hand, the setup itself has to be completely decoupled from the process to avoid any external or internal impact on the process. In the vicinity of these two contradictive requirements optical fiber applications gain more and more impact in vacuum processes, since optical fibers cover different necessary advantages: high mechanical and optical flexibility, low transmission losses and inherent immunity against external forces in combination with a high durability.

The focus of the present contribution is a new in-vacuum diagnostics solution enabled by customized high-temperature fiber optical feedthroughs featuring fiber Bragg gratings (FBGs) in the optical fiber. In a pioneering case study, the application of the feedthrough as an in-vacuum temperature sensor is demonstrated. The mechanism of the sensor is based on FBGs in the optical fiber. The FBGs are very sensitive to strain and temperature. In combination with the presented hermetical sealed UHV-suitable optical fiber feedthrough, an optical fiber containing a bunch of several FBGs becomes a compact, stable, robust, and flexible network of local sensors to simultaneously monitor temperature at different positions in vacuum with several km signal path and a measurement accuracy below 0.5 K.

Comparative study of IN600 superalloy produced by two powder metallurgy technologies: Argon Atomizing and Plasma Rotating Electrode Process

Jiayi Zhang

Two type products of IN600 alloy powders fabricated by Argon Atomizing (AA) and Plasma Rotating Electrode Process (PREP) were compared, in terms of microstructure, sphericity of powder, defects and mechanical properties. The interior morphology of AAed IN600 powder was mainly composed of cellular dendrites, and the dendrites were discontinuous and disordered. While, the interior morphology of PREPed IN600 powder was mainly composed of dendritic dendrites. The granularity of AAed IN600 powder ranged from 40 to 150 μm , in comparison that of PREPed IN600 powder ranged from 70 to 130 μm . The sphericity of PREPed powder particles were better than that of AAed powder particles. Large hollow powders existed in AAed IN600 alloy powder, while PREPed IN600 alloy powder did not exist. The AAed and PREPed IN600 alloy both exhibit equivalent tensile strength and yield strength after hot isostatic pressing and same heat treatment condition, but the section shrinkage rate of PREPed alloy (15.5%) was higher than that of AAed alloy (14.6%), indicating that the plasticity of PREPed IN600 alloy was better than that of AAed IN600 alloy.

Cavitation Assisted Hydrolysis of Waste Human Hair for Potential Use as Fertilizer

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Hair waste in India from saloons and temples amounts to a large value, India alone exported approximately 1 million kg of hair and its products in 2010. There are environmental concerns and problems of pollution when it comes to incineration of human hair, degradation of hair can cause foul smell and discomfort. This work concentrates on alkaline hydrolysis of hair assisted with acoustic cavitation (ultrasound) and hydrodynamic cavitation and further, it's comparison with conventional method of alkaline hydrolysis. In acoustic cavitation assisted hydrolysis of waste human hair, the effect concentration of hair and alkali solution along with the ultrasound power were investigated and optimised. Pressure was optimised for hydrodynamic cavitation. Viscosity reduction in the solution is caused during the process, hence optimization was predicted by studying the extent of viscosity reduction. Untreated and treated hair samples were characterized by Fourier Transform Infrared Spectroscopy (FTIR) to study the extent degradation of human hair and High Pressure Liquid Chromatography (HPLC) for amino acid analysis. In case of cavitation, it has been found from amino acid analysis that hair hydrolysate has a relatively more digestibility and relatively more nutritional value as compared to conventional process. Thus, acoustic cavitation or hydrodynamic cavitation assisted hydrolysis proved to have more stability, is an environmentally friendly technique and consumes less energy as compared to conventional methods. Cavitation assisted hair hydrolysate has a potential application in agricultural engineering as a fertilizer for improvement of the quality of the soil and land.

Investigation of the adsorption of nitrogen and ammonia on the surface of V3C2 using the methods of density functional theory and statistical physics.

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Azofra et al, showed that MXenes V3C2 exhibits a high catalytic activity in the reaction of nitrogen to ammonia.

We investigated the surface properties of MXenes V3C2 by methods of statistical physics. The thermodynamic properties of the adsorption layer and the temperature stability of the phases were investigated. The adsorption isotherms and thermal desorption spectra were constructed using the SuSMoST program code [2].

The potential of lateral interactions of ammonia and nitrogen molecules on the surface of V3C2 was investigated using local potentials. The lateral interactions were calculated using the methods of the density functional theory using the QUANTUM ESPRESSO [3] and GPAW [4] packages.

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Cold plasma activation of BPDA-PPD polyimide for improved biocompatibility

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Polyimide is commonly used for packaging of medical devices due to its thermal and chemical stability, mechanical strength and flexibility and low moisture absorption [1]. Although it is known to be biocompatible [2], a cold plasma treatment has been applied for the activation of BPDA-PPD polyimide in order to enhance the interaction and integration of the device with the surrounding tissue to minimize the foreign body reaction after implantation. The influence of different parameters of the plasma activation on the surface composition of polyimide has been studied (exposure time, discharge power, plasma gas) as well as the hydrophobic recovery of optimal treatments over the 24 h following the exposure. For all gases (air, He, N₂, Ar) short treatment times (1.0-32.0 s) and low discharge powers (1.5-3.0 W) revealed to be enough to introduce oxygen-containing functional groups, with an increase of 40-70% in the O/C ratio. Hydrophobic recovery stabilized fast (2.0-4.0 h after exposure) although the functionalities introduced onto the surface were not significantly affected. Eventually, it was confirmed that air or nitrogen plasma activation of polyimide can substantially increase fibroblasts attachment and viability, showing the potential of cold plasma treatment to improve the interaction of polyimide with the body tissue.

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Using ambient pressure x-ray photoelectron spectroscopy to measure the spatial gas composition above a catalytic active surface

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Recently, planar laser-induced fluorescence (PLIF) was used to simulate an ambient pressure X-ray photoelectron spectroscopy (APXPS) setup and measure the size of the CO depletion layer once it is mass transfer limit (MTL) for the CO oxidation reaction [1]. In this contribution, we will demonstrate how APXPS can be used to measure the size of the CO depletion layer directly and probe the gas composition within it for the same reaction.

Our APXPS experiments were performed in the flow cell of the HIPPIE endstation at the MAX IV Laboratory. By moving the sample backward in the cell while recording series of O 1s and C 1s spectra we probed the gas composition of a small volume further and further away from the sample surface. From such experiments performed at different flow and pressure settings we will discuss the size and composition of the CO depletion layer.

At the HIPPIE endstation it is possible to measure the gas composition with mass spectroscopy at the cell inlet, at the cell outlet, and of the gas that is pumped into the electron analyzer through the small aperture. Using these data, we will demonstrate how the flow distribution, apparent conversions, and the overall conversion in the cell can be found. Finally, the knowledge from our APXPS and mass spectroscopy experiments will be combined to give a complete picture of flow and gas composition in the cell.

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Plasma-enhanced Atomic Layer Deposition of Molybdenum Oxide using Molybdenum Hexacarbonyl and O₂ plasma for Silicon Solar Cells

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MoO_x is used for hole-selective contacts layer in silicon solar cells. But, MoO_x is sensitive to temperature, plasma, and air exposure. In this study, MoO_x is deposited by plasma-enhanced atomic layer deposition using Molybdenum hexacarbonyl (Mo(CO)₆) is selected as precursor for Mo and O₂ is adopted as precursor for plasma. To obtain high-purity sub-stoichiometric MoO_x film, the deposition temperature was varied from 50 °C to 170 °C and plasma power was also varied.

X-ray photoelectron spectroscopy (XPS) analysis confirmed the binding and film quality of the MoO_x films as a function of deposition temperature and plasma power. The thickness and MoO_x/c-Si interface was investigated by transmission electron microscopy (TEM). The lifetime and implied open-circuit voltage (V_{oc}) were measured by quasi steady state photoconductivity (QSSPC).

Synthesis and characterization of polymer stabilized-iron oxide nanocomposites for doxorubicin delivery in neuroblastoma therapy

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The development of multifunctional drug delivery systems (DDS) as nanocarriers for the delivery of cancer drugs to specific cancerous tissues has received considerable attention in the field of nanomedicine. In this study, a magnetic nanocarrier made up of iron oxide nanoparticles (MNPs) coated with Pluronic F127 for the delivery of doxorubicin (DOX) for neuroblastoma treatment was synthesized. The F127-MNPs were synthesized through co-precipitation method. The HR-TEM images showed spherical and uniformly dispersed particles with sizes between 10–30 nm. The XRD pattern of synthesized magnetic nanoparticles at $2\theta = 35.44^\circ$ corresponded to that of magnetite (Fe_3O_4) (311), consistent with Joint Committee on Powder Diffraction Standards (JCPDS) database. XANES spectra of Fe atom demonstrated an absorbance feature (Fe = 7113 eV), of 1s to 3d transition. Irrespective of the differences in Pluronic concentration and the dimensions of MNPs products, all the samples displayed negligible coercivity and remanence, suggesting their superparamagnetic properties. The MTT assay results showed no significant cytotoxicity of the prepared nanocarrier on treated cells. The in vitro drug release profile displayed a pH dependent drug release with a faster DOX release rate in acidic conditions than in a neutral environment.

Comparison of PVD coating topography at different deposition techniques

Typical application-oriented research in hard protective coatings is concentrated on a particular applied property, such as hardness, toughness, corrosion resistance, etc. While these properties depend on the coating as a whole, there are several other properties where the surface topography plays an important if not decisive role. Friction coefficient and tendency for workpiece adhesion are among the most relevant ones. The surface topography can be greatly improved by various post-treatment methods, such as wet blasting or polishing, nevertheless, the initial condition after deposition remains an important feature. It allows the coater to decide to which extent, if any, a post-treatment is necessary.

Though general physics background of, say, droplet formation in cathodic arc evaporation is well-known, there are several important relationships where the explanation is not that straight-forward. On the deposition side, there are parameters like vertical position in the chamber, rotation mode, coating type, and the deposition parameters themselves (both etching and coating phases). Regarding topography, in addition to the ubiquitous roughness there are several statistical parameters related to the growth defect density.

In this study we are looking for influences of the deposition parameters on the topography. We compared three deposition techniques: magnetron sputtering, cathodic arc evaporation and electron beam evaporation. Standard industrial coatings were deposited (TiN, TiAlN, TiAlSiN, DLC) on tool steel coupons and cemented carbide endmills. Their surface topography was evaluated using stylus profilometry, confocal optical microscopy and SEM.

Band structure of two dimensional electron gas at InAs(001) surface

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2D electron gases (DEGs) are formed at surfaces and interfaces of semiconductors as a result of the in-plane confinement of conduction electrons, caused by a surface electric field and the associated band bending. A characteristic quasi-2D surface electronic structure (a set of 2D subbands) is then observed. Such 2DEGs have extremely high technological relevance (c.f. the famous statement: the interface is the device). We have studied the band structure of 2DEGs formed at surfaces of InAs(001) with the aid of sulphur atoms adsorption, using angle resolved photoelectron spectroscopy. A care has been taken to prepare systems with smooth surfaces and not containing electron scattering centers in the bulk. Such systems present particularly clear pictures of 2D subbands. These subbands are explained within the one electron Poisson-Schroedinger scheme, however, taking into account the surface reflection phase effect seems necessary. In contrast to these observations the measured electron effective mass appears much larger than the tabulated values for InAs and varying with the surface band bending suggesting many electron effects at play.

Successive direct stacking of CVD synthetic graphene for twisted van der Waals heterostructures

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Controlled stacking method of 2 dimensional (2D) materials into van der Waals (vdW) heterostructure is key factor of design and fabrication of new devices based on 2D materials. With the recent increase in interest for twisting bilayer graphene, accurate angle control with clean interface is required. Many researchers are mainly using exfoliation graphene from HOPG, which can create vdW structures more easily than synthesized graphene on catalysts. However, for application development and industrialization, it is advantageous to use large scale CVD synthetic graphene. We report that stacking method of CVD synthetic graphene by successive hBN direct transfer. Using the interaction of hBN and graphene, graphene can be easily picked up from germanium, a synthetic catalyst. Also, successive pick & release also enables clean interface and controlled angle vdW heterostructure. This method can be a suitable method for creating applications, as well as studying the properties of the vdW structures.

A new STM-induced light emission apparatus applied to the study of 2D materials

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Light emission processes induced by the tunnelling current in a Scanning Tunnelling Microscope (STM) can be explored to study luminescence with a spatial resolution much higher than possible by optical microscopy. Also, STM-induced light emission (STM-LE) in semiconductors and colour centres, among others, has already been reported.[1,2] We report on a novel light detection scheme which aims to be highly efficient and yet compatible with an ultra-high vacuum, low-temperature STM. Our light detector uses a small mirror accurately positioned with a 3-axis piezo nano-manipulator. Supposing an isotropic semi-spherical light source, light ray optical numerical simulations predict about 70% collection efficiency, similarly to patented solutions.[3] We aim to apply this facility to the study of two-dimensional (2D) materials like transition metal dichalcogenides (TMDs) such as MoS₂ and WS₂ and WSe₂. These materials are receiving extensive relevance due to their great and tuneable optical properties.[4] Particularly, the properties of these materials can be further tailored by defect engineering, including on-purpose added point defects in monolayers.[5] We will present the first results obtained with our systems and expected direction of this project.

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SIMS study of hydrogen adsorption on TiFe alloy surface

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Secondary Ion Mass Spectrometry (SIMS) is a well-known technique of surface analysis that allows obtaining depth and spatial distribution of elements and isotopes in studied samples on micro- and nano scales. Another advantage of SIMS is that, among a few other methods, it allows the direct detection of hydrogen isotopes with high sensitivity and in a wide dynamic range.

In this work, we present the results of the application of SIMS to study hydrogen interaction processes with the surface of hydride-forming TiFe alloy. The experiments were carried out with a UHV capable custom built secondary ion mass spectrometer.

In the presence of chemisorbed hydrogen atoms on the surface of the alloy, emission of a variety of hydrogen-containing positive and negative secondary ions was observed. The studies of the influence of such experimental parameters as hydrogen partial pressure in the sample chamber, current density of primary ions, and temperature of the sample have shown that these parameters affect the hydrogen concentration on a surface. However, the yield of hydrogen-containing secondary ions is affected practically only by the hydrogen concentration on the surface, whatever the mentioned above parameters are. Although the yield dependencies of different kinds of hydrogen-containing secondary ions on hydrogen concentration were usually qualitatively similar, they were quantitatively different. The connection of secondary ion yields with hydrogen concentration on a surface allows studying processes that can change its concentration, namely adsorption and desorption. Thus, some characteristics of those processes and estimates of their kinetic parameters were obtained.

Magnetic and optical properties of metal filled luminescent porous silicon

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In today's research activities magneto-optics is intensely investigated and thus the purpose of this work is to influence the photoluminescence of microporous silicon (PSi) by filling with a magnetic metal (e.g. Ni). The samples are prepared by self-organization concerning both, the pore formation as well as the metal filling. The influence of the optical properties happens in two ways. On the one hand the surface plasmon of the metal deposits is exploited to modify the luminescence and on the other hand they are influenced by an external magnetic field. Due to the metal filling of the PSi the photoluminescence is blue-shifted and furthermore an increase of the intensity is observed. The influence of the magnetic metal filling on the optical properties is discussed and the magnetic characterization of the nanocomposites is presented. Photoluminescence spectra of bare PSi show a maximum around 620 nm whereas in the case of Ni filled samples the peak is blue-shifted to around 580 nm and the luminescence intensity is increased.

Field dependent magnetization measurements performed with the magnetic field applied perpendicular and parallel to the sample surface show a high magnetic anisotropy. It can be clearly seen that the samples offer a film-like behavior due to the interconnected Ni structures which is represented by the easy axis parallel to the surface. Furthermore the influence of an external magnetic field on the optical properties is elucidated. The presented systems are promising candidates for applications in optoelectronics and also for magneto optical integrated devices.

Experiencing NEG technology on radio frequency (RF) cavities for the Elettra 2.0 project.

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Elettra 2.0 is the upgrade project of Elettra, the third generation synchrotron radiation light source operating at Trieste (Italy). In order to obtain an ultra-low emittance storage ring, a new magnetic lattice has been studied. As a consequence, the entire storage ring vacuum system will be replaced with small aperture vacuum chambers because of the reduced bore size of the magnets. Large (and heavy) sputter ion pumps (SIPs) will be no longer used: they will be replaced mainly by non evaporable getter (NEG) pump technology in long and narrow vacuum chambers (as internal coating) as well as in lumped pumps in order to reduce size and weight and, consequently, to simplify their installation. When NEG pumps are coupled with small SIPs, all the gas species present in UHV systems can be effectively pumped. Some combined pumps were tested on the first component already defined for the Elettra 2.0 project: the radio frequency (RF) cavity. Results of this experience are reported and compared to theoretical simulations.

Study of nitrogen ion doping of titanium dioxide films

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This study reports on the properties of nitrogen doped titanium dioxide (TiO₂) thin films considering the application as a transparent conducting oxide (TCO). [1] Sets of thin films were prepared by sputtering a titanium target under oxygen atmosphere on a quartz substrate at 400 or 500°C. Films were then doped at the same temperature by 150 eV nitrogen ions. The films were prepared in Anatase phase which was maintained after doping. Up to 30 at% nitrogen concentration was obtained at the surface, as determined by in situ X-ray photoelectron spectroscopy. Such high nitrogen concentration at the surface leads to nitrogen diffusion into the bulk which reached about 25 nm. Hall measurements indicate that average carrier density reached over 10¹⁹ /cm³ with mobility in the range of 0.1–1 cm²/Vs. Resistivity about 0.31 Ohm cm could be obtained with 85% light transmission at 550 nm, similarly or better to other studies.[2,3] The Anatase band gap, 3.29 eV, was not modified by the nitrogen doping, in agreement with the literature.[4] These results indicate that low energy implantation is an effective technique for TiO₂ doping that allows an accurate doping that is independent of the film growth. [4]

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Chemical Bonding in MAX phases and MXenes Investigated by X-ray Spectroscopy and ab initio calculations

Martin Magnuson

The electronic structures and chemical bonding as well as the crystal structures in 2D ceramic MAX-phases and MXenes are investigated by X-ray spectroscopy and compared to ab initio electronic structure calculations. Calculated spectra using hybrid functional density-functional theory (DFT) including core-to-valence dipole matrix elements are found to yield consistent spectral functions of experimental data. By varying the constituting elements and structures in MAX-phases and MXenes, a change of the electron population cause a change of covalent bonding between the laminated layers, which enables control of the macroscopic properties of the materials. For MXenes, the role of functional –O, –F and –OH termination groups at the interfaces and their local symmetries at different adsorption sites are discussed. Synchrotron radiation techniques such as bulk-sensitive soft X-ray absorption and emission spectroscopy are shown to be particularly useful for detecting detailed symmetry in the electronic structure that yield anisotropic information about internal monolayers and termination groups at the interfaces. Angle- and polarization-resolved measurements are shown to reveal differences in orbital occupation across and along the laminate basal plane.

Temperature Dependent Electronic Structure of Wurtzite GaAs Nanowires

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Semiconductor nanowires can adopt both the zinc blende and the wurtzite crystal phase, while only the zinc blende is stable in bulk. A rapid development of growth methods allows growing pure wurtzite, pure zinc blende nanowires, and even switching crystal phases during the growth with atomic layer precision.(1,2) It has already been shown that wurtzite III-V semiconductors possess a second conduction band and three non-degenerate valence bands.(3) Despite general interest in such materials, in many cases the fundamental material parameters are still under debate.

In this work we studied the temperature dependence of the band structure of wurtzite GaAs nanowires with diameters up to 500 nm. In this study we employed resonant Raman scattering (RRS) spectroscopy to improve accuracy, escape defect influence, and temperature broadening of the emission characteristics. The RRS showed strong ingoing and outgoing resonances of 1LO, 2LO, and 3LO Raman lines. In contrast to previous work(4) we found that the two polytypes have very similar bandgaps throughout the studied temperature range. We further find that the energy difference between the first and the second valence bands is constant, around 100 meV. Due to fortunate spacing between the two topmost valence bands, we also observed an unexpected and very strong quadruple resonance of 3LO line.

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Polymer Membrane device for the application of air dehumidification

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For the countries in tropical or sub-tropical areas, removing heat and moisture consumes lots of the energy. According to American Society of Heating, Refrigerating and Air-Conditioning Engineers (Standard-55, about thermal comfort), temperature and relative humidity affect the thermal comfort level significantly. The requirement of proper humidity is increasing not only for life of human beings and animals, but also for operation and maintenance of equipment in the industries of semiconductor and clean room. Based on the previous researches, 40 to 60 % of the energy consumption is for removing the moisture, which means the latent heat occupying a lot of energy. There are some ways for removing the humidity, such as condensing, absorption and adsorption. The condensing method needs the surface temperature lower than the air's dew point temperature. The absorption method needs the surface pressure gradient of air below the water vapor gradient. The condensing method causes the energy consumption of 539 kCal/kg for phase change. The absorption method needs additional energy to regenerate the dehydration material. Therefore, the polymer membrane device for air dehumidification is designed. The membrane has the good selectivity for water vapor and air, and it is able to dehumidify air continuously without the need of regeneration. The properties of membrane device are introduced in the paper.

- Keywords: Polymer membrane; Plane type membrane dehumidifier; dehumidification; Air conditioning;

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unravelling uniaxial strain effects on electronic correlations, hybridization and bonding in transition metal oxides

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The interplay among spin, lattice, charge and orbit is of central importance for several rich and fascinating properties of oxides, and is the subject of intense research at present. Here, we present an approach to manipulate this interplay by Sn doping to effectively apply uniaxial strain on the TiO₂ lattice. The evolution of this interplay in pseudo-homoepitaxial Ti_{1-x}Sn_xO₂ films is measured using a combination of X-ray absorption near edge spectroscopy at the O K and Ti L_{3,2}-edges. Supported by various theoretical calculations, we find that the multiplet-type electronic correlations, long-range bonding and hybridization in the system can be controlled by independently modifying uniaxial strain, thereby allowing us to establish the correlations among these effects, doping concentration, and strain. This significantly widens the phase space for experimental exploration of predictive models and leads to new possibilities for manipulation over materials' functional properties. The methodology presented here can be applied in general to study the nature of the multiplet-type electronic correlations and bonding properties in octahedral-coordinated 3d^N transition metal oxides.

Ti_{1-x}Sn_xO₂ Nanofilms: Layer-by-layer Deposition with extended Sn solubility and Characterization

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High quality rutile Ti_{1-x}Sn_xO₂ nanofilms were successfully grown in a layer-by-layer mode at a moderately low temperature of 400°C using pulsed laser deposition (PLD). High solid solubility of up to $x = 0.216$ has been achieved in the Ti_{1-x}Sn_xO₂ films despite theoretical prediction by Density functional theory (DFT) of large formation energy (~5.64 eV) required for the substitutional alloy to exist at such high Sn concentration. The resultant films have smooth interfaces and step-terraced surfaces with well controlled stoichiometry and are optically transparent. Sn L₃-edge Extended X-ray absorption fine structure (EXAFS) reveals the substitution of Sn⁴⁺ in the Ti⁴⁺ lattice sites of TiO₂. The lattice spacing along [110] increases linearly with increment in x due to substitution of Sn⁴⁺ ions in the Ti lattice sites of the Ti_{1-x}Sn_xO₂ films. X-ray photoelectron spectroscopy (XPS) and Rutherford backscattering (RBS) show that Sn is uniformly distributed on the surface and in the bulk of the films. These results are crucial when considering Ti_{1-x}Sn_xO₂ with suitable composition for making TiO₂ based quantum structures in advanced optoelectronic devices and solar energy materials, where high-quality crystalline thin film-substrates are important.

Linear array of cesium atoms dominated by uracil molecules via electrostatic interactions on Au(111)

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Electrostatic interactions have attracted pervasive interests for its non-directional and non-saturable properties along with the highly flexible bond lengths and geometries, which indicate the advantage of dynamic characteristics for structural transformation and would have potential application in molecular switching devices. Alkali metals, as the typical active metals, can easily stir metal-organic structures via electronic interactions. Among others, the cesium (Cs) possesses the strongest metallicity, which shows the highest tendency to lose electrons and turns into cation (Cs⁺). Herein, by the combination of scanning tunneling microscopy (STM) and density functional theory (DFT) calculations, we choose an organic molecule, i.e., a nucleobase uracil (U), as a potential candidate to interact with Cs atoms on the inert Au(111) surface. By controllable regulating metal/molecule ratios, we achieve a series of structural transformations of supramolecular nanostructures stabilized mainly by electrostatic interactions. More importantly, with the assistance of U molecules, we successfully realize the on-surface linear array of alkali metal atoms. These experimental findings may provide fundamental insights into the intrinsic dynamic characteristic of electrostatic interaction and also the controllable fabrication of novel nanostructures.

magnetic properties of aerosol fe87.5cr12.5 ferrite nanoparticles generated by spark ablation

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Magnetic nanoparticles (NPs) have been a developing topic over the last years due to the wide variety of applications such as cancer therapy, data storage and environmental remediation. Here we present a structural and magnetic characterization of aerosol FeCr ferrite NPs produced by spark ablation [1], a method capable of generating particles with a narrow size distribution (<10%) and good control of the surface coverage. High-Resolution Transmission Electron Microscopy (HRTEM) reveals similar lattice parameters as magnetite spinel structure (Fe₃O₄) and Pair Distribution Function (PDF) measurements point in the same direction. XPS studies indicate the presence of a mixture of Fe(II), Fe(III) and Cr(III) species, with no metallic Fe. Furthermore, TEM analysis shows homogeneously mixed particles with the 87.5 to 12.5 Fe-Cr ratio. Magnetic properties of different coverages and particle sizes were studied by the use of SQUID magnetometry. The low coverage systems (with 3% coverage) of 10 nm particles exhibit SPM behaviour with a blocking temperature TB=58K and no coercivity present at room temperature. Three times higher coverage samples account for a mixture of SPM and super spin glass (SSG) behaviour. In the case of high coverage systems with cluster formation, inter-particle interactions seem to govern the samples' magnetic response. At a particle size of 30 nm, hysteresis is still detected at temperatures up to 400K. XMCD measurements were employed and the analysis reveals magnetic contributions from both Fe and Cr ions. Furthermore, the data from the Cr substituted Fe₃O₄ is compared to pure Fe₃O₄ NPs and the differences will be discussed.

Enhance boiling heat transfer performance by micro/nanostructures

Zhen Cao, Zan Wu, Bengt Sundén

Climate change has been one of the world's grand challenges. It has a global objective to construct an energy-efficiency and sustainable society. Boiling, one of the most common and important processes in energy-relevance activities, attracts more and more attention. The enhancement of boiling can improve the efficiency of an energy-relevance equipment or system, e.g., an Organic Rankine Cycle system and a heat pipe. With the development of micro/nano technologies, micro/nanostructures fabricated on surfaces show their big potential to enhance the boiling performance, i.e., heat transfer coefficient and critical heat flux. In the present study, two deposition methods were used to generate coatings on copper surfaces and pool boiling performance of dielectric liquids was experimentally studied on the coating surfaces. One method is electrophoretic method, by which, commercially available nanoparticles were deposited on copper surfaces due to the electric field between two electrodes. Experimental results indicate that the nanoparticle coating can enhance the heat transfer coefficient by 100%, but the critical heat flux is not enhanced by this type of coating. The other method is electrochemical deposition method, by which, Cu^{2+} ions in copper sulfate solution were reduced on the cathode, forming a microporous coating. Experimental results show that the microporous coating improved the heat transfer coefficient by 600%, while the critical heat flux is enhanced by around 54.9%. In addition, the mechanisms of the enhancement of heat transfer coefficients and critical heat fluxes are investigated, e.g., from the surface characterization, quantitative measurement of concerned parameters and theoretical models.

Fabrication of Tunnel FETs demonstrating sub-thermal subthreshold slope

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Tunnel Field Effect Transistor (TFET), based on band-to-band tunneling, overcomes the thermal limit (subthreshold slope (S) > 60 mV/decade) of the MOSFETs by filtering the high-energy Fermi tail, thereby allowing a substantial reduction of supply voltage and power consumption. Despite the steep slope behavior, TFETs can suffer from ambipolarity wherein carriers tunnel into the channel at both high positive and negative gate voltages. In this work, we demonstrate the fabrication of InAs/InGaAsSb/GaSb vertical nanowire TFET devices and present experimental data showcasing suppressed ambipolarity and a minimum $S = 39$ mV/decade at $V_{ds}=0.05V$. The nanowires were grown using MOVPE where the 100nm long InAs drain was n-doped with TESn followed by a 100nm undoped InAs channel and a 100nm/300nm DEZn doped InGaAsSb/GaSb source. After growth, the InAs was selectively digitally etched using citric acid to reduce the channel diameter from 40nm to 25nm. The electrostatics was improved, compared to our previously reported devices, with a gate stack of ALD bilayer of 1nm/3nm Al₂O₃/HfO₂ (EOT~1nm) followed by 30nm sputtered W. To decrease the ambipolar conduction, a gate-drain underlap of approximately 20nm was used which widens the tunnel barrier at the drain junction. Since the gate length is defined by the bottom spacer thickness in vertical transistors, the underlap provides a shorter gate positioned close to the source-channel junction. Thus the new process scheme has improved the slope and reduced the OFF current by one order of magnitude compared to our previous devices [1].

[1] E. Memisevic et al., IEEE Trans.ElectronDevices,vol.64,4746–4751, 2017.

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The high resolution diffraction beamline P08 at PETRA III

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The high resolution diffraction beamline P08 at PETRA III is dedicated to studies of surfaces, interfaces and thin films by high resolution x-ray diffraction and scattering methods.

The beamline operates at photon energies ranging from 5.4 to 29.4 keV with beam sizes ranging from 20x2 micrometer² to 1500x100 micrometer² depending on the focusing.

The experimental hutch contains two diffractometers. First, a high precision 6-circle diffractometer with Eulerian cradle serves for investigations at hard condensed matter samples. It can fit sample environments up to 15kg weight and rotate with a precision of 0.0005° and wobble of 20 micrometer. The second diffractometer is dedicated to studies of liquid interfaces. It can change the incident angle of the x-ray beam without moving the sample, which makes it perfectly suited for reflectivity experiments on liquid interfaces. In addition custom setups can be mounted on an optical table.

Development of an ambient pressure microreactor for in situ soft XAS analysis

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Establishing relationships between structure and activity is a main question in fundamental and applied catalysis research owing to the complex structures displayed by heterogeneous catalysts. It is well known from ex situ structural characterisation that the morphology, composition and crystalline structure of the catalysts evolve during catalytic reactions. Undoubtedly significant progress has been made in using in situ X-ray diffraction, hard X-ray absorption spectroscopy (XAS) and X-ray tomography studies.[1,2] However, taking into account that the metal active site loading in the sample is often only a few percent, the measured signal mainly originates from the bulk volume and not from the surface where the reaction takes place. Thus, the main scientific challenge for identifying the nature of true active species during reaction is the ability to accurately determine the structure of the surface or species at the surface under operating conditions. In situ soft XAS is capable of providing such data.

We have successfully designed and constructed a new in situ reaction cell for soft XAS analysis that is operational at pressures 1 -3 bars. Measurements are performed in the Total Electron Yield (TEY) detection mode, making the setup sensitive to the first few nanometres of the sample. The sample environment will be tested using catalysts for industrially important processes like Fischer-Tropsch (FT) synthesis above ambient pressure operating conditions on the B07 beamline of the Diamond Light Source.

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Iron-based magnetic nanoparticles by spark ablation

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Magnetic nanoparticles have shown great potential for use in drug delivery and bioimaging applications and are prospective building blocks in future high-performing permanent magnets. Today, magnetic nanoparticles are most often produced in batches by chemical methods resulting in the risk of chemical impurities and production of vast amounts of chemical waste. Aerosol generation methods on the other hand, particularly spark ablation, are promising for future generation of magnetic nanoparticles since they are simple, fast, continuous, scalable, provide good control of size and composition, and offer the possibility to form alloys of material combinations not miscible on the macroscopic scale. High controllability is of utmost importance when generating magnetic nanoparticles since small deviations in size can significantly alter the magnetic coercivity. Also, the composition of the particles is of high significance since the magnetic properties can be completely transformed by changes in elemental composition or the oxidation state of the particle.

In this work, we present the successful generation of monodisperse bimetallic FeCr and FeMn nanoparticles by spark ablation, and the results from the thorough characterization of individual particles with aerosol instruments, transmission electron microscopy, and synchrotron-based X-ray photoelectron spectroscopy. We demonstrate how the carrier gas can be used to dictate the oxidation and how to alternate between self-passivated and completely oxidized nanoparticles. We also show how the produced particles can be deposited to yield a low surface concentration which is critical for minimizing interparticle interactions during magnetic measurements. Finally, as a proof of concept, measurements using a magnetometer equipped with a SQUID on samples with different particle coverages are presented.

Numerical investigation for entropy generation in hydromagnetic flow of fluid with variable properties and slip

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This modeling and computations present the study of viscous fluid flow with variable properties by a rotating stretchable disk. Rotating flow is generated through nonlinear rotating stretching surface. Nonlinear thermal radiation and heat generation/absorption are studied. Flow is conducting for a constant applied magnetic field. No polarization is taken. Induced magnetic field is not taken into account. Attention is focused on the entropy generation rate and Bejan number. The entropy generation rate and Bejan number clearly depend on velocity and thermal fields. The von Kármán approach is utilized to convert the partial differential expressions into ordinary ones. These expressions are non-dimensionalized, and numerical results are obtained for flow variables. The effects of the magnetic parameter, Prandtl number, radiative parameter, heat generation/absorption parameter, and slip parameter on velocity and temperature fields as well as the entropy generation rate and Bejan number are discussed. Drag forces (radial and tangential) and heat transfer rates are calculated and discussed. Furthermore the entropy generation rate is a decreasing function of magnetic variable and Reynolds number. The Bejan number effect on the entropy generation rate is reverse to that of the magnetic variable. Also opposite behavior of heat transfers is observed for varying estimations of radiative and slip variables.

2342-A-1902

Scroll pumps “on demand” usage for reduction of operating costs

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TRIUMF is Canada's particle accelerator centre. The facility produces and delivers a variety of beams to targets and experiment stations through beam lines. The total length of beam lines operating at TRIUMF is about 700 meters. The vacuum in these beam lines is supported by turbo pumps backed by scroll pumps. There are more than 114 scroll pumps operating continuously and TRIUMF spends more than 50 days of maintenance related activities per year. A new mode of operation, permitting the usage of the scroll pumps only when they are needed was proposed, tested and it is in process of implementation. Under the new mode of operation the pressure in the backing line of a turbo pump is permitted to rise to 500 mTorr before turning on the scroll pump and evacuating the backing line. The savings in reduced maintenance activities and electrical power consumption are expected to exceed 50%. Details of the new operating mode are presented.

In-situ Bragg Coherent X-ray Diffractive Imaging Study of Flexo-Photovoltaic Effect in SrTiO₃ Crystals

Bragg Coherent X-ray Diffractive Imaging (BCDI) developed during recent years enables investigation of real material science problems at nanoscale [1, 2]. The reconstruction of 3D strain profile within a single sub-micron crystal can be recovered with 10s of nm spatial resolution. We have applied BCDI to study lattice distortions within a single SrTiO₃ (STO) sub-micron crystal upon in-situ nano-indentation. This enables a better understanding of newly discovered flexo-photovoltaic (FPV) effect in centrosymmetric crystal structures [3]. The FPV effect refers to a photovoltaic current that is generated in a bulk STO crystal by illuminating the area of local indentation with a visible light laser (405 nm wavelength). The strain gradient induced within the crystal breaks the symmetry of the material inducing the local bulk photovoltaic effect. The FPV is not affected by the thermodynamic Shockley-Queisser limit which defines the maximum efficiency of a solar cell using a single p-n junction and can be realized in any semiconductor including silicon. Therefore, a large variety of materials can be a subject of improved photocurrent generation and find new applications. We reveal the 3D strain distribution induced by the local indentation of STO sub-micron particles and correlate it to the strength of the FPV effect. Our work highlights the applicability of BCDI to complex in-situ problems in material science and contributes to establishing structure-functionality relations which drive the development of nanoscale devices.

observation in-growth nano film of beta-fesi2 with reducing boundaries.

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Epitaxial growth of nano-films on solid substrates induces step and domain boundaries in general; the step boundaries arise from the substrate steps and the domain boundaries arise from nuclear growth of individual domains. Recently our group found a unique structure of a nano-film with a little number of the boundaries for beta-FeSi₂(100) on Si(001) [1]; different height surfaces are continuously connected at the substrate-step area in the nano-film, which drastically reduces the step boundaries. Such a boundary-less nano-film has carpet structure (hereafter we call as "nano-carpet"). "Nano-carpets" will improve carrier transport properties because of less scattering at boundaries, compared to general nano-films.

The understanding of the growth mechanisms of the beta-FeSi₂ nano-carpet is quite important, in order to create nano-carpets of other two-dimensional materials. To find key concepts for the nano-carpet formation, we have studied snap shots of atomic images in scanning tunneling microscopy (STM); changing from Fe clusters to a beta-FeSi₂ nano-carpet by short-time annealing for a clean Si substrate deposited of Fe at room temperature. From the results we propose several processes toward the nano-carpet: (1) the formation of clusters of most likely beta-FeSi₂ unit, (2) the aggregation of the clusters forming beta-FeSi₂ nano-domains, (3) the diffusion of extra clusters on the nano-domains, and (4) the crystal merging between different nano domains from restricted area. We will present the details with results of depth-profiled X-ray photoelectron spectroscopy.

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Mechanism of subnanometer-level flattening of Cu surfaces with low-energy Xe⁺ ions

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To develop a surface flattening method for surface activated bonding at room temperature with no pressurization, where root mean square roughness, R_q , of the surfaces is rigorously required to be below subnanometer levels, the interaction between Cu surfaces with initial $R_q = 2.9$ nm and low-energy rare gas ions was investigated by a photoemission-assisted plasma ion source, in which DC discharge is triggered with photoelectrons emitted from the Cu surface irradiated with 7.2-eV light. Cu surfaces treated with 26-eV Xe ions showed a decrease in R_q to 1.3 nm, although they were not flattened at all but roughened with Ar⁺ ions. The sputtering yields of Ar⁺ and Xe⁺ ion were measured by using a Mo mask with a 1.0-mm opening as 5.6×10^{-3} and 2.8×10^{-3} atoms/ion at 26 eV, respectively. In addition, it was observed from the line profiles of the sputtered Cu surfaces that the flying distance of Cu atoms sputtered with Xe⁺ ions is much smaller than that with Ar⁺ ions which is ~ 150 nm. These results imply that the energy transfer from Xe⁺ ion to Cu surface results predominantly in the formation of Cu adatoms rather than sputtered Cu atoms in comparison to Ar⁺ ion. Although sputtering of Cu atoms is accompanied with the creation of deep holes, giving rise to surface roughening as observed for Ar⁺ ion, Cu adatoms are able to contribute the surface flattening as demonstrated for Xe⁺ ion, because of small energy barriers of surface migration, 0.05-0.5 eV.

Transient photocapacitance measurement for characterization of deep defects in B-doped diamond films

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Diamond is expected as a potential material for high-performance devices in the next generation, because of its various interesting physical properties. For the realization of diamond semiconductor devices, it is essential to investigate the nonradiative defects of the diamond films which have not been clarified in detail. In this study, we have developed a highly-sensitive transient photocapacitance measurement system for deep defects in wide bandgap materials, and applied it to characterize the boron-doped (100) diamond film and its MIS structure.

Using a high-power MWCVD apparatus, undoped buffer and B-doped diamond layers were homoepitaxially grown on mechanically polished HPHT Ib (001) diamond substrates with an off angle of 5 degree tilted from the [001] and [111] direction, respectively. As a Schottky electrode, some Au electrodes were fabricated by an electron beam evaporator. The insulating layer of a diamond MIS diode was fabricated by depositing Si film, followed by a subsequent oxidation at 650 degree C.

We clearly observed a steep increase in photocapacitance, due to hole emissions from hole trap states in the depletion layer of the (100) diamond Schottky diode. Signal intensity was increased by the photon irradiation in the energy range above 1.2 eV, indicating the presence of an acceptor-type defect around 1.2 eV above the valence-band edge. In addition to this deep defect, we observed an interface state at the SiO₂/B-doped diamond interface of the diamond MIS diode by the photon irradiation in the energy range above 1.8 eV.

Surface structure analysis of micropatterned Si(110) by nano-beam Weissenberg Reflection High-Energy Electron Diffraction

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It is important to understand the surface of micro- or nano-domains that we can see abundantly in nanotechnology. We have developed a technique to analyze the surface structure of such small domains, combining the scanning electron microscope and the Weissenberg Reflection High-Energy Electron Diffraction [T. Abukawa, T. Yamazaki, K. Yajima, and K. Yoshimura, Phys. Rev. Lett. 97, 245502 (2006)]. In order to demonstrate the method, we prepared a grating-like structure on Si(110) substrates by photolithography and etching [A. N. Hattori, K. Hattori, S. Takemoto, H. Daimon, and H. Tanaka, Surf. Sci. 644, 86–90 (2016)]. The grating consists of rectangular ridges, whose cross section are 20 “micro”m in width and ~10 “micro”m in height. The ridges aligned along [1-12] so that the top and the side of the ridges were (110) and (111) surfaces, respectively. The sample substrate was cleaned in UHV by 1200°C flash and annealing. We observed 16x2 super structure patterns on the top (110) surface, and 7x7 patterns from the side (111) surface. The 16x2, in general, can take two equivalent rectangular unit cells with x2 direction along with [1-12] or [-112]. However, one of the two orientations, whose x2 direction was along with the ridge, i.e. parallel to [1-12], was dominantly observed near the edge of the top surfaces. As was the same for the bottom (110) surface between the ridges. The structure analysis by W-RHEED will be presented.

Nonlinear etching process of Si(110) revealed by Kuramoto-Sivashinsky equation

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Over the past ten years, attention has been paid to Si(110) surface because it is an anisotropic surface and a suitable substrate for three dimensional silicon devices. In order to obtain a flat (110) surface on the atomistic scale, a possibility of a wet chemical process has been considered. In this study, we have observed the etching time dependence of the surface morphology of Si(110) surface by atomic force microscope (AFM). The AFM images show the growth of ribbon-like structure, which extends along [1-10] direction and have a step and terrace structure along [001] direction. Based on these AFM images, we calculate the one-dimensional power spectrum density (PSD) along [001] direction and found the following five features of the PSD; a peak at critical wavenumber q^* , an increase in the intensity at q^* , a peak shift to lower wavenumber side, a broadening of the peak, and a slope of q^{-4} on the high wavenumber side. Furthermore, we derived a generalized one-dimensional nonlinear Kuramoto-Sivashinsky (KS) equation for the roughening of an almost flat surface including the effects of thermal fluctuation. We first derived the free energy functional of the rough surface and then performed a numerical simulation on the etching process with the KS equation by finite difference method. In the simulation, we determined the three coefficients of the model equation, i.e. the Onsager kinetic coefficient, the surface tension, and the surface elasticity. These coefficients were determined using the experimentally obtained PSD. The simulation successfully reproduced the experimental results including the above-mentioned five features of the PSD. These results indicate that the etching process of the Si(110) can be described by the KS equation.

Dynamic heterointerface formation in magnetic few monolayers

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Heterostructures have been widely studied for interest in the emergence of novel phenomena and their promising practical potentials. However, in the case of magnetic metal heterostructures, severe intermixing at the interface often hampers the realization of desirable functions. Thus, the quantitative characterization on the interface formation is necessary. In the present study, we have investigated the structural, electronic, and magnetic properties of the Mn-Fe thin-film heterointerface in few-monolayer range.

Combining element-selective soft X-ray magnetic circular dichroism with scanning tunneling microscopy, we find, in the heterostructure with increasing the Mn coverage, a two-step spin-reorientation transition (SRT) of the fcc Fe layer on Cu(001) accompanied with successive formation of interface ordered-alloys. [1] At low Mn coverages (<1 ML), a considerably rough heterointerface due to the formation of disordered alloy drastically weakens the out-of-plane magnetization of the fcc Fe film, triggering the first step of the SRT. In the second-step SRT, the in-plane magnetic anisotropy is gradually enhanced up to 3 ML Mn coverage. With the help of the first-principles calculations, we attribute the stabilization of the in-plane magnetization dominantly to the electronic hybridization of the Fe layer with the ordered alloy at the heterointerface. Furthermore, the Fe magnetic domain structures at the interface are studied by spin-polarized STM through the anti-ferromagnetic Mn overlayer with an in-plane magnetic anisotropy. A strong magnetic anisotropy is suggested by the observed narrow width of the magnetic domain wall.

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Tribological enhancement of a cutting process using Hafnium and Vanadium Nitride thin films as protective coating.

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Hafnium nitride (HfN) and Vanadium nitride (VN) coatings have been deposited and characterized onto diverse substrates by different authors in the world; finding outstanding properties desired for tribological applications in an industrial environment, for example as a protective coating for high-temperature and high-speed cutting tools.

In this research, HfN monolayer, VN monolayer, and Hafnium nitride-Vanadium nitride multilayer ([HfN/VN]*n*) thin films were deposited, by means of physical vapor deposition technique (PVD), as protective coatings onto High-speed steel (HSS) cutting tools, for dry turning of AISI 1020 steel. To evaluate coating performance and identify changes in the workpiece material removal process, the following procedures were carried out: optical microscopy and scanning electron microscopy (SEM) to assess workpiece surfaces integrity and tool wear, machined surface roughness quantification, and cutting temperature measurement with a non-contact sensor.

Results show these coatings do not only increase tool lifetime, in addition, a tribological enhancement of the tool/workpiece system was also achieved, showing an increase of the manufacturing productivity and quality. As coating performance was higher as a multilayer, bilayer number influence was also studied, by means of X-ray spectroscopy (EDX) of the worn edges, tool weight measurement, corrosion test of machined steel, chip samples inspection and chip compression ratio estimation.

In conclusion, these protective coatings cause a tribological enhancement in a cutting process, reducing cutting temperatures, which increase workpiece integrity and tool lifetime, due to the mechanical and tribological properties of HfN and VN thin films, which also increase wear resistance, as a function of bilayer number.

Measurement of the adsorption isotherms and the mean residence time of D₂ physisorbed on a cold copper surface

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Cryopumping is a usable means to achieve an extremely high vacuum (XHV), where H₂ is the main residual gas. In order to reveal the pumping characteristics of H₂, we have investigated the adsorption isotherms and the mean residence time of D₂ physisorbed on a cold copper surface. This is because to avoid the effect of residual H₂ in the experimental chamber, water and hydrocarbons chemisorbed on the substrate, and H contained in copper.

The density of D₂ physisorbed on the copper surface was determined from the intensity of desorbed D⁺ ions using the Electron-Stimulated Desorption (ESD) method and the Time-of-

Flight (TOF) method. The adsorption isotherms showed Henry's law like behavior in the submonolayer region at substrate temperatures of 4 - 7 K and equilibrium pressures, p , of 3×10^{-10} - 3×10^{-7} Pa. The mean residence time, τ , was obtained from the time constant of the transient state approaching equilibrium. When the system was approaching equilibrium state at $p = 3 \times 10^{-8}$ Pa at the substrate temperature of 6.0 K, we found τ of 1500 s and obtained the adsorption energy E_d of 1.9 kJ/mol from $\tau = \tau_0 \exp(E_d / kT)$, where $\tau_0 = 10^{-13}$ s was assumed. The comparison between the results of D₂ and H₂ will be discussed.

2369-A-1902

Molecular Behaviour of thiamine hydrochloride moiety in aqueous mixtures of D-glucose and D-fructose at different temperatures

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Molecular Behaviour of thiamine hydrochloride moiety in aqueous mixtures of D-glucose and D-fructose at different temperatures

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Abstract:

Thermodynamic, ultrasonic and transport studies have been conducted for thiamine hydrochloride in aqueous mixtures of D-glucose and D-fructose at various concentrations and temperatures. Density, ultrasonic velocity and viscosity have been determined and used for obtaining different thermo-acoustical and transport parameters. The analysis of the obtained data has been done by using Masson's equations, Jones Dole equation and using Feakin's model and finally interpretation was done in terms of solute - solute and solute - solvent interactions. From the current study it has been concluded that thiamine hydrochloride acts as a structure breaker in water as well in binary aqueous mixtures of D-glucose, D-fructose.

Keywords: Partial molar volume, partial molar adiabatic compressibility, partial molar expansibility, transition state theory and structure breaker.

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Ravi Sharma, R. C.Thakur, Balwinder Sani and Harsh Kumar: "Properties of L-ascorbic acid in water and binary aqueous mixtures of D-glucose and D-fructose at different temperatures".Russ. J. Phys. Chem., 91(12), 2389–2396(2017).

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Growth, characterisation and thermoelectric properties of $\text{CaMn}_{1-x}\text{Nb}_x\text{O}_3$ ($x = 0 - 0.1$) thin films.

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Oxide based thermoelectric modules can be an important alternative to conventional thermoelectric modules, commonly based on tellurides for low to moderate working temperatures. Tellurium has drawbacks such as being toxic and scarce, preventing commercialising. Instead, perovskite (e.g. CaMnO_3) oxide based modules employs environmentally friendly, easily available materials with positive economic impact. The perovskite CaMnO_3 is a promising n-type thermoelectric compound, and in this study, $\text{CaMn}_{1-x}\text{Nb}_x\text{O}_3$ thin films ($x=0-0.1$) were synthesised using a two-step sputtering/annealing procedure. Rock-salt-structured $\text{Ca}_{0.5}(\text{Mn}_{1-x}\text{Nb}_x)_{0.5}\text{O}$ films were deposited by reactive magnetron sputtering from elemental targets operated in metallic mode. The as-deposited $\text{Ca}_{0.5}(\text{Mn}_{1-x}\text{Nb}_x)_{0.5}\text{O}$ films were annealed at 700 °C, leading to the formation of the CaMnO_3 phase. Despite a high Seebeck coefficient of $-270 \mu\text{VK}^{-1}$, CaMnO_3 suffers from its poor electrical resistivity, 2.7 Ωcm . The obtained $\text{CaMn}_{1-x}\text{Nb}_x\text{O}_3$ films were characterised by a number of techniques, with a focus on structure, morphology and thermoelectrical properties. X-ray diffraction and transmission electron microscopy (TEM) showed textured films grown in the (220) direction with local epitaxy to the sapphire substrate. Atom resolved TEM revealed the presence of a secondary phase identified to the Ruddlesden-Popper ($\text{Ca}_{n+1}\text{Mn}_n\text{O}_{3n+1}$) which was collaborated by electron energy loss spectroscopy. $\text{Ca}_{n+1}(\text{Mn}_{1-x}\text{Nb}_x)_n\text{O}_{3n+1}$ films demonstrate enhanced overall performance of these films, by mainly reducing the electrical resistivity by more than 30 times compared to pure CaMnO_3 although the secondary RP phase caused an increase in electrical resistivity.

Towards two-dimensional Van Der Waals stacked heterostructures via Electron Assisted Growth

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Stacked Van Der Waals heterostructures of two-dimensional (2D) materials are promising building blocks for a wide range of applications [1]. These 2D materials, such as hexagonal boron nitride (h-BN) or graphene (Gr), are usually grown in-situ on active single crystal surfaces by chemical vapor deposition (CVD) [2]. However, this growth technique is self-limiting to one monolayer. Therefore, scalable mass production of high-quality stacked 2D layers cannot be achieved.

With this contribution, we will present a variety of CVD that overcomes such limitations; Electron Assisted Growth. Using STM and XPS we will demonstrate that borazine dosing within an electron shower results in adsorption of borazine radicals and formation of 2D BN islands atop an otherwise inert Ir(111) supported Gr film. Furthermore, we will discuss the thermal stability of the islands by probing their composition with XPS and their structure with STM. Finally, we will demonstrate how a focused LEEM electron beam can be used to spatially control the formation of the 2D BN islands onto the Gr layer.

As an outlook, the scalability of electron assisted growth to other substrates and materials will be discussed for two additional systems; Gr islands on a Gr substrate and Gr islands on h-BN.

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Enhanced photocatalytic efficiency of visible light active PVA/Ag-TiO₂ nanocomposites via plasma modification

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TiO₂ nanoparticles (NPs) are excellent photocatalytic materials due to its high surface area. However, use of unsupported NPs for photodegradation of organic dyes is not advisable because it forms a stable colloid when dispersed in water, making it difficult to recover and reuse after the treatment process. Immobilizing the NPs will allow reusability of the photocatalyst. Poly(vinyl alcohol) /silver-titanium dioxide (PVA/Ag-TiO₂) nanocomposites were synthesized using the electrospinning method. Ag-TiO₂ NPs were prepared via wet impregnation followed by reduction using a custom-built dielectric barrier discharge plasma system. Transmission electron microscopy (TEM) and elemental mapping confirmed presence of Ag and Ti in the samples. 1% (w/v) <25 nm Ag-TiO₂ NPs were suspended in 12% (w/v) PVA solution and was electrospun using the following parameters: applied voltage = 15 kV, tip-to-collector distance = 15 cm, and flow rate = 0.5 mL/hr. The nanofibers were deposited on an aluminum foil mounted on a 3 in diameter grounded electrode rotating at ~850 rpm. The nanofiber mats (NFMs) were irradiated with 13.56 MHz radio frequency sub-atmospheric pressure plasma using oxygen at 20 W incident power for 5 min. Plasma exposure allowed the controlled etching of the NFMs to expose the Ag-TiO₂ NPs on the surface. Using a 3x3 cm² NFM, photodegradation of reactive black 5 (RB5) as the test analyte under simulated solar light (1 sun) was conducted. UV-vis spectral analysis was used to monitor the change in concentration of RB5. After 6 hr illumination, plasma-treated NFMs exhibited higher RB5 removal compared to the untreated NFMs.

Extraction and transport of broad hyperthermal Ar ion beams

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Low-energy ion beams continue to attract interest due to its potential for materials engineering applications. Ion beam-assisted and direct-ion beam deposition techniques have been done to grow ultrathin high quality films. In addition, as electronic devices approach atomic-scale dimensions, control of incident ion energy becomes increasingly important for ion implantation processes. In this work, an ion source system was designed, assembled, and tested for the extraction of 100 eV ion beams. The stainless steel cylindrical chamber which can assume different multi-cusp magnetic configurations to confine a discharge was used as an ion reservoir. The discharge was excited by a pair of thermionically-heated tungsten (W) filaments to produce a quiescent plasma. To extract the ions, a two-electrode extraction configuration was used with ~90% transparency and effective ion beam cross-sectional area of 4 cm. The extractors were made from 0.1 mm diameter W wires. The gap between the powered and grounded electrodes was maintained at 0.8 mm. Ion beam extraction tests using argon revealed the extraction of ions from 70 to 130 eV extraction potentials and with current densities in the microA/cm² range. Ion beam profile measured from a moving Faraday cup indicated center-to-edge uniformity of less than 20% with low extraction potentials having better uniformity. The uniformity is attributed to the compensation of the primary electrons seeping downstream to neutralize space-charge. The custom-built ion source system capable of producing 100 eV ion beams may find applications in thin film deposition and ion implantation for ultra shallow junction formation.

Flexible Ca₃Co₄O₉/PPy particles/PEDOT: PSS hybrid thin films for thermoelectric applications

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Flexible thermoelectrics, including the development of inorganic/organic hybrid materials, is an emerging area of research, in particular, for wearable applications (e.g. harvesting power from body heat to power wearable electronics). Inorganic/organic hybrids materials, which have good flexibility and fascinating interfacial transport properties, have displayed promising growth in flexible thermoelectrics. Here, nanoporous Ca₃Co₄O₉ thin films have been grown on mica substrates using rf-magnetron reactive cosputtering from metallic targets of Ca and Co followed by annealing at 700 °C in air. Then, we take the advantage of the nanoporous structure to hybridize the Ca₃Co₄O₉ thin films with polypyrrole (PPy) by filling the nanopores of the former with the nanoparticles of later. The nanopores of Ca₃Co₄O₉ thin films is also filled with PEDOT: PSS to prepare the inorganic/organic hybrid films. The structural properties of the films were determined by XRD, SEM and TEM. XRD and TEM results showed clearly single crystalline Ca₃Co₄O₉ in the nanoporous thin films. SEM results showed that there were many nanoscale pores in the smooth surface for the Ca₃Co₄O₉ thin films and PPy nanoparticles clearly filled in the nanoporous in the hybrid films. The hybrid films show good flexibility and thermoelectric performance.

Multifunctional vacuum dry pump test bench control system

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The multi-function, high-span vacuum pump test bench provides theoretical data support for the dry pump design phase or design completion phase, improving quality and yield. In this paper, a control system for integrated vacuum dry pump test bench is established. distributed control system consists of upper computer, PLC and control level, The system adopts modular design and consists of flow control module, temperature control module, pressure control module and test module to be tested. Through the control of temperature, flow, vacuum and speed, the vacuum pump's pumping performance, such as pumping rate, leakage, compression ratio, etc. can be studied by simulating a specific vacuum environment. The system is based on an expert system, using existing expert knowledge and experience as a control strategy to achieve high-precision control of the system. According to the experimental data obtained after the operation, the system has good robustness and fast response speed. The visual interface monitors the operation of the system in real time, and the measured quantity is accurately measured. The fully automatic control system avoids the error of human operation and realizes the original intention of design.

Kinetic approach for simulation of gas adsorption-desorption phenomena

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Adsorption on solids is frequently used for the separation and purification of gases. There are different adsorbent types with pores size of molecular dimensions, like activated carbons and zeolites, which give them a certain selectivity for molecules of the specific size and shape. Another application of the adsorption phenomenon is the chromatographic analysis, where different species of a gaseous mixture can be separated due to their different residence times. Adsorption is finally the only method which is practically available to measure the surface area of porous or powdery solids. Steady one-dimensional flows of a polyatomic gas in the presence of an adsorbing-desorbing surface are studied by DSMC solutions of the Boltzmann equation.

Borgnakke-Larsen model is used to describe inelastic collisions dynamics for a gas with rotational degrees of freedom. Adsorption and desorption phenomena are described by a kinetic reformulation of Langmuir model, leading to an additional equation for the time evolution of the surface coverage.

The influence of several parameters, like the adsorption time and the heat of adsorption, on the non-equilibrium evolution of the surface coverage in time is analysed. Besides, for the case of gas flow between two parallel surfaces, where one of them is an adsorbing and the other one is a reflecting surface, the analytical solution for free molecular flow regime was developed. The results show that the analytical and numerical solution presents deviation smaller than 1% for all the evaluated cases.

Application of nanopositioner for magnetic resonance force microscopy

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Conventional magnetic resonance imaging (MRI) has been persistently used due to its prominent spatial resolution and nondestructive method. Nevertheless, this inductive method using pick-up coils cannot resolve objects smaller than several microns. MRFM has been proposed as a new technique that could improve the sensitivity and spatial resolution of magnetic resonance to the single spin level. MRFM is based on the detection of the magnetic force between a ferromagnetic magnet and spins in a sample. To detect a force by magnetic resonance, MRFM uses a micro-fabricated cantilever as a mechanical oscillator and the oscillation of the cantilever is detected using a high-sensitive fiber-optic interferometer based on the optical interference. However, MRFM has not become a commercialized technology up to now in contrast with AFM.

In this study, we introduce an MRFM probe equipped with a nanopositioner which is helpful for low temperature experiment which can rapidly enhance signal-to-noise ratio. A variety of measurement options and superconducting magnets for the convenient characterization of nanomaterials offer highest flexibility. Depending on available infrastructure on-site in the laboratory, our probe offers a broad portfolio of research cryostats. The extreme stability of the measurement head allows also for combinations with cryogen free pulse-tube based cooling systems for applications where liquid helium is not available or desired.

2404-A-1902

A transportable dual Fabry-Perot cavity refractometry system

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In this poster presentation we will present a technical overview of our transportable dual Fabry-Perot cavity system which utilize the gas modulation refractometry methodology (GAMOR).

In short, the system is built in modules that can easily be individually packed and shipped. The system is also to a large extent built using commercially available components, which includes turn-key operational lasers and electronics. The system was originally set-up at Umeå University and later transported to RISE in Borås (~1000 km). After the transport the system was successfully installed and fully operational after 3 hours. The system has since been further optimized, and in order to evaluate its performance and characterizing its stability and accuracy, the system has been compared to a dead-weight piston balance which is used as a primary reference at the National Metrology Institute at RISE. To investigate the aspects of transportability, and how transportation might affect the performance of the system, it was shipped back to Umeå University, where it was characterized using a different dead-weight piston balance in order to verify that it can be transported without any significant loss of performance. The results of these measurements will be presented as well as future outlook and the planned upgrades to the system.

Dynamic XPS Measurements for Observing and Monitoring Surface Reactions

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X-ray Photoelectron Spectroscopy (XPS) is a widely used measurement technique with applications in many research fields where surface sensitivity combined with chemical state and quantitative elemental information are required. Typically, XPS measurements are carried out with the premise that the sample is not altered during the data acquisition.

Often, however, XPS is used to analyse surfaces in its original and altered state after an applied process. This can be a laborious procedure and misses out the observation of the transformation itself.

Furthermore, in many cases sample preparation requires a careful procedure followed by an analysis to verify the required outcome of the preparation. This is often time consuming and the outcome is not always guaranteed to be satisfying.

Here, we present a unique acquisition mode, Multi Peak Monitoring, based on multi-channel snapshot detection and the ability for switching the electron binding energy fast. Important parameters for using this acquisition mode to study dynamic processes down to the millisecond range are discussed and the capability of this measurement technique demonstrated.

Utilising the benefits of XPS on a sample under controlled and variable process conditions presents a completely new tool set for observing, monitoring and even tailoring surface reactions. Dynamic XPS measurements can be used not only to find and optimise parameters for controlled and reproducible processes, but also to gain fundamental understanding of the underlying reaction dynamics.

Templated ordering of C60 and C70 fullerenes on reconstructed SrTiO3 (111) surfaces

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Organic nanomaterials such as fullerenes provide a versatile synthetic base for a variety of applications in (opto)electronics [1]. In order to further exploit their properties there is a desire to arrange these molecules into particular ordered patterns [2, 3]. This is achieved through molecular self-assembly and organisation on surfaces with specific surface periodicities and chemical reactivity that can act as templates. We have used the polar (111) surface of SrTiO₃ for this purpose because it shows a variety of surface reconstructions [4]. The work presented here focuses on the self-assembly of C₆₀ and C₇₀ on the 4×4, 5×5 and 6×6 reconstructions of SrTiO₃ (111). We show that fullerenes produce epitaxial monolayer structures on the 4×4 and 5×5 reconstructions. However, disordered islands with random orientations are observed on the 6×6 reconstruction. This demonstrates that the 6×6 reconstruction interacts less strongly with the fullerenes than the other reconstructions and hence indicates that the 6×6 surface is less reactive.

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Self-cleaning glass surfaces based on chemically grafted photosensitizers

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Hospital-acquired infections, so-called nosocomial infections, are the case for 8.7% of patients and result in at least 37 000 deaths in Europe and in 99 000 deaths in the USA each year, as stated by WHO. The economic impact of such infections is also considerable, since they cause prolonged stay of patients in hospitals. Thus, high attention is put nowadays on the introduction of antimicrobial self-cleaning coatings in the health-related areas in order to decrease the number of patients gaining nosocomial infections.

In this work, we present the straightforward procedure, based on chemical grafting of 3-aminopropyltriethoxysilane (APTES) followed by surface post-modification steps, for the formation of photoactive layers able to generate singlet oxygen, 1O_2 , strong antimicrobial agent. The resulting covalently bound organic films were widely characterized by means of spectroscopic techniques: XPS, UV-Vis, Raman. The efficiency towards singlet oxygen photogeneration was determined by DPBF - chemical trap, while the antimicrobial activity of the thin layers was tested using the most common bacterial strains, like *Staphylococcus aureus* and *Escherichia coli*.

sustainable dye-sensitized solar cells based on wine pigments

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Solar energy production has been the fastest growing sector with the biggest share in newly created jobs in the past few years.[1] Among the different solar cell technology, dye-sensitized solar cells (DSSCs) have drawn a lot of attention due to their ease of fabrication, low-cost and competitiveness with different photovoltaic systems.[2] Several types of pigments such as the original ruthenium(II) complex,[3] and organic dyes,[2] have been used as light absorbers. Anthocyanins are the main polyphenolic dyes found in young red wines, which are transformed into more stable structures such as pyranoanthocyanins, during wine ageing. Compared to anthocyanins, pyranoanthocyanins are more resistant to hydration and constitute a photosensitizer family with great potential for bio-inspired DSSCs.[4] Still, the best known efficiency reported for pyranoanthocyanins, prior to the present work, was 0.006%.[4]

Herein, a series of bio-inspired pyranoanthocyanin derivatives were designed, synthesized and applied for the first time as dye sensitizers in DSSCs. A relation was established between dye structure and cell efficiency. Specifically, the presence of the catechol unit was shown to increase electron injection to the TiO₂ semiconductor. An overall efficiency of 1.15% was obtained for the best performing compound, with no further optimization.

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Temperature distribution on the active surfaces of Bayard-Alpert type ionization-gauges

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The accuracy of ionization gauges is limited by processes on their active surfaces. The composition and coverage of the surfaces with chemisorbed and physisorbed molecules is a function of temperature. The ion-induced secondary electron-emission yield at the collector depends on the work function and thus on sputtering by ions and adsorption rates of gas molecules. Electron-stimulated ion desorption at the anode is influenced by chemi- and physisorbed molecules.

Calculations of the temperature distribution on the ion collector and the anode are presented together with temperature measurements. For the simulations, a generic 1-dimensional model based on heat-transfer and heat-generation mechanisms as well as material properties is derived. This model can be transferred to other ionization-gauge geometries.

Influence of process parameters on CrFeCoCuN_x multicomponent alloy films deposited by magnetron sputtering

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Use of multicomponent alloy thin films on fuel cells and batteries can act as corrosion and wear resistant coatings [1]. In the present study, CrFeCoCu films were grown on silicon substrates by a combination of DC and RF magnetron sputtering with segmented targets.

Films with high Cu and Cr content (Cr_{14.7}FeCo_{1.9}Cu_{44.7}) deposited at room temperature were found to be dense but rough. Addition of nitrogen gave rise to square-shaped intergrowths which further increased the roughness of the films. In order to reduce roughness and increase the density of the films, deposition temperature (300°C-500°C) and concentration of Cu and Cr were varied. Films deposited at 300°C with composition Cr_{3.1}FeCo_{2.7}Cu_{5.6} showed a growth morphology which consisted of domed columnar clusters of ranging height (700 nm-1000 nm) separated by gaps through the film. Addition of nitrogen (0-9%) brought down the surface roughness significantly (rms≈2.5nm) while retaining the columnar growth and increasing grain size whereas increasing the deposition temperature did not favour reduction of roughness (rms≈11nm). The complex surface morphology may be due to the presence of mixed FCC and BCC phases. The coatings showed resistivity values ranging between 23μΩ.cm-73μΩ.cm. By performing electrochemical, mechanical, and optical characterization the nitride films, are proposed to be used as corrosion resistant coatings.

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thermally-driven crystallization of titania amorphous nanotubes by in situ transmission electron microscopy

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Anodically grown TiO₂ amorphous nanotubes (TANs) are among the many materials obtained by amorphous and crystalline titania (TiO₂) showing interesting properties that make them promising candidates in a wide range of fields. However, their thermally-driven crystallization has only been studied under ambient pressure on large populations. This approach lead to averaged responses, without granting a deep understanding of the role of user-defined parameters on the amorphous-to-crystalline transition and its outcomes. On this basis, we studied the crystallization of TANs by High Resolution Transmission Electron Microscopy (HRTEM) in situ at a single nanotube level by annealing them upon different environmental and electron beam energy conditions and we could observe the local evolution of the crystallization process with an unprecedented level of detail. We repeatedly applied this in situ approach with different electron beam energies in high vacuum regime and in inert (N₂) and reducing (H₂) atmosphere to study their effect on the crystallization temperature and on the crystallization of different TiO₂ phases. The HRTEM studies were subsequently combined with analogous pre- and post- crystallization compositional in situ investigations of the TANs by Electron Energy Loss Spectroscopy (EELS) to study the how the amorphous-to-crystalline transition influenced the Ti/O stoichiometry, The combination of these techniques provided us with novel insights on the role played by electron beam energy, pressure and chemical environment on TANs' evolution during annealing processes.

Single-stage vacuum pump performance measuring method

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Traditional dry pump measurement devices usually focus on the entire vacuum pump performance parameters other than vacuum pump interior flow situation. This paper propose a performance test method for testing a single stage of a vacuum pump, concentrating on four basic physical quantities; flow, vacuum degree, temperature and rotating speed. For a better description of the measurement method, this test method is divided into six modules: the pump inlet test doom module, the pump outlet test doom module, the pressure measurement module, the temperature measurement module, the flow measurement module and the rotating speed measurement module. This method ensures the normal operation and parameter measurement of the single-stage vacuum pump by adjusting the pressure range of the front and rear vacuum dooms so that we can measure the flow field inside the single rotor and the specific measurement parameters to fit pumping speed - pressure curve and other parameter curves. The pressure, flow, temperature and rotating speed measurement ranges of the test method are 10-3~105 Pa, 20 SCCM~5000 SLM, 20°C~300°C and 100 rad/s~3000 rad/s. Compared with the traditional vacuum pump measurement method, the measurement method of the single-stage vacuum pump proposes a performance parameter to measure the internal flow field of the first-stage rotor of the multi-stage vacuum pump and the related parameters to provide design reference and experimental data support and rotor profile design for the rotor combination of the multi-stage vacuum pump.

Characterisation of intermediate and product structures of an Ullmann-type reaction on Ag(111): A combined X-ray standing wave and scanning tunnelling microscopy study

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On-surface synthesis protocols, including those based on Ullmann coupling reactions, are a promising route towards fabrication of customisable 1D and 2D structures [1]. Ullmann-type reactions, often performed on well-defined metallic substrates whose catalytic properties initiate the reaction, progress to covalently bonded products via a metal-organic intermediate state incorporating atoms from the supporting surface. However, the exact adsorption geometry, and alignment with the substrate, of the intermediate and final structures is difficult to obtain experimentally using scanning probe methodologies (often used to investigate such systems). In particular the nature of the carbon-metal bond within the intermediate structures is difficult to ascertain; i.e. whether the incorporated metal atom resides within the top layer of the substrate or is an adatom species.

Here we investigate the Ullmann-type coupling of 1,3,5-Tris(4-iodophenyl)benzene (TIPB) and 4,4''-diiodo-m-terphenyl (DITP) on Ag (111). Characterisation of intermediate and product structures is facilitated by high-resolution photoelectron spectroscopy (C 1s and I 3d regions) and normal incident X-ray standing wave (NIXSW) measurements utilising the (111) and (200) Bragg reflections of the Ag crystal. This allows adsorption sites, and heights above the (111) surface, of key atomic species within the reactant molecules to be determined. These results are also directly compared to our scanning tunnelling microscopy (STM) investigations [2-3], of the same molecule-substrate systems, providing insight into the underlying reaction mechanism.

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Investigating the atomic layer deposition of TiO₂ growth on InAs(100) using real-time monitoring by ambient pressure XPS with millisecond time resolution.

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Atomic layer deposition (ALD) is a thin film deposition technique for depositing uniform and conformal layers on complex three-dimensional topographies. ALD is highly used in different fields of technology, e.g. in microelectronics and solar cell technology. The understanding of the atomic and molecular surface processes is far from complete. A thorough investigation for the identification and role of surface species, impurities and vapour phase reactions are therefore very much needed [1].

We performed ambient pressure x-ray photoelectron spectroscopy (APXPS) to study the ALD growth of TiO₂ on the clean native oxide-covered InAs(100) surface. We have chosen tetrakis (dimethylamido) titanium (TDMAT) and water as precursors. It is for the first time that APXPS has been applied to this subject with millisecond time resolution. The time resolution is illustrated in Fig. 1, which shows As3d spectra with the native oxide signal at around 44.5 eV binding energy and the bulk As signal at around 41 eV. The spectra were measured with a time resolution of 0.058 s. Here we can follow in detail how the native oxide is removed [2]. We have also used other spectral regions to identify the nature of surface chemical species during the TDMAT half-cycle. In particular, from the N 1s region we can identify methyleneimine as well as the surface-bonded Ti-amido complex.

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2432-A-1902

leak testing technology in general assembly of large satellites based on the mass spectrometry

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The special leak testing technology of the assembly of large satellites is very important to ensure the reliable operation of large satellites in orbit. The local and total leakage testing technique was developed which based on quadrupole mass spectrometer and helium mass spectrometer. For large satellite electric propulsion system requirements of a local leakage detection, The leak testing system was mainly composed of quadrupole mass spectrometer with a sniffer, xenon positive pressure standard leak. A xenon calibration device with known leakage rate is developed to calibrate test system from 10^{-6} Pa·m³/s to 10^{-8} Pa·m³/s, and synthetic standard uncertainty is better than 5%. And After many experiments of detectable gas analysis machine, and based on the GAM500 on-line mass produced by Germany IPI, we developed alternate circle sampling system and get over the instability of long-time measure. The multi-system leak detector by mass spectrometer has been developed and used in the large satellite successfully. Several large satellites have been tested in the process of AIT with these testing equipment. The quality of the large satellite has been effectively guaranteed.

Self-organization of silicon surfaces for the production of nanoscale standards

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It was possible to initiate a reproducible self-organization process on mono-crystalline Si (111) surfaces by a suitable process control in the UHV. The aim is to generate crystalline structures at surfaces which can be traced back to a well-known parameter of the crystalline sample, e.g. lattice constant. In this case the crystalline sample and its features can be used for the calibration of microscopes with ultra-high resolution. By this the smallest achievable linear dimension could be reduced by more than one order of magnitude. The uncertainty is also reduced by more than a factor of ten, compared to the previously available commercial standards, thus opening new areas of application.

The basis for the production of nanoscale standards is the lattice parameter of silicon, which has a very high reproducibility. The variations of the (bulk) lattice parameter between individual crystals can be measured with relative measurement uncertainties well below 10^{-6} . Also, if we take into account some unknown properties of the crystalline surface, e.g. rearrangement of the atoms at the surface, the achievable step height and its uncertainty is less than 10 pm for a step height of 313 pm!

In the first working section this new approach for the production of crystalline standards is successfully demonstrated. The main focus was on the identification of the individual process steps and the experimental determination of the associated process parameters. In the subsequent characterization of the samples, further important properties such as the stability of such delicate samples under laboratory conditions could be demonstrated.

After this proof-of-principle, further approaches for targeted surface modification by self-organization are investigated in order to extend the application spectrum of these standards, e.g. to increase to number of steps or the size of step free areas to diameters of more than 100 μm .

Another important point is related to the handling and use of such samples for the calibration in, e.g. AFM or high-resolution optical microscopes (phase-shifting, coherent scanning, confocal).

2434-A-1902

Enhanced Scroll pump for very large volume and continuous high pressure operation

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¹ Edwards

The XDS35 range of scroll pumps have been applied for over 15 years in a wide range of vacuum applications including surface science, electron microscopy, cryogenic dilution, mass spectrometry and general R&D across a wide range of pressures. One limitation has been continued high pressure (~200 mbar) operation. A novel and patented internal 'relief-valving' technique has been developed to overcome this. The mechanism will be described in detail.

The comparative performance of the 'Enhanced' scroll pump will be illustrated with data from large volume (7.5 m³) evacuation and continuous high operating pressure. The positive performance impact on specific examples, including rapid cycling and carrier gas flow will be discussed.

Optical and electrical properties of (Al,Ga)N/GaN LED structures in nanowires with switching growth polarity

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III-N compound nanowires (NWs) are promising building blocks for novel optoelectronic nano-devices including light-emitting diodes (LEDs) and lasers. The MBE growth process of NWs with embedded axial LED structure consists of many stages intended to achieve various chemical compositions, majority charge carrier polarities etc. in subsequent layers. This requires changes in growth conditions, i.e. element fluxes and temperatures, which may lead to changes of NW growth polarity, from N-terminated to Ga-terminated. That may markedly influence functionality of the obtained structure.

In this work we provide the nano-scale correlation of morphological, structural, electrical and optical properties of GaN/(Al,Ga)N nanowire LEDs as observed by a combination of scanning electron microscopy, spatially and spectrally resolved cathodoluminescence (CL), electron beam induced current (EBIC) technique, atomic force and Kelvin probe force microscopies. GaN/(Al,Ga)N LED nanowire structures with three GaN quantum wells in the p-n junction and (Al,Ga)N barriers were grown on silicon (111) substrates without any catalyst by plasma-assisted molecular-beam epitaxy. Two kinds of the NW morphology, appearing in the same growth process, were observed and correlated with the polarity of the top part of the NWs. The EBIC signal as well as the CL spectral features recorded for individual NW proved that a p-n junctions were deactivated and quantum-well luminescence suppressed in N-terminated NWs. Physical mechanisms responsible for that are discussed.

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2437-A-1902

The Biological Laboratory at MAX IV

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The biological laboratory at MAX IV is the central laboratory facility to support of life science related experiments at various beamlines and also a platform to carry out in-house life science research. The lab complements those beamline-attached sample preparation units and are designed and constructed to offer extended instrumentation access and top-notch supports with continuous upgrading possibility.

The Biolab is now available for users and in-house researchers to perform fundamental protein preparation, including limited protein analytics (UV-vis spectroscopy, gel electrophoresis etc.) which allow a critical entry check for protein samples before the experiments at MAX IV. The lab is also equipped with a glovebox for sample preparation under anaerobic conditions, and storage of chemicals and protein samples. The lab's biosafety level is now classified as Biosafety Level 1 and restricted to work with well-characterized agents. The lab also has the capacity to be upgraded to Biosafety Level 2 in the future. The latest status of the MAX IV Biolab will be presented.

As more new beamlines enter the operation mode, the usage of the Biolab is also expected to correspondingly increase on account of the growing number of life-science users at MAX IV. The synergy between the Biolab and relevant beamlines will continuously improve ones' user experiences and cover the new needs.

2438-A-1902

ISO9001 (QMS) and Vacuum System Support

Thomas Weston¹

¹ Science and Technology Facility Council

ISO 9001 is the international standard that specifies requirements for a quality management system (QMS).

ASTeC Vacuum Solutions Group provides vacuum system support for accelerators (e.g. AVO, CLARA, VELA, ESS) of various sizes and cleanliness requirements. To achieve a constant approach to cleaning vacuum components, processing vacuum components, record keeping and supporting accelerator systems we have developed a QMS system which manages our needs and our customers' (in house or commercial) requirements.

This presentation provides an overview of how the QMS keeps track of vacuum system support at STFC, Daresbury Laboratory, Warrington, Cheshire, WA4 4AD, UK.

AVO Advanced Oncotherapy.

CLARA Compact Linear Accelerator for Research and Applications.

ESS European Spallation Source.

VELA Versatile Electron Linear Accelerator.

Author: Thomas Weston.

Mechanical Properties and Corrosion Resistance of Magnetron Sputtered Co-Cr-Fe-Mn-Ni-C Thin Films

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In this project we aim to deposit thin films that combine high hardness with high ductility and corrosion resistance. This combination of material properties is rare as there is often a trade-off between hardness and ductility. The starting point for this study is CoCrFeMnNi, a well known multicomponent alloy. To this alloy we have added small amounts of carbon, something that is known to simultaneously increase the ductility and the hardness of sputtered metallic thin films [1].

The CoCrFeMnNi system, and the reduced system CrFeNi at near-equimolar compositions, were studied at different carbon contents. Thin films were deposited by combinatorial magnetron sputtering, creating gradients in the composition [2]. This allowed for studying the effect of composition and carbon addition on the mechanical and electrochemical properties, which were evaluated by nanoindentation and scanning droplet cell microscopy respectively.

In the CrFeNi system, the addition of up to 10 at-% of carbon gave an increase in both hardness and ductility, reaching a hardness of 11 GPa. The hardness of the CoCrFeMnNi films at 10 at-% C was 15 GPa, an increase compared to the carbon free film at 7 GPa. The corrosion resistance of CrFeNi films increased with the addition of carbon. The electrochemical behavior of both systems will be described in more detail.

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2442-A-1902

Sputter-deposited highly (001)-textured WS₂-x films

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Highly (001)-textured layered WS₂-x films were sputter deposited from a WS₂ target onto oxidized silicon substrates by reactive sputtering in H₂S as well as in pure Ar. It was concluded that the film quality was increased with higher substrate temperature and higher processing pressure. X-ray diffraction Θ - 2Θ measurement reveals the formation of high quality films showing only (002), (004), (006) and (008) peaks. Raman peaks were observed at 355 cm⁻¹ and 419 cm⁻¹ when the film was illuminated with 532 nm laser. Photoluminescence (PL) measurement using the same laser resulted in a broad signal between 605-636 nm. The transmission electron microscope (TEM) image shows distinguishable layers of the deposited film. The layer separation calculated from diffraction was 0.63 nm. Rutherford backscattering spectrometry (RBS) reveals that the films were clearly substoichiometric (sulphur deficient). The deposition rate was measured to be 3.8 Å/min.

Thermodynamic Model of the Single-stage Gradational Lead Screw Vacuum Pump used in the Chemical Engineering

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¹ Northeastern University

Compared with the constant lead screw (CLS) vacuum pump, the gradational lead screw (GLS) vacuum pump, widely used in the chemical engineering, has the advantage of heat dissipation and saving energy. A thermodynamic model can provide a well explanation on these phenomena. The single-stage GLS (SGLS) vacuum pump is suitable for mass production owing to the simple construction and easy manufacture. Taking the SGLS vacuum pump as the research object, this paper divides the pumping process into four successive stages and proposes a thermodynamic model to analysis quantitatively. The characteristic curves of thermodynamic parameters are drawn and explained in detail. Moreover, the power consumption under diverse operating conditions are plotted and illustrated. The performances with different design structures are contrasted and discussed. A comparison between the SGLS vacuum pump and CLS vacuum pump with the same pumping speed is presented at the end of this paper.

Electron mobility studies of InGaAs III-V MOSFETs

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The quality of modulation doped In_{0.63}Ga_{0.37}As quantum well channels on InP have been studied by Hall electron mobility measurements. The channels are grown by metalorganic vapor phase epitaxy on an InP substrate. Quantum wells with high electron mobility combined with high carrier concentration are important for high performance III-V MOSFETs. The modulation doping increases the carrier concentration multiple times with a small penalty of reduced electron mobility in the channel, this enables a low resistance channel access region and high on-currents. When the thickness of the InP top barrier was decreased, the influence of remote scattering from the surface increased and the mobility degraded. Samples with no InP top barrier was also fabricated, these channels exhibited a comparatively lower electron mobility. Passivating the exposed InGaAs channels in these samples with an high-k oxide greatly increases the electron mobility.

Determination of pumping properties and surface resistance of quaternary alloy of non-evaporable getter of TiZrVAg

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Non Evaporable Getter (NEG) has been employed extensively in the particle accelerator especially where the conductance of the vessel is severely restricted and ultra-high vacuum condition is required. NEG coating will significantly reduce the rate of outgassing and at the same time provides active pumping surface for H₂, CO and CO₂. In addition, it has been proven that NEG coated surfaces have a very low secondary electron yield, as well as low photon stimulated desorption and electron stimulated desorption yields. However the existing NEG film increases the impedance of the beam pipe by an order of magnitude which can the beam pipe wakefield impedance.

In order to increase NEG conductivity, at ASTeC we have commenced to study alternative NEG composition by adding more conductive element such as silver. In this study, we report on the pumping properties, activation temperature, sticking probability (H, CO, CO₂) and surface resistance of new NEG quaternary alloy of TiVZrAg as function of the film structure, morphology, and composition.

Film bulk composition was determined using Rutherford Back Scattering RBS while the surface composition and surface chemical state as function of activation temperature was determined with X-ray photoelectron spectroscopy XPS. Surface structure and its morphology was determined by Scanning electron Microscope and X-ray diffraction.

Current and Future Improvements of the NEG Coating Test Facility at DESY: Pumping Speed Measurements

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The NEG coating technology has been introduced at DESY in the framework of the PETRA III project when a facility for internal coating of vacuum chambers was built. NEG coatings have first been applied to narrow gap insertion device chambers with subsequent positive experiences about their performance. A detailed knowledge about the pumping, saturation and outgassing behavior of the coatings was not in the scope at that time. In the light of the PETRA IV project this has changed. DESY is currently preparing tests for synchrotron radiation induced activation of NEG coated dipole chambers in one octant of PETRA III. Pumping speed measurements of coated as well as uncoated chambers thus need to be performed in order to interpret upcoming data on their conditioning behavior in the storage ring. The setup together with first results of corresponding measurements is described in this contribution. Since a baseline proposal for PETRA IV excessively relies on NEG coatings, further improvements of the coating test facility, which will enable PSD/ESD and impedance measurements, are necessary and outlined herein.

Catalytic gasification of pighair biowastes using nanophase NiO/Al₂O₃ catalysts with hydrogen production

Kuen-Song Lin, You-Shen Lin, Chao-Lung Chiang, Sat Septian Dwitya

Hydrogen can be affectively turned out through the gasification of biomass such like pighair biowastes (PBs). Gasification has been considered as potential methods that are beneficial in the treatment of PBs. Hydrogen is also a clean and new energy carrier to generate power through the PEMFC system. Therefore, the main objective of this study was to present an analysis of the catalytic gasification of PBs for the generation of high purity hydrogen in a lab-scale fixed-bed downdraft gasifier using 10-15 wt% NiO/Al₂O₃ catalysts at 760–900 K. By using thermogravimetric method, gasification of PBs can be satisfactorily described by the corresponding rate equation: $\frac{dX}{dt} = (4.51 \times 10^{13}) \exp \left(\frac{-33.48}{(1.987 \times 10^{-3} T)} \right) \times (1-X)^{0.4}$. $\frac{dX_2}{dt} = (1.70 \times 10^{16}) \exp \left(\frac{-48.587}{(1.987 \times 10^{-3} T)} \right) \times (1-X)^{-2.49}$. In the catalytic gasification process, reduction of Ni(II) catalyst into Ni(0) has been confirmed through XANES spectra and consequently EXAFS data shows that the central Ni atoms have Ni–O and Ni–Ni bonds with bond distances of 2.04 ± 0.05 and 2.45 ± 0.05 Å, respectively. The PBs were partially oxidized and ultimately converts into hydrogen rich syngas (>90% dry basis, CO and H₂) and increases of the reaction temperature are favored the generation of hydrogen with lower CO. In addition, based on a simulated pilot-scale ASR catalytic gasification process with >99.9% hydrogen generation in an integrated fuel processor, the generation of 100 kW electric powers for an internal combustion engine and 150 kW for a PEMFC were obtained, respectively.

Evaluation of Composite Film Morphology by Image Analysis

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The paper presents efficient tools for research morphological properties of various composite structures. It focuses on the composites that are created by metal particles in a dielectric matrix. Nevertheless, the results could be used for other similar two-phase systems. Physical properties of the composite films are given not only by a concentration of the metal component but also by a spatial distribution of the metal objects. It was demonstrated in the literature that an image analysis obtained for the composite films (from their sections or projections) brings a valuable source of information about further film properties. The particles are assumed to be more or less randomly distributed in the matrix, and a low metal volume fraction is supposed. The hard-sphere model for generation of the composite structures is described. The Voronoi tessellation and other methods were chosen to study the composite film morphology. All the methods chosen are able to precisely describe the three-dimensional composite structure morphology simply using one two-dimensional section of the given structure. To evaluate the degree of disorder of the structure, novel scalar measures are introduced. Results for homogeneous as well as inhomogeneous composites are presented. It is shown that the scalar measures give the possibility to precisely evaluate the degree of disorder of the composite structures. The sensitivities of the methods are compared to each other. It is shown that the methods are independent of the section chosen.

Silver nanoparticles on cellulose surfaces: quantitative measurements

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It is common to find in the literature characterization studies of chemically modified surfaces frequently based on incomplete analyses that lead to biased interpretations.

The development of new, straightforward and green methodologies to functionalize the surface of biopolymers with metal (or metal oxide) nanoparticles led us to examine the complementarity of very different techniques of analysis [1] seeking for coherent results and, as far as possible, full descriptions of the different systems.

In this work, cellulose films pre-activated with carbonyldiimidazole (CDI) and grafted with 1,6-hexanediamine, were decorated with silver nanoparticles (AgNPs). The generation of AgNPs was followed in real time by quartz crystal microbalance (QCM). The obtained films were characterized by X-ray Photoelectron Spectroscopy (XPS) and imaged by atomic force microscopy (AFM). XPS confirmed the synthesis in situ of AgNPs on the film attesting their oxidation state [2]. The results from the three techniques were quantitatively compared and, despite the different approximations made in each of the techniques to extract quantitative information, a very good agreement was obtained showing how sound they are for quantitative reasoning.

Acknowledgments

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Growth of Fe islands on Si(111)7x7 surfaces modified with ammonia

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The interaction between adsorbed molecules with metal deposition on substrates has attracted much attention for a new type of molecular-controlled artificial growth. The molecule adsorption sites will restrict to the subsequent metal adsorption and growth process. Some metals directly deposited on reactive semiconductor substrates form three-dimensional (3D) island. When metals are deposited on the semiconductor surface partially covered by molecules, we expect larger crystalline domain size of the 3D metal islands owing to the small density of the nucleation center if the molecules prevent and survive during the metal deposition. So far, such a molecule-modified metal growth is not clear yet. At the initial stage of the growth, a scanning tunneling microscopy (STM) study revealed that the adsorbed molecule remains after the metal deposition, and the metal adsorbs on an uncovered substrate [1]. However, in a large amount of metal deposition, no systematic observation has been done yet. The understanding for the behavior of much thicker deposited metal on molecular modified surfaces is important toward a future electrode patterning application controlled by sub-nm sized molecules. In order to prove the hypothesis, the average domain size of the three-dimensional cluster can be estimated from the width of diffraction spots using transmission electron diffraction, such as Reflection high-energy electron diffraction (RHEED), which is sensitive to nano-meter material grown over monolayer deposition. In addition, we present the chemical properties of the molecule in the interface.

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Reduced retinal glial cell proliferation on nanowire arrays

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Several retinal degenerative diseases lead to neuronal cell loss and eventually blindness. Retinal implants are being developed to restore sight in patients with loss of photoreceptors, however, their long-term functionality is limited. We investigate the interactions of retinal cells with vertical nanowires as these might be used to improve the performance of implants. We have shown that vertical gallium phosphide nanowires (GaP-NWs) support long-term survival of retinal neurons in vitro. Here, we analysed the fate of retinal glial cells on GaP-NWs, since one factor limiting the functionality of current implants is activation of these cells, which migrate towards the implant site, destabilizing electrical signal transduction at the neuron-implant-interface.

Glial cells derived from 6-day-old mouse retina were cultured on GaP-NWs (3-5 μm long, 80 nm diameter, 1 NW/ μm^2) and control GaP-flat (no NW) substrates. Qualitative and quantitative assessments were performed at 2-12 days in vitro to investigate cell morphology, proliferation, cell viability, and expression of glial-specific proteins.

Consistent differences were observed in cell and nuclear morphology among glial cells between GaP-NWs and GaP-flat. Over time, the total number of glial cells and degree of glial proliferation were lower on NWs than on flat substrates, while cell death tended to be higher on NWs. Nanowires seemed, however, to have a smaller effect on microglial cells as they remained unchanged, whereas the number of macroglial cells diminished. The study shows that the NW topography tested reduces macroglial cell proliferation, while a modified array design may be necessary to control also microglial cells.

Double quantum dots fully defined by polytype structures in semiconductor nanowires

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Double quantum dots (DQDs) are promising systems for quantum technology as they allow for two electronic states to coherently couple [1]. Defining QDs with materials rather than the more commonly used electrostatic gating method [2] allows for hard-wall confinement potentials and less coupling to external noise, leading to more robust charge/spin states.

Until now, a missing ingredient of these material-defined DQD systems has been the ability to address each of the dots individually which is necessary to control the quantum states. We have defined DQDs using the conduction band edge offset at the interface of the wurtzite and zinc blende polytypes in InAs nanowires [3]. By selectively growing a GaSb shell on the zinc blende phase [4], we can use simple SEM imaging to identify our structures and precisely align gate electrodes to each dot.

The gate electrodes allow us to control each individual QD and using them we were able to, for the first time, measure the characteristic DQD honeycomb charge stability diagram in a fully material-defined system. We could also observe a discrete energy spectrum and extract parameters such as charging energy, finding them relatively unchanged over a large range of gate voltages. In addition, we found the tunnel barriers tunable by changing the electron numbers of the dots.

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Ab initio study of zinc silicate surfaces and interfaces

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Silicate films can form at the interface between silica and oxides or metals, potentially altering the interface properties. However, detailed understanding of surface and interface properties of silicates is in many cases missing. Here, motivated by the technological problem of poor adhesion between silicon-rich steel and zinc coatings, we focus on zinc silicate that can form at this interface. Applying density functional theory, we study the stability and electronic structure of the Zn_2SiO_4 surface terminations, and show that the formation of siloxane rings, which is the main responsible for suppressing adhesion at silica-zinc interfaces, is absent at silicate surfaces. The properties of the interfaces between the silicate and metallic zinc are determined by those of the zinc oxide-rich surface terminations. Finally, I will discuss the factors that influence the stability of a silicate layer with respect to the binary oxides.

Physical properties of MgCl₂ activated CdSe thin films for solar cell applications

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The grain size in absorber layer to the Cd-based solar cells may be enhanced along with the passivation of grain boundaries by the chlorine treatment. In this paper, the study on the physical properties of the MgCl₂ activated CdSe thin films is reported. The CdSe thin films were deposited employing electron beam evaporation technique followed by chloride treatment using MgCl₂ and then thermally annealed in air atmosphere at temperature 170 °C, 320 °C and 470 °C. The pristine and annealed thin films were subjected to the X-ray diffraction (XRD), scanning electron microscope (SEM), source meter and UV Vis spectrophotometer for micro-structural, electrical and optical properties respectively. The structural analysis reveals that the pristine and films annealed at temperature 170 °C, 320 °C are crystallized in cubic phase with (111) predominant reflection while films annealed at 470 °C have hexagonal phase along with reflection (002) . The structural and optical parameters like inter planar spacing, lattice constant, grain size, dislocation density, internal strain, number of crystallites per unit area and optical band gap, absorption coefficient, refractive index and extinction coefficient are calculated. The experimental results demonstrate that treated CdTe thin films may be used as an absorber layer thin film solar cells.

Gas Transporting Tubes Failure Prediction

Evgeny Deulin, Ekaterina Ikonnikova, Roman Emelianenko

The investigations results were used for the intensity of tube "hydrogen illness" estimation also as for the arterial transporting gas tube failure date prediction. The Secondary ION Mass Spectrometry[1](SIMS) and Russian Electron Microscopy, УЭМБ100K were used in the experiments. Process of hydrogen dissolution is the result of so-called "dry friction". In our case, it is a result of micro size gas particles contacting with tube inner surface and hydrogen penetration into the near surface volume. It is shown, that the described process being considered on nano scale level increases the dissolved hydrogen concentration 100-300 times on the depth 20 microns, after 2 min [2]. The main SIMS analysis results shows[3], that the process of arterial gas tubes hydrogen illness and its destruction are the result of hydrogen dissolution at friction. The plastic properties of the gas tube metal deterioration was done with Electron Microscopy on Azov Steel (Ukraine) by Ikonnikova, and the results of sulfide inclusions and its hydrogen transformation we may see on Fig.1 and Fig.2, where the black areas of sulfide particles in result of hydrogen diffusion transforms into "roundish" form particles, where hydrogen concentration is less. As it goes from the theory, the friction process may leads to mechanical properties of the gas tube discrepancy and sometimes is a reason of the tube failure.

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3. Applied Surface Science, 144-145, (1999), pp.258-268

ZnSnN₂ by RF magnetron sputtering: A potential photovoltaic absorber for thin film solar cell

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In the past few decades, new materials identification with impending applications to an extensive variety of technologies has swiftly increased. Especially for solar cell technology, many new absorber materials have predicted based on earth abundant and non-toxic. One such material is zinc tin nitride (ZnSnN₂), an II-IV-N₂ analog of the III-nitride materials, which has been identified as a potential solar absorber due to its direct bandgap and large absorption coefficient. Owing to these advantageous, polycrystalline ZnSnN₂ thin films were successfully synthesized by reactive radio-frequency (RF) magnetron sputtering with different Sn concentrations at 450°C. The orthorhombic ZnSnN₂ grew along the (120) direction with higher grain size (15.88 nm) which is confirmed by X-ray diffraction technique. The surface morphology and the film composition were determined using FESEM and energy dispersive X-ray spectroscopy (EDAX) analysis. The optical band gap of our films with different growth conditions is in the range of 2.0 to 2.30 eV. The refractive index and extinction coefficient were also calculated from the reflectance spectra obtained by UV-Vis-NIR spectroscopy. The deposited ZnSnN₂ films showed n-type conduction with carrier concentration in the range of 10¹⁹ cm⁻³ to 10²⁰ cm⁻³, resistivity between 10⁻¹ Ωcm and 10⁻² Ωcm and the maximum mobility of 3.44 cm² V⁻¹ s⁻¹. The collective results show that ZnSnN₂ is a promising candidate for photovoltaic absorber and alternative material for III-nitrides.

Keywords: ZnSnN₂, Photovoltaic, III-nitrides, Absorber, Mobility

From biosensor to photodetector; biomarker controlled fabrication of a photosensitive gold-nanoparticle/porous silicon device

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Photodetector devices incorporating gold nanoparticles (AuNPs) on porous silicon (PSi) structures have been fabricated. The dosage of AuNPs incorporated on PSi is achieved by a sandwich reaction relying on a capture antibody immobilized on PSi, a calibrated amount of a cancer biomarker and a detection antibody conjugated to AuNPs. Relevantly, the dosage is key in the final photosensitivity of the device. To optimize its performance, a three electrode configuration, analogue to a field transistor is used. The I-V characteristics between the two surface electrodes on PSi have been acquired for different amounts of AuNPs and for common gate bias voltages of 2.5 V and white light illumination. It is patent that the control system (with no AuNPs) presents a weak photoresponse. On the other hand, by loading the device with AuNPs, an increase of the sensitivity is achieved, with gradual gain of response for increasing loading of AuNPs. This response is gate voltage sensitive. The photogenerated current has also been measured along time for pulses in the gate voltage (from 0 to 2.5 V, each 5 s). This time response demonstrates the relevance of the gate bias in the sensitization of the device and its stability in the short term for dissipated electrical power reaching 0.4 mW. The combination of spectroscopic and functional information suggests that the plasmonic effects induced by AuNPs are responsible of the enhanced photosensitivity of the loaded devices.

Effect of single walled carbon nanotubes on the thermal and mechanical properties of polyurethane/ polyvinyl chloride blend

Abdelwahab rajeh alouiry, Rizk Mostafa Shalaby, I. S. Elashmawi, A. M. Hezma

Structural, thermal, and mechanical properties of pure blend and nanocomposites based on polyurethane (PU) and polyvinyl chloride (PVC) doped with low different content of single walled-carbon nanotubes (SWCNTs) were studied. The nanocomposites at different concentration were prepared via casting technique. The interaction between PU/PVC blend and SWCNTs were examined via FT-IR studies. The changes in the structures of the nanocomposites were examined using X- Ray Diffraction (XRD), and the results indicated that the amorphous domains of nanocomposites increased with increasing SWCNTs content. Transmission electron microscope (TEM) observation indicated that SWCNTs surface was wrapped with the polymer. The thermal properties of nanocomposites was improved after addition of SWCNTs. The mechanical behavior of the nanocomposites was evaluated as a function of SWCNTs content. The main enhancement in tensile properties was observed, e.g., the tensile strength and elastic modulus increased compared with the pure blend, which may be attributed to the interaction and adhesion between CNTs and the polymer matrices due to the hydrogen bonding between carbonyl groups (C=O) of polymer blend chains and carboxylic acid (COOH) groups of CNTs. This paper studies the influence of SWCNTs doping on the structural, thermal and mechanical properties of PU/PVC with its potential to stand strongly to work in the field of wind turbines blades for electrical power generation.

Water dynamics in hydrated nanocellulose membrane by quasi elastic neutron scattering

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The solid electrolyte membrane is a key component in Polymer electrolyte fuel cells. It must be both an ionic conductor and an electronic insulator. Cellulose nanofibre membranes (CNM) are promising in this respect while being thermally and mechanically stable at high temperature and high humidity. However, unlike the commercial standard Nafion, CNMs show important proton conduction with only carboxylate groups as opposite to the very acidic groups available in commercial membranes. Moreover, they are cheaper and environmentally benign, and have better gas barrier properties than the commercial alternative. In this work, we use quasielastic neutron scattering (QENS) to study how the density of surface functional groups on CNMs influence the water dynamics as a function of relative humidity and temperature. Elastic window scans show a clear sigmoidal-shaped decaying for hydrated membranes with the transition temperature around 280 K. QENS data below and above the transition temperatures could be well fitted with two-component Lorentzian function in combine with Bayesian analyses, suggesting two types of water movement at different time scale. One could be associated to confined water in the porous system and the other is related to diffusion of bulk-type water. The nanoscale membrane structures were studied with small angle X-ray scattering at the similar water content. The results in this work shed light on the understanding of water-cellulose interaction and the development of novel fuel cell applications.

Adsorptive Removal of Ciprofloxacin from Aqueous Samples using Zr MOF

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Abstract:

Increasing concentration of antibiotics in water bodies is a topic of concern due to various harmful effects of these on both flora and fauna. Therefore, it is imperative to remove these emerging water contaminants from water bodies. In this manuscript, performance of hydrothermally synthesized porous Zirconium Metal Organic Framework (Zr-MOF) was evaluated for adsorptive removal of ciprofloxacin (CIP) antibiotic from aqueous samples. The resultant sample was characterized by various techniques such as powder X ray diffraction (PXRD), scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), ultraviolet spectroscopy (UV) and N₂ adsorption desorption analysis. The adsorption behaviour of CIP on Zr MOF was investigated with different initial concentration of CIP and amount of adsorbent, varying pH and contact time. Adsorption kinetics, isotherms and thermodynamics were studied to explain the adsorptive behaviour and mechanism of CIP on porous Zr MOF. From the obtained results, significant removal of CIP was observed, which presents Zr MOF as a promising candidate for removal of CIP from wastewater.

KEYWORDS: Adsorption, Ciprofloxacin (CIP), Zr MOF, Wastewater

2503-A-1902

Interface engineering of p-doped layers with new family of hexacyano-[3]-radialene anion-radicals

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Interface engineering of p-doped layers with new family of hexacyano-[3]-radialene anion-radicals

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Organic electronics utilizes pi-conjugated organic materials as semiconductors and their electrical properties can be controlled by a doping process. Solution-based technologies, which promise potentially cheaper and higher throughput production (than vacuum deposition) of large-area devices, are still at a premature state. One of the main difficulties is degradation (dissolution) of proceeding layers during the processing of the next ones and uncontrollable intermixing of layers. Dopants reduce contact resistance thus improving their performance of field-effect transistors. To this end, it is essential to introduce dopant molecules only at electrodes and not in the channel avoiding expansive lithography. In organic depletion transistors, there is a need for dopants to be introduced into the channel. Other devices may require deposition of dopants atop of semiconductors. This poster demonstrates how these challenging tasks can be solved with our ionic dopants. We used recently introduced family of hexacyano-[3]-radialene-based anion-radical dopants [1,2] and demonstrated that the dopants can be selectively attached to oppositely charged surface (Si-substrates modified with polycations or protonated amino-silanes (Fig 1).

References:

[1] Y. Karpov, et al. Adv. Mater., 28, 6003 (2016)

[2] Y. Karpov, et al. Chem. Comm., 54, 307 (2018)

2508-A-1902

Status of the Super-Fragment Separator (Super-FRS) Vacuum System of the GSI future accelerator facility FAIR

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The Super-FRS will be the most powerful in-flight separator for exotic nuclei up to relativistic energies [1] and is currently under construction in the framework of the FAIR project [2]. It consists of a pre separator, a main separator, high-energy branch, low-energy branch and the ring branch. Overall length of the vacuum system is about 350 m. Some components are already in the test phase, some others commissioned and others specified. The Super-FRS requires a vacuum in the range from 10^{-6} to 10^{-8} mbar. This machine presents different challenges: the high radiation area close to the target where new sealing solutions has to be developed, the 62 super conducting magnets including their insulation vacuum, the Beam Catchers, and the wide radius of the beam pipes (DN400). The design status of the vacuum system will be presented.

[1] H.Geisel, M.Winkler, et al, Technical Design Report on the Super-FRS

[2] <https://fair-center.de>

Enhanced Tunable Light Harvesting in Nanostructured Si Arrays Based on Double-Quarter-Wavelength Resonance

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Antireflective (AR) property is of crucial importance for light-harvesting that is critical for many optoelectronic devices including solar cells and photodetectors. For the traditionally layered AR coatings, the optical thickness of an AR coating determines the absorption peak wavelength based on the quarter-wavelength rule, and the effective refractive index (n_{eff}) of that, such as the square root of that of the substrate, determines the absorbance due to Fresnel law. However, it is extremely difficult to find the desired pair of the AR coating and the substrate to satisfy the square root requirement.

In this presentation, we introduce the cost-effective fabrication of large area nanostructured Si arrays based on monolayer colloid crystal templates which show excellent antireflection performance with tunable fashion. A new double-quarter-wavelength resonance (DQWR) model can unveil the underline mechanism of the enhanced full spectrum light-harvesting performance. Based on DQWR, one can quantitatively engineer light-harvesting regions and absorbance in any wave band from ultraviolet to the near infrared region by adjusting the thickness and diameter of the nanostructured Si arrays. And an enhanced full spectrum absorbance of more than 99% can be readily achieved, which is stronger than that of black silicon in the near-infrared region. In addition, the antireflective property of the nanostructured Si arrays is independent of the substrate and the angle of the incident light. Such novel optical properties provide an opportunity to achieve excellent AR performance by tuning the structure of nanostructured array instead of searching for a hard-to-get n_{eff} of the optical substrate.

ALD of HfO₂ on InAs: new insight by time-resolved in-situ studies

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Atomic layer deposition (ALD) is a powerful technique for the deposition of thin films with atomic-scale precision. The ideal ALD scheme, which relies on the assumption of a self-limiting surface reaction during deposition [1], is of crucial importance for modern metal-oxide-semiconductor (MOS) devices. III-V semiconductors are excellent candidates for future MOS-based applications; however, defects at the semiconductor-oxide interface limit device performance. ALD of the high-k material HfO₂ has been shown to remove the native oxide through the so-called self-cleaning effect, but many details of the surface chemistry remain unknown and the interface quality still needs to be improved.

We studied the HfO₂ ALD on InAs from tetrakisdimethylamido-hafnium (TDMAHf) and water fully in situ and operando by ambient pressure X-ray photoemission spectroscopy at the SPECIES and HIPPIE beamlines of the MAX IV Laboratory (Sweden). A complete removal of As-oxides was confirmed during the first ALD half-cycle [2]. Importantly, we observed a two-step chemical reaction including molecular adsorption of the TDMAHf precursor prior to oxide removal and HfO₂ formation, which shows that the established ligand exchange model of ALD needs to be revised. Recent studies with improved time-resolution, monitoring simultaneously As3d, In3d, In4d, Hf4f, and C1s core-levels, reveal the time sequence of the removal of different As- and In-oxide components, Hf surface chemistry, and Fermi level unpinning. These results have significant potential to improve the performance of III-V MOS devices.

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[2] R. Timm et al., *Nature Commun.* 9, 1412 (2018)

2520-A-1902

High Electron Affinity Molecular Dopant CN6-CP for Efficient organic electronic devices.

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High Electron Affinity Molecular Dopant CN6-CP for Efficient organic electronic devices.

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Doping is one of the most important processes to control the electrical properties of organic semiconductors. It involves the partial oxidation (or reduction) of a pi-conjugated system to generate free charge carriers. This leads to a significant increase of the conductivity in otherwise poorly conductive pi-conjugated organic semiconductors. This process has found numerous applications in organic electronic devices. For example, the doping of semiconductors has shown to improve the performance of organic light-emitting diodes (OLEDs), field-effect transistors and solar cells. Recently, we reported a new powerful p-dopant based on a [3]-radialene structure. [1]

Precise positioning of dopants is desirable for many applications. For example, doped layers may reduce contact resistance in field-effect transistors. To this end, it is essential to introduce dopant molecules only at electrodes and not in the channel and desirably avoiding expansive lithography processes. In other devices, such as in organic depletion transistors, the dopants are needed to be introduced into the channel that is at the dielectric-semiconductor interface. In this poster, we report a highly efficient 2D (interfacial) doping of organic semiconductors, poly(3-hexylthiophene) (P3HT) by a polyelectrolyte-supported layer-by-layer assembly of the dual-mode functional dopant CN6-CP^{•-}-K⁺, having an anionic group for its fixation onto oppositely charged surfaces/molecules as well as electron-deficient groups providing its p-doping ability.

[1] Y. Karpov, et al. Adv. Mater., 28, 6003 (2016)

catalyst-free covalent coupling of nonfunctionalized organic molecules on-surfaces

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On-surface Synthesis has consolidated as an efficient and elegant strategy toward the controlled synthesis of atomically-precise low-dimensional nanostructures. It is based on the hierarchical colligation of tailored precursor monomers through the realization of chemical reactions directly on a surface. So far, a plethora of low-dimensional nanostructures have been realized by means of different chemical reactions [1]. So far, they are based on the use of catalysts which drive and increase the efficiency of the thermally- or light-induced reaction.

Here, we report [2] on the catalyst-free covalent coupling of nonfunctionalized PAHs adsorbed on a relatively inert surface in the presence of atomic hydrogen. The underlying mechanism has been characterized by high-resolution scanning tunnelling microscopy and rationalized by density functional theory calculations. It is based on the formation of intermediate radical-like species upon hydrogen-induced molecular superhydrogenation which favors the covalent binding of PAHs in a thermally activated process, resulting in large coupled molecular nanostructures. The mechanism proposed in this work opens a door toward the direct formation of covalent, PAH-based, bottom-up synthesized nanoarchitectures on technologically relevant inert surfaces.

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[2] C. Sanchez-Sanchez et al. *J. Am. Chem. Soc.*, feb. 2019, DOI: 10.1021/jacs.8b12239

Formation of tungsten oxide nanowires by electron-beam-enhanced oxidation of tungsten disulfide

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Oxidation of van der Waals-bonded layered semiconductors plays a key role in deterioration of their superior optical and electronic properties. The oxidation mechanism of these materials is, however, different from non-layered semiconductors in many aspects. Here, we will show a rather unusual oxidation of tungsten disulfide (WS₂) nanotubes and nanoplatelets in a high vacuum chamber at a presence of water vapor and at elevated temperatures. The process results in formation of small tungsten oxide nanowires on the surface of low-dimensional WS₂. Utilizing real-time scanning electron microscopy we are able to unravel the oxidation mechanism, which proceeds via reduction of initially formed WO₃ nanoparticles into elongated W₁₈O₄₉ phase. Moreover, we show that the oxidation reaction can be localized and enhanced by an electron beam irradiation, which allows for on-demand growth of tungsten oxide nanowires.

Elaboration and characterization of undoped and La doped ZnO thin films by the spray pyrolysis technique

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¹ University of ouargla

Transparent conductive oxides technology has been accelerated since the 1980's with their interesting physical properties. Zinc oxide (ZnO) considering among the most promising materials for use in various fields such as piezoelectricity, photovoltaic effect, optoelectronics...etc. The principal aim of our work is elaboration and characterization of undoped and La doped ZnO thin films, with concentrations: 1, 2, 3 and 5 %wt. The solution was obtained by dissolving zinc acetate in methanol-double distilled water with concentration of (0.5 M), after it was pulverized on heated (375°C) and precleaned glass substrates using spray pyrolysis technique. A fundamental study of structural and optical properties such as crystallization, optical transmittance spectra, energy gap and grain size of prepared samples were realized using x-ray diffraction (XRD), Vis. UV and FTIR spectroscopies. XRD analysis showed polycrystalline and hexagonal wurtzite structure with (002) preferred orientation (wt%=0, 1, 3). The analysis show that the structure defects increase with the increase of grain size. Spectrophotometric measurements in Vis and UV wave lengths range have showed that all the films have a high transmission at the wavelengths range (300-900 nm), about 85% in the visible zone. Measured band gap energy ranged in 3.28 and 3.21 eV. It was found that the disorder of defects in the structure surveyed by deducting the Urbach energy, which ranged in 56.05 and 86.98 MeV, did not affect the energy band gap. FTIR measurements showed Zn-O vibration bands at 400 to 700 Cm⁻¹range. The addition in doping concentration leads to light deviation of bands range.

Keys words; TCO, Thin film, ZnO; La; Spray

Unraveling the Atomic Structure of Fe Intercalated under Graphene on Ir(111)

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The corrugated graphene on metal substrates is naturally a complex system and its atomic structure determination represents a challenge from the theoretical and experimental point of view [1,2]. Herein [3], the interaction of Fe deposited on graphene grown on Ir(111) was studied in detail to better understand the growth, intercalation, and oxidation of Fe ultrathin films on and under graphene. The study has combined a multiple technique approach that allows extracting at once the chemical, topographic and the precise atomic structure of the system submitted to different conditions of growth and atmospheric environment. For instance, scanning tunneling microscopy (STM) measurements allowed us to follow the formation of Fe nanostructures during Fe deposition and intercalation. Synchrotron-based high-resolution photoelectron spectroscopy (HR-XPS) untangled the different chemical environments for C-Fe bonds. We have also used photoelectron diffraction experiments to site-specifically unravel the atomic structure of the intercalated Fe under graphene. Oxidation experiments were also performed for samples prepared under different conditions which revealed that indeed one can set the thermodynamic parameters to selectively protect or oxidize the intercalated/supported materials which open interesting possibilities to engineer complex metal-oxide graphene-based devices.

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2554-A-1902

Nanophase wetting layer and formation of the metal/ silicon contact

Results of investigation of the initial stages of the formation of a transition metal-silicon contact at room temperature by means of the complex structural-chemical analysis by AES and EELS methods and the low-temperature method of physical vapor deposition have been presented. A nanophase wetting layer of a metal/ silicide on a silicon substrate was detected and identified before the formation of the first bulk phase. Formation of nanophase wetting layer fundamentally changes the approach to initial stages of the formation of a metal contact with a silicon substrate.

Investigating Charge Transfer Mechanisms in the Heterostructures of Two-Dimensional Materials

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Heterostructures of two-dimensional (2D) materials such as graphene and transition dichalcogenide (TMDC) can be realized either by manual stacking or 2-step chemical vapor deposition (CVD) method. We were able to grow heterostructures of molybdenum disulfide (MoS₂) with graphene by the CVD growth of graphene followed by another CVD of MoS₂ for this study. On the other hand, similar heterostructures are also prepared by vertical stacking utilizing polymer-assisted transfer of individual nanomaterials for comparison.

MoS₂ is found to grow as small flakes (a few hundred nm to a few micrometers) on top of graphene, forming vertical heterostructures. Characterizations of as-grown structures using such tools as atomic force microscopy (AFM), Raman and PL measurements confirm the formation of heterostructures with mono- to few-layer crystalline MoS₂ flakes on graphene. Efficient charge transfers from MoS₂ to graphene upon visible light illumination are observed. By utilizing efficient light absorption and charge transfer in MoS₂ with high mobility channels (graphene), we demonstrate photodetectors with high responsivities. The effects of the interface between two materials are investigated by comparing results on the heterostructures which are grown and stacked. Especially, local electrical measurements utilizing AFM show non-uniform charge transfers depending on the characteristics of interfaces.

Surface Passivation Study of Single InP Nanowire Solar Cells

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Photovoltaics directly convert solar energy to electricity and thus play an important role in sustainable energy production. Nanowires have several superior properties compared to their bulk material and when arranged in an array with optimized periodicity it is possible to reach similar efficiencies of photon absorption like thin films by using only a fraction of the material. Electron-beam-induced current (EBIC) has been used to characterise as-grown photovoltaic nanowires in order to optimize growth parameters [1]. However, it has been shown that due to the high surface-to-volume ratio the surface passivation of InP nanowires can play a crucial role [2], even though the surface recombination velocity of native InP is quite low [3].

In this study, as-grown p-i-n doped single photovoltaic InP nanowires are compared with nanowires passivated by atomic layer deposited SiO_x and PO_x/Al₂O₃ in a nanoprobe system inside a SEM. In this way, key parameters for solar cells can be measured without the need to process samples into functional solar cells. Furthermore, time-resolved photoluminescence (TRPL) is used to compare the charge carrier lifetimes. The comparison of the different passivation schemes will help to manufacture InP nanowire solar cells with higher efficiencies and pave the way to a successful nanowire tandem junction solar cell.

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Development of nano-beam Weissenberg RHEED for nano- and micro-surfaces

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It is important to understand the structures of functional nano-surfaces, which is involved in a functional material complex. There is a large demand for the techniques to investigate the surface structures of such small surfaces. Here we utilize a nano-electron-beam of SEM (scanning electron microscopy) to investigate the surface structure. Weissenberg reflection high-energy electron diffraction (W-RHEED) is a powerful technique for surface crystallography, where hundreds of diffraction patterns were captured as a function of the sample azimuth rotation [T. Abukawa, T. Yamazaki, K. Yajima, and K. Yoshimura, Phys. Rev. Lett. 97, 245502 (2006)]. Surface structures can be analyzed from 3D reciprocal maps that were reconstructed from the hundreds of diffraction patterns. For rotating a nano surface without moving away from the electron beam, it is required to move the target on to the rotation axis, and to rotate the target precisely on the axis. Therefore, we have made a 4-axes UHV manipulator with a piezo rotator, and are developing a beam tracking software during the rotation.

We have tested the technique on a polycrystalline Ni film. 3D reciprocal maps were successfully acquired from a single grain of the Ni film. The crystal orientation and the crystal structure of the grains were unambiguously determined from their 3D reciprocal maps. We will present the details of the technique and its potential for the surface structure analysis.

Nanoscale Study of Luminescence from a Thermally-reduced Graphene Oxide

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Graphene oxide (GO) is known as a two-dimensional material, which is formed by the oxidation of graphene. The electronic and optical properties of GO are governed by the size of the sp² hybridized domain isolated in the sp³ hybridized matrix [1]. In this study, we altered the spatial distribution of the sp² domain in GO by the thermal reduction, and the nanoscale luminescence of the GO were investigated using scanning tunneling microscopy (STM) and STM light emission (STM-LE).

GO was deposited on Au(111) covered with the octanethiolate (C8S) self-assembled monolayer (SAM). Thermal reduction of the GO was performed at 6×10⁻¹⁰ Torr. We also utilized Raman and photoluminescence (PL) spectroscopies to check the sample condition. STM and STM-LE were measured in a UHV chamber at RT.

The general features of Raman spectra obtained from the GO/C8S-SAM/Au(111) at RT are similar to the previous report, appearing of the D and G bands. We found that this GO did not exhibit the PL. However, the strong PL was observed from the GO after annealing at 400 °C. Simultaneously, the D band intensity of the Raman spectrum was decreased, indicating that highly luminescent sp² domains were formed via the thermal reduction with C8S-SAM. Bias dependent STM-LE experiment of thermally-reduced GO on C8S-SAM/Au(111) revealed that GO emits light when the voltage exceeds 1.6 V. STM-LE mapping identified the luminescent sites of GO, which are localized in a few nm regions.

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Dehydrogenation of methanol on pure and transition-metal-doped cerium tungstate model catalysts

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Modern heterogeneous catalysts are based on active compounds incorporated in or supported by various oxides, considered inert or not in the relevant chemical reactions. The most important active supports contain cerium oxides of different stoichiometry. Cerium can be stabilized in Ce(III) chemical state by incorporating tungsten atoms in the crystal structure, forming cerium tungstate (Ce₆WO₁₂) that can be easily prepared in situ on W(110) as model thin films of the (100) surface orientation. We used this material to support palladium and platinum nanoparticles and study the reactivity towards methanol molecules by photoelectron spectroscopy of core levels and valence bands excited by laboratory and synchrotron photon sources. The adsorption of methanol was performed at 150 K, followed by a step-wise annealing up to 700 K. The role of tungsten was ascribed to the creation and stabilization of Ce(III) sites that were found to be active in dehydrogenation of methanol to methoxy while both deposited transition metal additives (Pd, Pt) helped to proceed the reaction further towards CO formation and its dissociation. Cerium tungstate was chemically intact during the reaction while palladium and platinum exhibited reversible changes. The stability and activity of the studied model thin film catalysts in decomposition of methanol is discussed.

Elastic Recoil Detection and ^3He Nuclear Reaction Analysis of fusion reactor materials and isotopic tracers

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First wall materials in controlled fusion devices undergo serious modification by several physical and chemical processes arising from plasma–wall interactions. This includes material erosion, transport of eroded species in the plasma and re-deposition leading to the formation of mixed-material layers. The driving forces for detailed study of plasma-facing materials and components are related to the assessment of: (i) material lifetime; (ii) accumulation of hydrogen isotopes in wall materials, i.e. fuel inventory; (iii) dust formation.

As opportunities to study materials is very limited special techniques are needed to study these mechanics. One very powerful tool is to use rare isotopes as tracers in important processes.

For maximum results a large variety of materials research methods are used to determine the properties of wall materials. Ion beam analysis techniques play a particularly prominent role because of their isotope selectivity in the low-Z range (1-20), high sensitivity and possible combination of several methods in a single run.

The role of ^3He -based Nuclear Reaction Analysis and Time of flight Elastic Recoil Detection in fuel retention and material migration studies along with the use of tracer techniques utilizing rare isotopes (e.g. ^{13}C , ^{15}N , ^{18}O) or marker layers on wall and diagnostic components is described. The development and optimisation of multiple anodes in the gas volume that detect the energy in the ERDA detector are discussed with examples from the world largest tokamak the world's largest tokamak: Joint European Torus (JET) operated with beryllium and tungsten on the plasma facing wall.

Fabrication and characterization of GaN nanocrystals with a metal core

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Properties of GaN, such as a direct band gap, high electron mobility, high thermal stability, etc., remain attractive both for research and application purposes, particularly for design of electronic and optoelectronic devices [1].

A unique, low-temperature ($T < 300\text{OC}$) preparation method of GaN was developed in our research group. The method is based on deposition of Ga atoms assisted by ultra-low energy nitrogen ions ($E = 50\text{ eV}$) [2] at substrate temperatures being significantly lower than in conventional GaN deposition technologies (e.g. MOCVD, 1000°C). We have applied this method for selective growth of GaN nanocrystals [3].

In [4] it has been shown, that the presence of Ag nanoparticles in close vicinity to GaN structures enhances its photoluminescence [4]. In our contribution we will report on GaN nanocrystals on the Si(111) substrate covered by the native oxide possessing an Ag nanoparticle (core) directly in each of them .

Gas Transporting Tubes Failure Prediction

Evgeny Deulin, Ekaterina Ikonikova, Roman Emelianenko

The investigations results were used for the intensity of tube "hydrogen illness" estimation also as for the arterial transporting gas tube failure date prediction. The Secondary ION Mass Spectrometry[1](SIMS) and Russian Electron Microscopy, УЭМБ100K were used in the experiments. Process of hydrogen dissolution is the result of so-called "dry friction". In our case, it is a result of micro size gas particles contacting with tube inner surface and hydrogen penetration into the near surface volume. It is shown, that the described process being considered on nano scale level increases the dissolved hydrogen concentration 100-300 times on the depth 20 microns, after 2 min [2]. The main SIMS analysis results shows[3], that the process of arterial gas tubes hydrogen illness and its destruction are the result of hydrogen dissolution at friction. The plastic properties of the gas tube metal deterioration was done with Electron Microscopy on Azov Steel (Ukraine) by Ikonnikova, and the results of sulfide inclusions and its hydrogen transformation we may see on Fig.1 and Fig.2, where the black areas of sulfide particles in result of hydrogen diffusion transforms into "roundish" form particles, where hydrogen concentration is less. As it goes from the theory, the friction process may leads to mechanical properties of the gas tube discrepancy and sometimes is a reason of the tube failure.

1. SIMS Europe 2010/ / Muenster Germany Sept 2010, p.110
2. Patent RF.№ 2391601 dated 21.07.2008
3. Applied Surface Science, 144-145, (1999), pp.258-268

Fig.1 Russian Steel 10G2FB ,before heat X 3200

Fig2 The same gas tube steel after heat 12500C

2574-A-1902

Core-shell Cu-Ag Nanoparticles Produced by Spark Discharge Generation

Namsoon Eom, Markus Snellman, Martin Ek, Maria Messing, Knut Deppert

The synthesis of core@shell nanoparticles has predominantly been carried out by chemical methods or physical deposition of a shell material post-growth onto core particles. By combining immiscible materials that differ in surface energy, we demonstrate the spontaneous atomic rearrangement to monodisperse Cu@Ag core@shell particles directly in the aerosol phase, starting from pure Cu and Ag electrodes with the spark discharge generation (SDG) method. The morphology and crystallinity were investigated by SEM and HRTEM, and the composition was confirmed by STEM EDX, which indicated that the Ag shell acts as an oxidation barrier for the Cu core. The current material system may find applications in antibacterial coatings. The method presented can be extended to other bimetallic systems with applications in catalysis, plasmonics and as seed-particles for nanowire growth. Owing to the simple, zero-waste and continuous production method, SDG is an ideal platform for such nanoparticle generation and investigation.

Building superlattices from aerosol nanoparticles via evaporative self-assembly

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Nanoparticle superlattices consisting of densely packed particles with periodic arrangements can exhibit interesting collective properties different from those of individual nanoparticles and thus have attracted great interest in research due to their potential applications in optoelectronic, plasmonic, and magnetic devices. Evaporation-induced self-assembly on solid substrates which employs nanoparticles produced by wet chemistry is one of the most widely used methods in nanoparticle superlattice fabrication. However, impurities are inherent in the popular wet chemistry-based method and are often a cause of lack of reproducibility. Here we present a simple but novel method to generate close-packed arrays of nanoparticles uniquely created by combining aerosol technology with evaporation-induced self-assembly. Metal and metal oxide aerosol nanoparticles (20 - 50 nm in diameter) are generated using a spark discharge generator and are subsequently deposited on liquid droplets. We demonstrate that this way of capturing aerosol nanoparticles in the gas-liquid interface of a droplet suppresses the ubiquitous 'coffee-ring' effect during evaporation leading to self-assemblies of nanoparticles. This simple, effective method provides a versatile strategy for fabricating various types of nanoparticle superlattices.

InSb Nanoparticles Produced by Spark Discharge Generation

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We present the synthesis of monodisperse aerosol InSb nanoparticles of high crystalline quality using the spark discharge generation (SDG) method. Apart from successfully using metallic In and Sb electrodes, we demonstrate the feasibility of using pure semiconducting InSb wafers as electrode material. We investigated the influence of carrier gas on the quality of the size selected particles. We show that addition of 5% hydrogen in the carrier gas (nitrogen or argon) reduced particle oxidation and drastically lowered the compaction temperatures. Further we found an influence of the compaction temperature on the stoichiometry and crystallinity. While uncompacted particles contained excess Sb, the InSb particles reached 1:1 molar ratio after full compaction. The spark discharge method shows promise for generating large quantities of high-quality InSb nanoparticles with applications in e.g. optoelectronics and plasmonics, and the method may be extended to generate nanoparticles of other semiconductor materials.

Surface analysis of microplastic and microplastic mixtures exposed to fresh water.

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The widespread presence of microplastic material (small synthetic plastic particles <5 mm) in the environment has gained considerable attention in recent years, as regulators, researchers, and manufacturers race to understand its sources and pathways, to assess its impact on ecosystems and human health, and to develop effective means to tackle the issue. However, the different human behaviour and different sources depending on geographical location make the microplastics monitoring and filtering difficult.

Amongst the different type of plastics, polyethylene and polyvinyl chloride are amongst the most commonly found in the aquatic environment being observed not only on the surface and sub-surface of sea, river and lake waters but also in several varieties of marine organisms (e.g. sea turtles, whales, mussels) and sea birds. However, up to now, most of the studies and investigations on the effects of microplastics have concentrated on the marine environment, with less attention being given to the behaviour of microplastics in freshwater ecosystems.

In this work, commercial spherical microplastics, namely polyethylene (PE), polyvinyl chloride (PVC) and polymethylmethacrylate (PMMA) have been analysed by Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and other analysis techniques such as X-ray photoemission Spectroscopy (XPS), FTIR and Raman spectroscopy, before and after exposure to fresh water with and without natural sand collected from the Lake Maggiore (Italy) to study their chemical interactions with the environment. Moreover, mixtures of microplastics were also analysed to investigate the influence of the microplastic composition

Oxidation of the NbO termination on Nb(110)

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Oxygen reacts strongly with niobium and temperatures in excess of 2200K are required to remove oxygen impurities. Oxides will clearly influence niobium's superconductive properties and its tunnelling characteristics in devices. Niobium oxides find relevance as catalysts in redox reaction and Nb₂O₅ sees application as a dielectric in capacitors with conductive NbO acting as the electrode.

When oxidised Nb(110) is vacuum annealed a NbO(111)/Nb(110) termination forms, which is extremely stable [1]. In this work, the in-situ oxidation of this oxide termination is examined by several surface sensitive techniques foremost of those being scanning tunnelling microscopy and spectroscopy (STS). The oxidation is strongly influenced by the structural and electronic properties of the NbO(111)/Nb(110) substrate. The NbO(111) is terminated by one-dimensional few-nanometer niobium nanocrystals, which form a regular pattern [1]. High-resolution STS measurements reveal regions of high density of states (DOS) at the edges of these nanocrystals. Very low-dosage oxidation and subsequent vacuum annealing results in the formation of resolved sub-nanometer clusters, which solely reside in-between the nanocrystals in the regions of high DOS. High dosage oxidation results in the formation of Nb₂O₅ confirmed by X-ray photoelectron spectroscopy measurements. The Nb₂O₅ is unsurprisingly amorphous at the atomic-scale. However, larger scale (tens of nanometers) structure is observed, which is dictated in part by the nanocrystals of the underlying NbO(111).

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Integrated Sandwich-Like Battery Design for Rechargeable Energy Storage: Optimizing the Compatibility of the Flexible Electrodes

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The booming development of wearable and implantable electronics proposes the persistent requirements for the high-performance flexible batteries. Despite the research efforts towards designing ingenuity of the electrodes, the simultaneous realization of mechanical flexibility and electrochemical performance remains a significant challenge for the battery design, especially in consideration of the component compatibility in the full batteries with the light-weight arrangement, structural robustness, and shape-conformability. In this talk, some battery models which integrated the flexible electrodes, modified separator and the flexible substrate will be introduced. the sandwich-like flexible battery with optimal integration could not only build an intimate component coupling without relative displacement but avoid the use of additional current collectors for the low interfacial resistance. Three prototype full cell configuration, including lithium-ion battery and metallic battery are demonstrated with good electrochemical performances. This sandwich-like configuration showcases its potential use in flexible electronic devices.

Emergence of form birefringent nanostructures during the ion irradiation of thin films

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Surface nanoscale features can modify the optical properties of materials. Developing techniques to produce these features, offers the possibility to engineer high-efficiency sensors [1].

Here we have investigated the optical reflectance of anisotropic nanostructures fabricated through ion irradiation of thin metal films. These nanostructures self-organize according to a dewetting scheme [2]: at each ion impact, the film is locally brought to the molten state, and the concurring actions of sputtering, surface tension and disjoining pressure produce an instability in the surface morphology.

Under broad-beam irradiation, the film develops an isotropic pattern of percolated patches exposing the substrate and showing a characteristic wavelength [3]. In the present experiments, this isotropy has been broken by focusing and rastering the ion beam. By choosing flux and dwell time for the rastering beam in a very narrow window of the experimental parameters, it was possible to induce the emergence of nanoscale gratings, with full in-plane anisotropy. Several other degrees of anisotropy were obtained by tailoring the irradiation parameters.

The spectral characteristics and the polarization dependence of the optical reflectance of the anisotropic structures were studied experimentally, and we report the evidence of form birefringence with an efficiency depending on the illumination wavelength. The sensing capabilities of these structures are demonstrated by showing that absorbates strongly increase the form-birefringence effect.

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Wettability Properties of Pineapple Leaf Fibers and Banana Pseudostem Fibers Treated by Cold Plasma

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Banana pseudostem fiber (BPF) and pineapple leaf fiber (PLF) for their excellent mechanical properties and biodegradability characteristics arouse interest in different areas of research.

In tropical regions, where the banana pseudostem and the pineapple leaf are transformed into hard-to-handle solid waste, they can be low-cost raw material and environmentally sustainable in research for composite materials. In terms of functionality of this type of fiber, an open structure would allow the adsorption and retention of organic, inorganic and metallic species. In general, natural fibers have closed structures on their surface with intricate internal arrangements that can be used for the solution of environmental problems and other technological uses, however it is not possible to access their internal structure and sublayers, exposing the fibers in the natural state. An alternative method to chemical and enzymatic treatment are the processes with the plasma treatments, which have known to be clean, economical and controlled. In this type of treatment, a gas contained in a reactor in the form of plasma acts on the fiber generating changes in their physical structure, morphology and topography.

This work compares the effects on fibers of PLF and BPF treated with cold plasma, alternating time and current. These fibers are grown in the regions of Antioquia-Colombia. The morphological, compositional and wettability properties of the fibers were analyzed by Contact angle measurements, Scanning Electron Microscopy (SEM), and Raman microscopy. The treatment with cold plasma on PLF and BPF allowed increasing their hydrophobicity, and they showed changes in their roughness.

Sputtering Damages in Metal Sulphide Dichalcogenides

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Sputter deposition is a commonly used process and the possibility of using it in conjunction with 2D materials would constitute an enormous advantage for the industrial scale production in Europe. This is the objective of the LaMeS project (FLAG-ERA - Graphene - Basic Research 2 – 2017) where sputter-deposition of high quality layered sulphide structures, such as WS₂, MoS₂, SnS₂ and combinations thereof, is developed.

The crystal structure of the layers obtained has been characterized by XRD and TEM. The precise composition has been obtained from Rutherford Backscattering Spectrometry, and indicates a reduced sulfur concentration. This may be associated with the growth process. The drawback of sputter deposition onto sensitive 2D-materials is indeed that the energetic bombardment associated with the sputtering process typically exceeds the level needed to break the chemical bonds, resulting in the loss of lighter elements, the damage of the material and the deterioration of its properties.

In order to get detail of the sputtering damages, we have used Scanning Tunneling Microscopy to study the surface structure of either samples prepared by the sputtering deposition or commercial samples. In particular, microfocused ion beam has been used to study the impact of low energy ions (typically Ar⁺ of a few eV) on the layered sulphides, and the results were compared to those obtained on metal surfaces.

Results on a vacuum chamber with amorphous carbon coating subjected to synchrotron irradiation from 12.5 to 1250 eV critical energy

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In the framework of the HL-LHC project design, the vacuum performance of new surface material needs to be studied in details. In particular, amorphous carbon (a-C) coating is proposed as an anti-multipactor surface with the objective to minimize the beam induced electron cloud heat load deposited on the shielded beam screen and the background to the experiments due to proton scattering onto the residual gas. Since the protons in the HL-LHC final focusing triplets generates synchrotron radiation with ~ 10 eV critical energy and $\sim 10E16$ ph/m/s flux, it is therefore of great importance to study the impact of such photons on a-C coating held at room and cryogenic temperature and compare the results against present LHC material. This paper presents results on quantitative measurements of photon stimulated gas desorption, relative measurements of photo-electron yield, photon specular reflectivity and azimuthal distribution of diffusely scattered photons. All the measurements are done at room temperature in the range of synchrotron radiation critical energy $12.5 \div 1250$ eV for a tube with a-C coating irradiated at grazing incidence angle and a simple Cu tube used as a reference.

Development of a new taxis assay using micro-patterned scaffolds

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To determine how three-dimensional (3D) shapes influence the direction of cell migration, micro-patterned scaffolds incorporating different shapes were fabricated on a silicon substrate. When we had imaged the migration of NIH3T3 cells on the micro-patterned scaffolds over 72 h, we found that the cells adhered to and extended along the edge of the upper surface of the scaffold. The angle at which the migrating cells turned differed markedly and correlated with the unit shape within the scaffold. We next identified a 3D shape that induced cells to migrate in only one direction. 3D scaffolds were constructed that bore sharp-edges, all of which faced in almost the same direction. NIH3T3 cells cultured on the 3D scaffolds migrated only in the direction faced by the sharp edges. We postulated that this phenomenon may be a new form of taxis induced by topological stimuli. We also partially identified the mechanism that caused the NIH3T3 cells cultured on these 3D scaffolds to migrate in only one direction. Confocal laser scanning microscopy revealed that the sharp edges induced cells to put forth protrusions in a single direction. Thus, it appears that the 3D scaffold regulates the direction of these protrusions, thereby inducing unidirectional migration. I have now succeeded in separating different cells using this new technology.

Metal nitride nanoflake thin films grown by dc-magnetron sputtering for high-performance supercapacitor applications

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Transition-metal nitride thin films are recognized as the leading electrode material for new generation, high-performance, stable, flexible, smart supercapacitor because these films exhibit wider voltage range, good sustainability and high electrical conductivity. Herein, we have deposited high quality thin films of metal nitride in controlled vacuum level by using reactive DC-magnetron sputtering for enhanced performance supercapacitor. These films were grown on 304 Stainless Steel (304 SS) substrate at 2000 C for 15 minutes in Ar-N₂ atmosphere. These films of gamma-Mo₂N@SS and VN@SS were tested as an electrode material in aqueous solutions of KOH and Na₂SO₄ at various scan rates. Scanning Electron Microscopy (SEM) revealed the film thickness and confirm the nanoflake type structure for both the films, while composition was confirm by the EDAX attached with SEM. X-ray photoelectron spectroscopy (XPS) revealed the good stoichiometric and electronic state of all the elements present in the as-deposited films, while X-ray diffraction (XRD) showed the phase orientation and crystal structure of films. These metal nitride based electrodes exhibited super hydrophilic nature (with contact angle 6.7 degree for VN@SS and 11.3 degree for gamma-Mo₂N@SS) in presence of used electrolytes and revealed enhanced volumetric capacitance with an excellent rate performance.

Keywords: gamma-Mo₂N and VN thin films, sputtering, cyclic volumetric, contact angle, XPS.

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Vacuum Technology in Pakistan

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In the recent years, rapid industrialization has taken place due to the promising policies of the government for the private sector. The increasing demand of innovations in industrial products has given considerable impetus to the growth and development of vacuum technology in the country. This technology has proved its usefulness in a number of scientific, industrial and technological disciplines. The extensive use of vacuum technology in over 10,000 industrial units has raised the profit rates of the manufacturers as well as provision of quality products to the consumers. In research side, over 500 high-tech universities have been launched to the high-tech research world-over. Pakistan Vacuum Society (PVS) is doing remarkable efforts in promoting vacuum technology in the country. Realizing the importance of vacuum technology, the Govt. of Pakistan has established National Institute of Vacuum Science and Technology (NINVAST) in Islamabad-Pakistan. This paper reviews the use of vacuum in advanced research and industrial sectors as well as high-lights the present and future role of NINVAST in the development of vacuum technology in Pakistan

STM and XPS Studies of PTCDI on Sn/Si(111)- $2\sqrt{3}\times 2\sqrt{3}$

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We have studied PTCDI on Sn/Si(111)- $2\sqrt{3}\times 2\sqrt{3}$ using scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). The substrate was prepared by evaporating ~ 1.4 ML Sn onto a Si(111)- 7×7 surface followed by 2 min annealing at 560 °C. PTCDI was deposited while the sample was kept at room temperature. STM images recorded at low coverages show a strong interaction between the molecules and the substrate since the molecules are locked into specific adsorption sites. The molecules grow in 1D rows along high symmetry directions of the $2\sqrt{3}\times 2\sqrt{3}$ surface, and these rows become increasingly common up to a coverage of 0.5 ML. The rows also grow at specific distances to each other which results in a PTCDI-induced $4\sqrt{3}\times 2\sqrt{3}$ superstructure. Three different row directions are identified, two of which involve intermolecular O \cdots H hydrogen bondings while the least common row type does not. At 1 ML coverage, several new 2D structures are formed as additional molecules are positioned between the molecules in the 1D rows. Above 1 ML the growth is characterized as island growth and the molecules are arranged in these islands according to the canted structure. The interaction between the substrate and the molecule was also studied using XPS, where a strong charge donation from the Sn atoms to the imide related carbons was identified. The observed changes in the XPS spectra at low coverages are saturated at about 0.5 ML coverage, which corresponds to the coverage where the molecules no longer can adsorb at the aforementioned specific adsorption sites.

Recent development in XPS and Ambient Pressure XPS techniques

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Many important processes such as energy conversion, electrochemical, corrosion and biological processes take place at solid-gas and solid-liquid interfaces [1-3]. X-ray photoelectron spectroscopy (XPS) is the most powerful technique for understanding of these processes at the atomic level and it is the key to improving the performance of novel battery generation or renewable energy sources such as solar, wind or hydropower energy conversion devices. We would like to promote the latest equipment, technology solutions and innovations for the photoelectron spectroscopies field. Here it will be presented an innovative and compact spectrometers for the routine X-ray photoemission spectroscopy and ambient pressure photoemission spectroscopy for study of important phenomena in the current research. The design, construction, and technical parameters of new analyser will be presented. We will report the research results of XPS measurements conducted on the photovoltaic [4], catalytical [5] or bio-materials. Moreover, it will be demonstrated the analyser operation in ambient pressure. Also the results of interaction of oxygen and surface alloy will be presented, in order to permit complete characterization for the different pressure and temperature conditions.

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Silicon-Nanographite Aerogel-Based Anodes for High Performance Lithium Ion Batteries

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To increase the energy storage density of lithium-ion batteries, silicon anodes have been explored due to their high capacity. One of the main challenges for silicon anodes are large volume variations during the lithiation processes. Recently, several high-performance schemes have been demonstrated with increased life cycles utilizing nanomaterials such as nanoparticles, nanowires, and thin films. However, a method that allows the large-scale production of silicon anodes remains to be demonstrated. Herein, we address this question by suggesting new scalable nanomaterial-based anodes. These are based on a three-dimensional porous structured silicon-nanographite aerogel fabricated by a novel cost-efficient chemical method using polyvinyl alcohol as a precursor. These silicon-nanographite aerogel electrodes have stable specific capacity even at high current rates and exhibit good cyclic stability. The specific capacity is 455 mAh g⁻¹ even at 200th cycles with a coulombic efficiency of 97% at a current density 100 mA g⁻¹. If further optimization of materials is performed, this method has the potential for the future large-scale production of high-performance anodes for lithium-ion batteries.

Thermally- and electron-induced self-assembly of biphenyl-4,4'-dicarboxylic acid on Ag(111)

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Self-assembly of organic and metal-organic species is an exciting field using principles of supramolecular chemistry to construct complex molecular objects [1]. Recently, this approach has been implemented at surfaces [2], where numerous two-dimensional structures with various functional properties can be created. At the moment, there is copious information on resulting thermodynamically stable molecular architectures on diverse substrates, but knowledge of how intermediate kinetically trapped states form and how in general, self-assembly processes develop in time is still scarce. Even less is known about an impact of external stimuli other than thermal heating (e.g. low-energy electrons, photons) on self-assembly of surface-confined molecular networks. The use of low-energy electron microscopy (LEEM) may shed light on those yet unanswered questions. In this work we present an investigation of biphenyl-4,4'-dicarboxylic acid (BDA) self-assembly on an Ag(111) single crystal. Using LEEM we aim to reveal kinetics of the development of transitional and final BDA structures at different temperatures and electron beam energies. In addition, an influence of each external stimulus (thermal annealing and electron-beam irradiation) on the kinetics and structural transformations is discussed. Our results demonstrate significantly different self-assembly patterns when the process is dominated by one of the stimuli, which raises intriguing questions regarding the mechanism of low-energy electrons interaction with the on-surface molecular networks.

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Effects of photovoltaic nanowire arrays on human cancer cells

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Vertical nanowire arrays are attractive as cell culture substrates, as they can steer the behavior of cells cultured on the array. Hence, the effects of culturing cells on various vertical nanowire arrays have been extensively studied [Prinz, 2015; Bonde et al., 2014]. However, less is known about the effects of culturing cells on nanowires that have optoelectronic properties, such as nanowire solar cells. Here, we study the effects of photovoltaic nanowires on human cancer cells. Human A549 lung cells were cultured on vertical indium phosphide nanowire pn junctions (solar cells), and kept in light or dark conditions. Our results show that cells cultured on the nanowire solar cells exposed to light are present in lower density on the substrate compared to cells kept in the dark. Moreover, we could see a larger fraction of cells in the G0 cell cycle phase among cells cultured on illuminated solar cells. Altogether, this suggests that culturing cells on photovoltaic nanowires exposed to light can induce cell dormancy in a cell population subset. We also observed a recovery in cell proliferation after the illumination was turned off. Chemotherapeutic-induced dormant state has been observed for cancer cells, leading to treatment resistance [Barkan et al., 2008; Gao et al., 2017]. Future work will be directed to using photovoltaic nanowire arrays to study and manipulate cancer cell dormancy, in order to possibly use photovoltaic nanowires as a tool in cancer research.

Microwave plasma fabricated free-standing N-graphene sheets: electrical conductivity

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Microwave-driven plasmas were successfully applied in the selective synthesis of high quality free-standing graphene and N-graphene (nitrogen doped graphene) sheets via a single step process at atmospheric pressure [1,2]. A high level of control over sp²/sp³ carbons ratio (~15) has been achieved. The percentage of counts of monolayers is about 40%. The lateral size of the sheets is in the range 200 –700 nm.

Such self-standing graphene sheets are an alternative to surface-supported graphene. Many applications (e.g.: nanocomposites, batteries, supercapacitors) require free-standing graphene nanosheets or flakes consisting of a few atomic layers.

In this work the electrical conductivity of the N-graphene sheets compressed in tablets is investigated. The dependence on graphene sheets rearrangement upon compaction and packing density is studied. High electrical conductivity with values in the order of 1000 S/m was measured being much higher than the reported values of graphene sheets obtained by chemical methods. It is attributed to the formation of conductive network through the matrix of highly conductive sheets having multiple interfaces between them. The current flow mechanism was explored at low temperatures down to 10K. The charge transport exhibits a transition between thermally activated behavior at higher temperatures and variable range hopping at lower temperatures.

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Ni-TCNQ molecular network on the graphene

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Metal coordinated 2D molecular layers, where the metal ions are combined with organic ligands have potential for applications in spintronic and quantum processing. Recently the utilization of graphene layer as the substrate for molecular self-assembly proved to be a feasible approach. Apart for other advantages, graphene has low density of states near the Fermi level and can therefore electronically decouple molecules from the underlying metal substrate and allow high-resolution spectroscopy and imaging of molecular orbitals.

Here we present the preparation of a metal-coordinated network formed by the Ni-TCNQ (tetra-cyanoquinodimethane) on graphene grown on Ir(111) substrate. On metal surfaces, the Ni-TCNQ (7,7,8,8-tetracyanoquinodimethane) molecular network exhibit weak ferromagnetic coupling [1]. Recent work suggests the possibility to control magnetic interactions by adjusting the Fermi level position in the graphene [2,3]. We have grown Ni-TCNQ molecular network by simultaneous deposition of Ni and TCNQ molecules on Graphene/Ir(111) at elevated temperatures. The prepared samples were structurally characterized in-situ using RT scanning tunnelling microscopy (STM) and by low energy electron microscopy (LEEM). The X-ray photoelectron spectroscopy (XPS) was utilized to verify the chemical bonding of the Ni atoms.

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Minimum layers for graded-index porous silicon anti-reflective coating

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Porous silicon (PSi) is an inorganic photonic crystal known for its tunable physical and optical properties. This led to a multitude of studies investigating its potential for waveguide, biosensing and anti-reflective coating. Current limitations on its fabrication is the realization of thin PSi due to the innate constraints of electrochemical etching and the restricted porosity range of silicon. This study aims to formulate a method of optimizing the number of layers to approximate a desired low reflectance curve within the boundaries of the current experimental results. The setup includes a slab of 1 micrometer thick silicon substrate with varying porosity from 25% to 75% following a linear refractive profile. The incident light of wavelengths from 400 to 700 nm was directed 0 to 90 degrees normal to the surface of the slab. The angular and spectral reflectivity of different slabs with increasing number of layers was calculated and compared using Mathematica. It was found that the minimum layers for angular and spectral reflectivity was 28 and 45 respectively. The designed graded-index with significantly less number of layers and porosity variation was shown to be comparable to the anti reflective performance of an ideal GRIN film.

Optical transitions of spherical and spheroidal core-shell semiconductor quantum dots

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The electronic transitions of core-shell semiconductor quantum dots were calculated using a model of effective mass approximation, having the thin shell a higher band gap than the semiconductor forming the core. Stepped infinite spherical and spheroidal quantum wells were used in the calculations, where the step inside the infinite quantum well is originated due to the band gap difference between two compound semiconductors type 1. It has done a lineup calculation of the band-offset between mismatched interfaces based on the solid model theory. The calculations were compared with Photoluminescence peaks observed on samples of core shell nanocrystals. We have shown with this simple analytic model that is enough to explain the optical transitions of very good quality samples.

Study on surface potential of QD photodiode under illumination

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We have studied on the quantum dot photodiodes with the structure of Ag/MoOx/QD layers/ZnO/ITO/Substrate. In this presentation we focus only on the surface potential of the QD layers/ZnO/ITO which is part of the photodiode structure. Here the ZnO layer is for hole blocking layer (HBL) at the same time as electron transport layer (ETL). The surface potential of QD layers/ZnO/ITO was compared with QD layers/ITO to investigate the role of ZnO layer. Surface potentials were measured by Kelvin probe force microscopy (KPFM) under dark or light illumination conditions.

In the case of QD layers/ITO, the surface potential under the illumination was about 0.2 eV higher than that in the dark. While the surface potential of QD layers/ZnO/ITO under illumination increased to only 0.09 eV. Compared to QD layers/ITO, a relatively small increase in surface potential of QD layers/ZnO/ITO is attributed to the efficient transfer of photogenerated carriers on QDs to the ZnO rather than ITO. As a result, a QD photodiode 10 times faster than normal can be obtained.

2622-A-1902

Molecular-Viscous Vacuum Pump (MVVN)

Elena Svichkar, Vladimir Klyucharov

Based on the analysis of the basic principles of the operating of a high-vacuum oil-free evacuation system, depending on the operating conditions and the design of modern pumps, a molecular-viscous vacuum pump has been developed, which is an independent evacuation facility. MVVN is a new modern product.

The operating principle of molecular-viscous vacuum pump wet end involves molecules of gas, entering the channels of rotor and stator, getting extra quantity of motion against the channels in the exhaustion direction. Extra quantity of motion gas molecules receive from the rotating rotor, while the gas is moving through the stator channels. Due to the deceleration of the gas molecules on impact with stator, they receive extra quantity of motion. Dynamic pressure increment in the rotor channels converts into static pressure in the immobile channels of the stator. There is an increment of generated pressure over the entire length of the channel.

The pressure drop affects the gas particles in the direction, close to the normal direction to the channel, and the angular momentum is being transferred to the gas molecules in a direction perpendicular to the normal axis, i.e. in almost mutually perpendicular directions. The channels' impact on the gas molecules leads to the motion of gas molecules along a spiral.

MVVN is able to provide the evacuation of the vacuum systems in the pressure range of 105 Pa to 10^{-5} Pa and as a part of forevacuum stages of the combined TMP in the range from 105 Pa to 10^{-8} Pa.

Oxygen intercalation in graphene encapsulated metal nanoparticles probed by work function measurements

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Graphene encapsulated metal nanoparticles (G@NPs) have come into the focus of applied research, with potential applications in surface enhanced Raman scattering, lithium ion batteries and hydrogen storage solutions. Furthermore, G@NPs are systems that can be potentially used for catalysis under cover, where catalytic reactions take place in the nanocontainer formed by the graphene wall and the NP facets. The reactant and product molecules must pass defects of graphene to access and leave the nanocontainer, which modifies adsorbate entropies and mass transfer effects.

Direct measurements of intercalated atomic and molecular species are desired but still challenging. A suitable experimental method for detecting adsorption on metal surfaces in general is an analysis of work function (WF) changes. One example is the increase by +0.8 eV of the Pd(111) WF upon adsorption of oxygen. The idea is therefore to monitor changes of the NP's WF during an exposure with a reactant gas. In this contribution, it is shown that Kelvin probe force microscopy (KPFM) adsorption experiments sensitively reveal oxygen adsorption and intercalation phenomena on palladium NPs (PdNPs) and same NPs covered by graphene (G@PdNPs). Thanks to its spacial resolution at the nanometer scale and mV resolution in WF, KPFM yields accurate WF information at the single NP level. The experiments are strongly supported by density functional theory (DFT) calculations, which explain basic mechanisms of adsorption and related WF changes for pristine and graphene covered Pd(111).

2626-A-1902

Electronic Properties of Transition Metal Diborides Investigated by X-ray Spectroscopy and Calculations

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Transition metal-borides are known to exhibit interesting materials properties from super hardness to superconductivity with high thermal and chemical stability. These materials have the potential to be used for the next generation of hard, wear- and corrosion-resistant coatings. In particular, this is the case for diborides with an AIB₂ type of structure (Strukturbericht notation C32), where the B atoms form honeycombed, graphite-like sheets that are interleaved between hexagonal close-packed Zr atoms. From a combination of ab-initio electronic structure calculations and analysis with XPS, XRD, XANES, and EXAFS, the local chemical bonding structure and structural properties with atomic distances are investigated in epitaxial ZrB₂ films and compared to properties to those of the ZrB₂ compound target from which the film was synthesized as well as bulk Zr references. Epitaxial films are promising for property determination of diborides and future exploration of other material classes.

Reactive Magnetron Sputtering of ZnO:Al and application to ZnO:Al/Ag:Al/ZnO:Al structures

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The reactive rf magnetron sputtering using H₂:Ar plasma on ZnO targets leads to highly transparent and conducting films [1]. In this work aluminum-doped zinc oxide (ZnO:Al) films have been deposited by rf magnetron sputtering using different H₂:Ar mixtures at room temperature. Significant reduction in the resistivity of the films is observed due to the effect of hydrogen. The aim is to optimize ZnO:Al layers to be used in dielectric-metal-dielectric (DMD) structures. These DMD structures may replace the indium tin oxide (ITO) layers, which is the most widely used transparent conductive oxide (TCO) in the market, but is expensive due to indium scarcity.

DMD structures based on ZnO:Al/Ag:Al/ZnO:Al have been developed to be used as transparent contact in solar cells. The Al-doped Ag layers were deposited by co-sputtering. By doping with Al, very thin layers (below 10 nm) that are ultra-smooth and thermally stable can be obtained [2]. Analysis of DMD structures with different doping concentrations and thicknesses will be presented. Electrical characterization by four-point probe measurements and optical transmission spectroscopy are used to assess the suitability of the DMD structures as TCO, by using the Haacke figure of merit (FOM).

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Characterization of diamond-like carbon films prepared by bipolar-type plasma-based ion implantation and deposition

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Diamond-like carbon (DLC) films have attracted much attention because of excellent mechanical properties, such as high hardness, low friction coefficients and high wear resistance. However, the properties are strongly affected by the preparation conditions and methods. This means the presence of the widespread characteristics of DLC films. Therefore, it is important to understand the characteristics of respective films for suitable industrial applications when some preparation equipment is employed.

Plasma-based ion implantation and deposition (PBIID) is one of chemical vapor deposition techniques and has some advantages, such as high adhesion strength due to ion bombardment effect and the ability of 3 dimensional coatings. In this study, DLC films are prepared by a bipolar-type PBIID and the characteristics of the films are examined as a function of preparation conditions, such as negative pulse voltage.

DLC films are deposited on Si substrate using C₂H₂ gas and the characteristics are examined by Raman spectroscopy. Positive pulse voltage is kept a constant of +1.2 kV and negative pulse voltage is varied from -0.2 to -5.2 kV. Raman measurements suggest that structural disorder is increased with increasing negative pulse voltage up to about -1.0 kV and then decreased with further increase of negative pulse voltage. On the other hand, a similar trend is also observed in topological disorder. H content is increased from 20 to 50 % with decreasing negative pulse voltage, which is also estimated by Raman analysis.

Quantifying crystallinity in carbon nanotubes and its influence on mechanical behaviour

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The different fabrication methods that have been developed for making carbon nanotubes will provide materials with different levels of crystallinity. As crystallinity is qualitatively known to have a profound influence on material properties, this raises the need for standardised quantitative analysis.

Here we show how transmission electron microscopy and selected area electron diffraction can be used to provide quantitative information about effective crystallite sizes in individual nanotubes and how this can be linked to the mechanical behaviour of the tubes.

The crystallinity of arc-discharge grown tubes was found to be high enough for the crystallite sizes (about 20 nm) to exceed the circumference of the carbon nanotubes. This enables the formation of continuous graphene-like cylinders which constitute the walls of the tubes. In contrast, the crystallite sizes for commercial catalytically grown tubes were found to be notably small (only about 5 nm), and much smaller than the tube circumference, implying that here the walls are made from a patchwork of small graphene-like grains with different orientations.

The differences in atomic structure between high- and low-crystallinity tubes have profound effects on their mechanical behaviour, and thus one should really treat these as two distinctly different materials. This type of quantitative information, together with a classification system for different material qualities, will be vital for a successful utilization of carbon nanotube materials in applications.

Oblique deposition of nickel thin films by HiPIMS

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We study the microstructure and magnetic properties of 50 nm thick Ni films grown by high power impulse magnetron sputtering (HiPIMS) and compare it with films grown by dc magnetron sputtering (dcMS). All the films are deposited on the thermally grown silicon oxide substrate and thus are polycrystalline. It is shown that both methods present in-plane biaxial magnetic anisotropy at small tilt angles while larger tilt angles result in uniaxial magnetic anisotropy. However, the angle of transition for biaxial to uniaxial magnetic anisotropy is different when depositing using dcMS (35 degrees) and HiPIMS (60 degrees). Besides, the HiPIMS deposited films are magnetically softer than dcMS deposited films for all tilt angles. Our thickness uniformity test illustrates that HiPIMS deposited films are up to 40% more uniform than dcMS deposited films. Scanning electron microscope (SEM) images taken of the film cross section reveal that the HiPIMS deposited films consists of smaller grains compared to the corresponding dcMS deposited film. Both films' grains are elongated towards incoming flux although this is more pronounced in dcMS deposited films. X-ray reflectivity (XRR) measurements show higher mass density and lower surface roughness for HiPIMS deposited films. By increasing the tilt angle, the films deposited by both methods exhibit lower mass density and rougher surface.

Surface X-ray science analysis of large scale facility data using a scalable community-driven data-model

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The full acquired data sets from X-ray surface science experiments performed at large scale facilities occupy sizes typically exceeding the memory capacity of standard computer platforms[1]. The off-line analysis therefore often in practice involve complex data inspection and reduction procedures. A single generalized representation of the data would be beneficial, that could allow for efficient and flexible multiple data subsets extraction and analyses together with access to the full acquired data set. Surface X-ray analysis routines were developed based on an open-source and instrument agnostic data model (Universal Spectroscopy and Imaging Data (USID)[2]), implemented in python (pyUSID-framework[2], pycroscopy[3]). The USID-model represents n-dimensional data as two flattened dimensions, of which one is assigned to spatial dimensions. The data set is stored alongside ancillary and auxiliary data in the open standardized hierarchical format (HDF5)[4]. Classes and functions were implemented covering functionalities for conversion of time-resolved X-ray diffraction (XRD) data to USID, q-space-units based subsets extraction and XRD-analysis. Example surface-XRD data sets were analyzed on a standard computer with the pyUSID-based approach. pyUSID and the HDF5-interface allowed for flexible data subsets extraction and optional writing of associated extracted data subsets to a single hierarchical analysis structure, encapsulating all data sets and auxiliary data from the desired analysis workflow steps. pyUSID supports CPU-parallelization. The pyUSID-framework provide a computer platform performance adaptive data representation and structure with potential for efficient and flexible analysis of extensive size data sets from synchrotron surface X-ray experiments.

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Magnetic and structural properties of one-dimensional arrays of endofullerene single-molecule magnet peapods

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Rare-earth-based endofullerene nanomagnets belong to the group of single-molecule magnets (SMMs) [1], a class of molecules that exhibits intrinsic magnetic bistability at low temperatures. One such example is Dy₂ScN@C₈₀ which magnetic hysteresis and significant remanent magnetization with a relaxation rate of about 1 h at 2 K [2]. Here we present a study performed using high-resolution transmission electron microscopy (HRTEM), X-ray magnetic circular dichroism (XMCD), and ab initio calculation of one-dimensional chains of endofullerene Dy₂ScN@C₈₀ SMMs packed inside single-walled carbon nanotubes (SWCNTs). X-ray absorption measurements reveal that the orientation of the encapsulated endofullerenes differs from the isotropic distribution in a bulk sample, indicating a partial ordering of the endofullerenes inside the SWCNTs. The effect of the one-dimensional packing was further investigated by ab initio calculations performed for the structural analog Y₂ScN@C₈₀, demonstrating that for specific tube diameters, the encapsulation is leading to energetically preferential orientations of the endohedral clusters. In the case of endofullerene SMMs, a preferential orientation of the endohedral units implies alignment of the molecular anisotropy axis and magnetic ordering. These results, therefore, demonstrate the feasibility of forming ordered and well protected one-dimensional spin chains that could be addressed through the creation of SMM/SWCNT hybrid devices. Additionally, element-specific magnetization curves reveal a decreased magnetic bistability of the encapsulated Dy₂ScN@C₈₀ SMMs compared to the bulk analog.

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plasma-induced surface crosslinking of chitosan-acrylic acid hydrogel

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Hydrogels are three-dimensional (3D) materials composed of networks of hydrophilic polymers crosslinked physically or chemically. These materials can absorb large amounts of fluids and swell without dissolving [1]. In this study, chitosan (Cs) hydrogel was synthesized with acrylic acid (AA) and ammonium persulfate (APS) as the gelling agent and initiator, respectively. Initial results of x-ray absorption spectroscopy (XAS) shows that chitosan has 4 electron transition regions in its structure: 1s- π^* in olefinic and aromatic carbon (284 eV), 1s- π^* of C=C in ene-ketone (286.5 eV), 1s-3p σ^* in aliphatic carbon (287 eV), and 1s- π^* in the amide carbonyl (288.5 eV). Surface crosslinking will be further induced using an atmospheric pressure plasma (APP). Chemical structure of the synthesized chitosan-based hydrogel was characterized by synchrotron radiation based-Fourier transform infrared (SR-FTIR) analysis and baseline was corrected to determine different absorbance ratios. Using SR-FTIR, degree of deacetylation (DDA) of chitosan, which is 67.53 percent, was calculated based on the absorbance ratios of the 1463 cm^{-1} (-CH₃ deformation) and 1383 cm^{-1} (amide III) spectral bands, and using the equation recommended by literature [2]. The effect of the initiator was observed by determining the water uptake capacity (swelling ratio) of the hydrogels by gravimetric method. In addition, the effect of APP treatment times and working gases will be assessed using contact angle measurement and surface free energy calculations.

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Two-terminal multibit optical memory via van der Waals heterostructure

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Two-dimensional (2D) van der Waals (vdWs) heterostructures exhibit intriguing optoelectronic properties in photodetectors, solar cells, and light emitting diodes. In addition, these materials have the potential to be further extended to optical memories with promising broadband applications for image sensing, logic gates, and synaptic devices for neuromorphic computing. In particular, high programming voltage, high off-power consumption, and circuit complexity in integration have been primary concerns in the development of three-terminal optical memory devices. This study describes a multilevel non-volatile optical memory device with a two-terminal floating-gate field-effect-transistor with MoS₂/h-BN/graphene heterostructure. The device exhibits an extremely low off-current of 10^{-14} A and high optical switching on/off current ratio of over 10^6 , allowing for 18 distinct current levels corresponding to more than 4-bit information storage. Furthermore, it demonstrates an extended endurance of over 10^4 programme-erase cycles and a long retention time exceeding 3.6×10^4 s with a low programming voltage of -10 V. This device paves the way for miniaturization and high-density integration of future optical memories with vdWs heterostructures.

Si dopant incorporation in MBE-grown InAs nanowires

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Recently, semiconductor nanowires (NWS) have drawn attention due to their exceptional optoelectronic properties and compatibility with current silicon-based technology. Thanks to their small diameter, they can accommodate a significant lattice mismatch and are efficient for strain relaxation without producing defects. A number of technically and scientifically interesting devices have been demonstrated using NWs, such as Field-Effect Transistors (FET), Light-Emitting Diodes (LED) or devices based on semiconductor-superconductor interface. However, for all device application, doping is crucial for achieving predictable electronic and optical properties and appropriate operation of opto-electronic components.

In our group, we aim to reach high doping concentrations for tuning plasmon resonance in InAs in infrared region, taking additional advantage of high mobility of charge carriers in this material. However, dopant incorporation turns out to differ significantly from bulk material, as the dopants tend to segregate close to the surface (which is common for many nanoscale systems). Moreover, it is natural to expect the mechanism of dopant incorporation into the growing nanowire being dependent on the nanowire growth conditions.

In this contribution we reveal effect of Si incorporation in InAs NWs on their crystal structure and optical properties. InAs NWs are fabricated in MBE chamber by two approaches: selective area epitaxy growth and gold catalysed growth. Synthesized nanowires are studied by TEM, XRD and Raman scattering. Furthermore, FTIR measurements are presented which allow to detect plasmon resonance in infrared spectral range and, indirectly, the doping level achieved.

Supported aerosol nanoparticles for catalysis: design, durability and activity

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Nanoparticles are widely used as catalysts because of the high surface-to-volume ratio and high surface energy. In addition, the catalytic properties are highly dependent on the size, shape and crystallinity of the nanoparticles, as well as on the support onto which the nanoparticles are deposited [1]. Conventional nanoparticle catalysts rarely possess the control needed to understand the, often complex, kinetics of nanoparticle catalysis. This understanding is crucial in order to use the influencing factors to control and optimize the reactivity and selectivity of catalytic reactions [2].

We develop highly controlled catalytic nanostructures by combining nanoparticles produced by an aerosol method, which enables freedom in terms of material, size and crystallinity [3], with designed nanostructured supports. We have also performed an extensive study of the durability of the catalytic chips under catalytic conditions which is important in order to maintain the control over the structure, but also for the catalysts to be re-usable. This study resulted in a map of compatible environments for the catalysts, as well as guided the development of the design for more durable catalysts.

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Bandgap Renormalization in CsPbBr₃ Perovskite Quantum Dot/MoS₂ Heterostructure via Charge Transfer at Room Temperature

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Many-body effect including mutual exchange and strong Coulomb interactions in monolayer transition metal dichalcogenides shrinks the intrinsic bandgap, originating from the renormalization of electrical/optical bandgap, exciton binding energy, and spin-orbit splitting. This phenomenon has been commonly observed at low temperature and requires high photon excitation density. Here, we present bandgap renormalization at room temperature via charge transfer in type-II heterostructure of MoS₂ monolayer and CsPbBr₃ perovskite quantum dots. The bandgap renormalization can be further elevated by photoexcitation of perovskite to promote the plasma screening effect in MoS₂. This yields the redshift of A exciton energy by 82 meV, which is the highest bandgap renormalization at room temperature. Our hybrid structure by directly provoking the electron transfer from perovskite to MoS₂, under minimal photoexcitation density, suggests possibilities in reducing the optical/electrical bandgaps in MoS₂ towards near infrared region. This will help realize practical devices for solar cell, photo-detector and LEDs.

fabrication and characterization of polyaniline-chitosan hydrogels

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Biomaterials are designed to improve healthcare devices and services. However, these materials are often expensive. This study utilizes polyaniline-chitosan (PAni-Cs) composites, which are among the low-cost biopolymer composites, to synthesize PAni-Cs hydrogels. Chitosan is naturally abundant mucopolysaccharide commonly used for biomedical applications since it is a biopolymer known to be non-toxic, biodegradable, and biocompatible. Polyaniline, classified under conducting polymers, is one of the most promising biomaterial because of its intrinsic electrical conductivity, good stability, and easy preparation and modification. Based on the simple processability of polyaniline and chitosan, fabricating polyaniline-chitosan hydrogels through a combination of the two as a cost-effective biomaterial is certainly possible. Hydrogels are polymeric chain networks which are able to retain water in three-dimensional networks due to its hydrophilicity. In this study, PAni-Cs composites were prepared via in situ polymerization of aniline, with varying aniline-to-acetic acid ratio (2:8 and 8:2), in the chitosan solution and crosslinked via gamma irradiation at a dose of 15 kGy. Preliminary characterization tests were done. FTIR results showed that characteristic peaks at 1638 cm⁻¹ and 1560 cm⁻¹, attributed to -NH and -NH₂ bending, are present to all PAni-Cs samples. Contact angles of the samples were observed to decrease significantly as polyaniline was increased in the composite where the measured angle for the pure chitosan, 2:8, and 8:2 samples were 115.97, 31.37, and 3.9 degrees, respectively. Degree of swelling, UV-Vis spectra, and the wettability of the samples will also be determined.

Optimization of Spindt-type emitter cathode shape prepared by high power pulsed magnetron sputtering: The effect of template cavity dimensions

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The Spindt-type emitter is one of the vacuum electron emitters which is prepared using the semiconductor-manufacturing technologies [1]. Its cathode, which should be sharp for efficient electron emission, is fabricated by the film deposition inside the microcavity structure with a hole on its ceiling. By aligning the direction of the depositing atoms along the substrate normal, the modest closure of the hole by the film is achieved and the sharp cone structure is formed inside the cavity. We have tried to deposit molybdenum by using high power pulsed magnetron sputtering and determined the optimum condition to form the sharpest emitter cathode shape [2]. However, in those deposition conditions, the deposited films had strong compressive stress which frequently resulted in the delamination of films and/or the deformation of the cavities. In this study, we first tried to suppress the stress by using different discharge gas. By sputtering the Mo layer by Kr, we successfully reduced the compressive film stress, but the obtained cathode structure was not sharp enough. Secondly, we attempted another approach to fabricate the sharp cathode structure by optimizing the cavity structure. It was found that the larger hole diameter and the shallower cavity depth, the sharper emitter could be fabricated. With these results, it is expected to fabricate a sharp cathode enough to work with a practical emitter within the conditions where the films do not delaminate.

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spectroscopy and electrical conductivity of polyaniline-chitosan (PAni-Cs) composites produced via solution casting method

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The biopolymer chitosan (Cs) has important biological properties such as biocompatibility. However, the applications of Cs are restricted due to its low electrical conductivity [1]. Cs is incorporated with conductive polymers like polyaniline (PAni) to enhance its electrical conductivity [2]. Many studies have been done on the electrical properties of PAni-Cs composites synthesized using crosslinking agents or in situ polymerization. However, this study is the first to report on the electrical properties of PAni-Cs composites produced via solution casting method, which is simpler and cheaper compared to previous synthesis methods. In this work, PAni was mixed into chitosan solution until blended together. Spectroscopic properties and electrical conductivity were investigated through Fourier Transform Infrared (FTIR) and Ultraviolet-Visible light (UV-Vis) spectroscopy, and two-probe method. Pure PAni, pure Cs, and PAni-Cs films were prepared. The FTIR spectra of pure PAni and PAni-Cs films suggested that electrons move due to the aromatic rings and conjugated systems in the structure. IR spectra of the pure Cs film implied that hydrogen from the amine and alcohol groups interact with the nitrogen atoms of the PAni via H-bonding. These movements of electrons make PAni-Cs conductive. UV-Vis spectra of PAni-Cs showed a broad electronic transition indicating PAni and Cs interaction. Two-probe method showed a conductive PAni-Cs film greater than Cs. Since PAni-Cs offers good conductivity, this biocomposite has potential for diverse applications such as biosensors, drug delivery systems, and wound seals.

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Synthesis and Characterization of Polyaniline-Chitosan Composite Film

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Composite materials are prepared from the combination of two or more different materials with distinct characteristics. The aim of a composite material is to exhibit properties which are distinct and hopefully superior to its constituent materials. In this study, polyaniline, an intrinsic conducting polymer which is known for its simple synthesis, will be combined with chitosan which is a widely used natural occurring polymer in the biomedical field to produce a Polyaniline-Chitosan (PAni-Cs) composite films. Over the years, strong acids such as hydrochloric acid are utilized to synthesize polyaniline. In view with this, the polyaniline to be used in this study will be synthesized using a weak doping agent, acetic acid. The composite films will be synthesized with varying chitosan and polyaniline concentrations via solution casting method with an experimental design of 2^k . The synthesized PAni-Cs films will be characterized via Synchrotron Radiation based - Fourier Transform Infrared Spectroscopy (SR-FTIR). The microscopic images generated by the SR-FTIR revealed that synthesized composite film have incorporated a nanowire structure of polyaniline in the chitosan films. The nanowire-like structure seen in the microscopic images have characteristic adsorption bands at around 1560 cm^{-1} and 1500 cm^{-1} which corresponds to the C=N stretching vibrations of quinonoid and C=C stretching vibrations of the benzenoid unit ring respectively. The presence of these peaks suggests that the nanowire-like structure incorporated in the synthesized film is PAni. The synthesized PAni-Cs films will be subjected to cell viability assay which will evaluate the film's potential for biomedical applications.

Mapping of charge distribution by Kelvin probe force microscopy on graphene field effect transistor at controlled relative humidity

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The Kelvin probe force microscopy (KPFM) allows to image the surface potential (SP) at nanometer scale which can be used to study graphene field effect transistor (FET) during its operation at controlled relative humidity (RH). These observations are important due to a high influence of water on graphene FET based on back-gated graphene/SiO₂/Si systems. It has been shown that the surface conductivity of silicon dioxide system exponentially increases with the relative humidity as a consequence of higher water coverage ratio which can influence the performance of graphene FET [1].

The graphene Hall bar structure for the measuring of KPFM was fabricated on the silicon (100) substrate with a 280 nm thick layer of a thermal SiO₂. The KPFM measurement of the graphene Hall bar structure was done in NTEGRA Prima, NT-MDT with the humidity chamber to perform the changing of humidity. We have studied the SP of graphene Hall bar and surrounding insulating SiO₂ layer during current flowing through the main channel. We have also measured the influence of applied gate voltage on the graphene Hall bar with the focus on charge leakage from the graphene into surrounding SiO₂ layer.

We would like to use the graphene Hall bar as a sensor for sensing the relative humidity and as a tool for the measuring the water bridge formation between the tip of the atomic force microscopy and the surface of the graphene.

enhance the true intrinsic spectral signals of suspended and pristine two-dimensional materials

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The properties of two-dimensional (2D) materials are readily affected by their surroundings. Therefore, the underlying substrates and surrounding materials always disturb the pristine properties of 2D materials. Herein, we describe how the pristine properties of suspended 2D materials can be precisely extracted from Raman and photoluminescence (PL) spectra with great signal enhancements by taking advantage of both air gap suspension and nanocavity enhancement effects. The modes of the Raman emission lines were enhanced to almost the same degree when the 2D materials were positioned over the nanocavity: the 2D/G peaks of suspended single-layer graphene (SLG) and the E_{12g}/A_{1g} peaks of MoS₂ were significantly enhanced almost equally. Moreover, recording Raman and PL spectra at different positions of the suspended 2D materials was a very powerful tool for observing charge transfer between the pristine 2D materials and the surrounding materials. We also found that the residual holes of the suspended SLG could be neutralized by aluminum (Al) at certain positions. By employing the air cavity structure, we could readily locate the charge neutrality point of the suspended 2D materials. In addition, the PL intensity of MoS₂ could be greatly enhanced when using the same nanocavity. The great enhancements in the PL signals from the suspended 2D materials allowed us to further investigate the spectral weights of both the A₀ exciton and A-trion peaks when MoS₂ was suspended or supported upon various metal films.

DFT study of gallium and water adsorption on free-standing graphene

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The adsorbents on graphene can give rise to interesting physical properties. Using density functional theory (DFT) calculations, we investigate influence of the gallium atoms and water molecules on the electronic properties of free-standing graphene. Especially, we focus on the shift of Fermi level position. These calculations are made to support in-situ transport property measurement performed on graphene field effect transistor (FET) structure. The gallium atoms are used to tune the graphene electronic properties related to plasmonic applications, and the interaction of water molecules and graphene is interesting due to graphene applications in biosensors.

In case of low coverages, the Ga atoms are adsorbed individually and they sit in a center of the graphene hexagon. For higher coverages, the Ga atoms start creating clusters. The most stable arrangements of clusters are in form of 3D structures over planar arrangement of atoms. The DFT results show a switch of doping behavior for higher Ga concentration (over 0.5 monolayer). It is caused by creation of clusters.

In case of water molecules, the adhesion energy between the water molecules and neutral or ionized graphene is studied together with the electronic property impact. These results can highlight the mechanism of resistance response and creation of hysteresis in ambient and water solution graphene based biosensors.

Electrical properties of CVD graphene covered by gallium atoms

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The graphene layers have been intensively studied because of their interesting electrical and mechanical properties. A deeper understanding of the interactions between graphene and metallic particles and semiconductor materials is important for successful implementation of graphene based systems into complex semiconductor devices. The knowledge of the relationship between the deposition conditions and physical properties of prepared films plays a crucial role in the fabrication of more complex electronic devices. A promising possibility can be utilization of gallium atoms. Gallium is a sp-metal that forms predominantly ionic bonds with graphene. It means that there is not a strong hybridization between the pz orbitals of graphene and valence electrons of Ga. Also, a weak bonding charge yields a minimal distortion of the graphene lattice. Furthermore, Ga and carbon atoms are insoluble, a characteristic that preserves the graphene structure. Ga may even produce a catalytic effect in preserving and reconstructing the sp² structure of graphene. The influence of adsorbed Ga atoms on transport properties of a graphene layer under different conditions of deposition (substrate temperature, deposition rate, etc.) has been studied in-situ. We have observed a Dirac point (DP) shift during Ga deposition at a substrate temperature of 50°C. In addition, the relationship between transport properties and surface topography of Ga on graphene will be discussed. The surface properties have been studied by analytic methods such as AFM, SEM, XPS and HRTEM.

Study on silicon carbide based metal oxide semiconductor capacitor with magnetron sputtered ZrO₂ high-k gate dielectric

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A silicon carbide (SiC) based two terminal metal oxide semiconductor (MOS) capacitors with magnetron sputtered zirconium oxide (ZrO₂) as a high-k dielectric material using titanium (Ti) gate has been synthesized at room temperature. The structural, morphological and compositional analysis of the dielectric layer has been carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM), Atomic force microscopy (AFM), energy dispersive spectroscopy (EDS) and X-ray photoelectron spectroscopy (XPS). The current-voltage (I-V) and capacitance-voltage (C-V) characteristics of MOS capacitor were studied at room temperature by applying the dc bias gate voltage swept from -3V to 3V for both, high and low-frequency operation using semiconductor parameter analyzer. The thermal stability of the MOS capacitor is of critical importance for use in the fabrication of electronics for deployment in extreme environments. Hence, the effects of post-deposition annealing (PDA) temperatures (200 -1000 °C) on the electrical properties of MOS capacitor have been investigated. MOS characteristics of Ti/ZrO₂/SiC/Ni capacitor were correlated with structural and morphological properties of an insulating dielectric layer at different PDA temperatures. It has been observed that a synergetic contribution of lowest effective oxide charge, semiconductor-oxide interface-trap density and total interface-trap density improve the electric breakdown field of MOS capacitor for PDA samples.

Transparent electronics using one binary oxide for all transistor layers

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The growing demand for transparent conducting oxides (TCO) has been driven by the fast-growing markets of flat panel displays, solar cells, smart windows, light-emitting diodes, and sensors. Many researchers have been focusing on the enhancement of the electrical properties of alternate TCOs to replace ITO due to the limited supply of indium and its increasing cost. In this work, we developed a novel process in which thin film transistors (TFTs) comprising one binary oxide for all transistor layers (gate, source/drain, semiconductor channel, and dielectric) are fabricated in a single deposition system at low temperature (160 °C). By simply changing the flow ratio of two chemical precursors, C₈H₂₄HfN₄ and (C₂H₅)₂Zn, in an atomic layer deposition system, the electronic properties of the binary oxide ($\text{Hf}_x\text{Zn}_{1-x}\text{O}_{2-y}$) or HZO were tuned from conducting, to semiconducting, to insulating. Furthermore, by carefully optimizing the properties of the various transistor HZO layers, all-HZO thin film transistors were achieved with excellent performance on both glass and plastic substrates. Specifically, the optimized all-HZO TFTs showed saturation mobility of $\sim 17.9 \text{ cm}^2/\text{V}\cdot\text{s}$, a low subthreshold swing of $\sim 480 \text{ mV}/\text{dec}$, high $I_{\text{on}}/I_{\text{off}}$ ratio of $>10^9$, and excellent gate bias stability at elevated temperatures. In addition, all-HZO inverters show high dc voltage gain (~ 470), and all-HZO ring oscillators show low stage delay ($\sim 408 \text{ ns}$) and oscillation frequency of 245 kHz. Our approach presents a novel, simple, high performance, and cost-effective process for the fabrication of indium-free transparent electronics.

Reference:

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2670-A-1902

Surface modification of sputter deposited monoclinic WO₃ thin film for scaled electrochromic behavior

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Here, we have reported the electrochromic properties of highly ordered monoclinic WO₃ nanoporous thin film grown directly on the indium tin oxide glass (ITO) coated glass substrate using DC magnetron sputtering in a reactive environment (Ar:O₂) at room temperature. To achieve the nanoporous-nanocrystalline behavior of the active material, a thermal treatment (250°) was given to the active material, which modified the compact film surface into nanospheres. This surface modification is responsible to alter the physical, optical and electrochromic properties of the active material. The physical properties of the active material were characterized in detail using X-ray diffraction, scanning electron microscopy, atomic force microscopy, and energy-dispersive X-ray analysis. The optical and electrochromic behavior of the active electrode material was analyzed using UV-Vis spectroscopy and cyclic voltammetry. The proposed device revealed large optical modulation, high reversible redox behavior and good cyclic stability at least upto 1000 cycles. The proposed This electrochemically active architecture allow one to fabricate the device for energy harvesting applications at an elevated temperature. Our work indorses human comfort with financial benefits and plays a crucial role in "green nanotechnology".

Structural and optoelectronic characteristics of co-sputtered ZnWO₄ thin films prepared by sputtering method

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In the present work, thin films of zinc tungstate (ZnWO₄) of different thickness (50-500 nm) have been fabricated on silicon (Si) and glass substrates at 300 °C by direct current (DC) magnetron reactive co-sputtering from Zn and W target in the Ar+O₂ reactive atmosphere. Film thickness was changed by regularly increasing the deposition time, keeping all the other deposition parameters constant. The influence of film thickness has been studied for their structural, morphological, optical and electrical properties using standard characterization techniques. A spectroscopic ellipsometry (SE) was used to probe the optical constants (refractive index n and extinction coefficient k) over the wavelength range of 246-1688 nm, thickness and bandgap of the investigated films. The experimentally observed SE parameters have been fitted by four different dispersion model for the best fit. The packing density of the samples is discussed using Lorentz-Lorenz analysis. The non-linear optical parameter (χ^3 and n^2) of the samples have been also calculated by using Tichy and Ticha relation rather than expensive Z-scan.

2673-A-1902

Three-terminal Hot Carrier Nanowire Devices

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Three-terminal Hot Carrier Nanowire Devices

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In the era of nanoscale electronics, investigations of hot carrier transport are important for realization of next-generation electronic/quantum devices. Nanowires have proven to be ideal for bandgap engineering and thus they offer the possibility of designing quasi-one dimensional potential landscapes through tuning of material composition along the length of nanowires during the growth [1].

In this work, we engineered the band structure of InAs_{1-x}P_x nanowires (InAs/InP: conduction band offset ~ 600 meV) to be able to define a ramp-like potential profile in the conduction band. The ramp-like carrier injector together with an energy filter (an InP-based barrier) in nanowires were grown with various separation lengths (L_{I-F}) followed by 3-terminal nanowire device fabrications to realize the hot carrier transport experiments. Electrical measurements (at room temperature) demonstrate the hot carrier transport as a function of L_{I-F}. Based on fitted line (See figure 1 in abstract pdf file), the estimated relaxation/coherence length of the hot carriers is in the order of 220 nm.

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Surface characterization of nanowire-based coalesced GaN layers for wafer development

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In this study we investigate the use of nanowire crystal properties and their 3D geometry to introduce an alternative method in which a coherent GaN-layer is coalesced from an array of nanowires. The current method sees two potential advantages over previous research: dislocation filtering, inherent to the nanowire growth-step, and a coalescence-step appreciably closer to thermodynamic equilibrium than conventional MOCVD-growth.

The typical structures investigated are based on a hexagonal array of GaN nanowires, selectively grown on a GaN/Al₂O₃ substrate. The structures are further comprising a GaN shell layer. The sample is annealed in an NH₃-rich atmosphere, in order for the 3D-structures to spontaneously reform and coalesce into a single, monolithic GaN planar layer. This reformation-step is consequently driven by differences in surface energy between the facets of the 3D-structures, in contrast to conventional MOCVD where crystal growth is enabled by elevated gas-phase concentrations of source material.

Morphology and electrical properties of coalesced GaN film is studied by atomic force microscopy and its derivatives. Kelvin probe microscopy is used to map the surface potential where we distinguish between the nanowire core (higher potential), shell (150mV below), and the coalesced layer (250mV below the core level). Good correlation is found between the growth structure, the local charge carrier distribution as obtained by scanning capacitance microscopy, and optical properties as observed by cathodoluminescence. We identify dislocations and inversion domain boundaries, relate them to the growth parameters, and show how improved growth parameters strongly reduce their number.

Iron-oxide based Nanoprobe for Magnetic Resonance Based detection of Cardiac Troponin T

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Myocardial infarction (MI) is one of the most common causes of death worldwide. The prognosis of the patient highly depends on the time between onset of MI and the start of treatment. Hence, it is very important to correctly and within short time differentiate between patients with acute MI and patients with less threatening conditions. Here we present a new sensor technology with potential for early point-of-care detection of MI. The tissue damage caused by MI leads to release of biomarkers for MI such as cardiac Troponins, cTn. Serum concentrations rise slowly following MI and high sensitivity troponin detection is needed to identify early cases of MI.

Our sensor system is based on 5 nm superparamagnetic iron-oxide nanoparticles (Fe-NPs) coupled to cardiac Troponin I antibodies (anti-cTnI) using EDC/sulfo-NHS coupling chemistry. The resulting size is measured by Dynamic Light Scattering (DLS). The coordination of cTnI to the anti-cTnI bound to the Fe-NPs is investigated with both DLS and relaxivity. Fe-NPs are used as contrast agents in Magnetic Resonance Imaging, MRI, due to their ability to induce relaxation. The ability of Fe-NPs to induce NMR relaxation allows the sensor to detect the interaction between cTnI and anti-cTnI on the Fe-NPs. In the near future, this will hopefully enable quantification of the amount of cTnI in the MI patient's blood. The design of the Fe-NP probe and cTnI binding to the probe involves several molecular parameters that requires detailed characterization. These effects on the iron-oxide based nanoprobe will be presented in this contribution.

Surface Modification of Polyurethane Sponge with Functionalized Silica Nanoparticles to Combat Oil Spills

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In this study, a nanoparticle-modified porous medium was used as a filter to remove oil from water phase. For achieving this purpose, we employed a polyurethane sponge as a porous medium. Unmodified sponge absorbs both oil and water phases at the same time. By TMCS-functionalized silica nanoparticles as surface modifier agent, and phenol-formaldehyde resin as the sticker agent, the wettability of absorber has altered from neutral wettability to strongly oil wet condition.

At the first stage, wettability of sponge was determined using contact angle measurement. Afterwards, unmodified silica nanoparticles was subjected to surface modification with TMCS, and then dispersed in the base fluid (i.e. Ethanol) using ultrasonic apparatus. Then, phenol-formaldehyde resin solution was prepared to stick nanoparticles onto the pore walls. The next stage was to coat the pore walls with produced solution containing nanoparticles and the sticker, and then drain the sponge. After coating the sponge, contact angle measurements and absorption efficiency was evaluated. The results demonstrated that the absorption time for oil phase was decreased from 5 seconds to less than half a second. Water contact angle measurements also showed an increase in contact angle from 74° to 133°. The resultant sponge was able to absorb oil phase spontaneously and could be used as a filter for oil removal from the water phase.

The coating method is also a controversial subject. Here, cost effective dip coating method was employed to coat pore walls with nanoparticles. SEM images prove that this method successfully coated pore walls throughout the sponge.

Transrotational crystal growth in thin amorphous films: “vacuum epitaxy” for lattice-rotation nanoengineering

Vladimir Kolosov

Exotic thin crystals with unexpected transrotational nanostructures [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films of different chemical nature (oxides, chalcogenides, metals) prepared primarily by vacuum evaporation methods. We use TEM bend-contour method [2] combined with selected area electron diffraction. HREM, AFM and optical microinterferometry were used in due cases (preferentially for correlative microscopy).

The unusual phenomenon was also traced in situ in TEM column during local e-beam heating or annealing: regular internal bending of crystal lattice planes in a growing crystal. It is dislocation independent. Such transrotation (translation of the unit cell is complicated by small rotation realized round an axis lying in the film plane) can result in strong regular lattice orientation gradients (up to 300 degrees/ μm) of different geometries: cylindrical, ellipsoidal, toroidal, saddle, etc.

The possible mechanisms of the phenomenon are discussed. Initial amorphous state and surface nucleation of the crystal growth are most essential factors. The last fact accompanied by anisotropy of crystal growth rate and obvious tendency for regular change of interatomic distances of the crystal propagating from the surface layers inside the bulk material resembles specific epitaxy, “vacuum epitaxy”. The transrotation phenomenon is the basis for novel lattice-orientation/rotation nanoengineering of functional, smart thin-film materials suitable also for strain nanoengineering. Transrotational micro crystals have been eventually recognized by different authors in some thin film materials vital in applications, e.g. phase change materials (PCM) for memory [3-5].

New model for the amorphous films is proposed.

Asymmetric Post Shapes for enhanced particle sorting in microfluidic DLD devices

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Deterministic Lateral Displacement (DLD) has been an established technique for precise fractionation of particles in continuous flow. Typically, the sorting device comprises of an array of vertical posts with circular cross sections, wherein the array design determines the flow behaviour of the particles. In recent years, some studies have attempted to characterize the flow behaviour of particles in arrays with alternate post shapes. The current work presents a systematic study of sorting dynamics in DLD arrays employing L-shaped posts, supported by dissipative particle dynamics (DPD) simulations to predict quantitative associations among post dimensions, array parameters, particle size and sorting dynamic.

We show experimental validation of the predicted sorting behavior of DLD arrays with L-shaped posts, at different array parameters. In contrast to circular post arrays, a difference in particle flow dynamics is observed due to asymmetry in post shape in flow axis. Further we observe the presence of mixed-modes in DLD with L-shaped posts.

For a given array parameters, it is possible to lower the critical diameter of a DLD array, by using L-shaped posts, while eliminating the need for smaller gaps or posts. Further, L-shaped posts present the advantage of asymmetry in flow axis in the system, thereby accentuating the flow hysteresis.

2699-A-1902

Design and application of an inert stagnation detector for sticking measurements of highly reactive gases.

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An inert stagnation detector that simplifies sticking measurements of highly reactive gases like halogens under UHV conditions has been constructed. The principle is based on the King and Wells beam reflectivity method. The inert detector is more than 500 times more sensitive to Cl₂ compared with the standard King and Wells set-up with an unmodified quadrupole mass spectrometer mounted in a stain-less steel vacuum chamber. In the first part of this work, the detector performance is demonstrated by measurements of the initial sticking coefficient for the reaction of Cl₂ with evaporated K films. In the second part we show how the inert detector is applied in a molecular beam scattering experiment where it has to be moved away from the molecular beam to give space for other scattering experiments.

2701-A-1902

Microfluidic softness sorting of cancer cells

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Due to their direct association with the physiology of cancer cells, physical properties are especially attractive as markers for sorting and characterization. Where molecular surface markers are lacking, the physical properties can instead serve as inherent markers for separation. Indications that soft cancer cells are more metastatic than hard cells make mechanical properties of specific interest. Our work provides a deeper understanding of deformability based sorting based on deterministic lateral displacement (DLD) and will be used to optimize DLD devices for the characterization and fractionation of cancer cells into subpopulations with different mechanical properties. Our aim is to develop a device to help oncologists gain more accurate prognoses and better monitoring of the effect of treatment.

2702-A-1902

Vacuum acceptance testing of integrated cryomagnetic dipole and quadrupole modules of the SIS100 synchrotron at FAIR

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The series production of both the cryomagnetic dipole as well as the cryomagnetic quadrupole modules for the new SIS100 heavy ion synchrotron at FAIR in Darmstadt, Germany, is currently under way and is projected until 2021 (dipole modules) and 2023 (quadrupole modules), respectively. Concurrently, the series production of the dedicated, cryogenically cooled dipole and quadrupole ultra-high vacuum chambers is in progress. After meticulous integration of the vacuum chambers into the corresponding magnet cryostats, during which a multitude of challenging mechanical tasks have to be performed, final vacuum acceptance testing of the insulation vacuum as well as the beam vacuum system of the cryomagnetic modules will assess the suitability for use in the SIS100 synchrotron. The procedures of the complex interplay between production, integration and final vacuum acceptance testing are presented where key aspects will have to be conducted by external partners like industrial contractors and associated institutes.

Robust Superhydrophobic/Superoleophilic Nanomaterial Coated Porous Medium for Selective Separation and Expulsion of Oil Pollutants from Water

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Oil spills have caused significant environmental and ecological problems. Therefore, the development of methods for effective decontamination and cleanup is necessary for the protection of the environment and human health. The use of 3D porous materials for oil removal in oil industry has a long history, but with surface modification of these materials in the first of 21st century, new approaches for surface modification was introduced. However, Obtain a robust method for oil removal and water purification is challenging in oil industry.

Metal organic frameworks (MOFs) are used in various applications including hydrocarbon, Hydrogen, and CO₂ storage and also drug delivery. In this study, a polyurethane sponge was used as the porous medium. As a robust and novel hydrophobe coating agent, new class of MOFs (ZIF-8) was first synthesized, and then was coated on wall surfaces of porous medium with PDMS polymer using dip-coating method. This sponge was then coated with functionalized nanoparticles is used for expulsion of oil contaminant from water continuously.

Contact angle measurement results before and after coating with nanoparticles prove that wettability of the sponge has altered to strongly oil-wet conditions. Also SEM images before and after coating proves that pore walls have coated with nanoparticles. In addition, EDAX results from different points of porous medium proves that our nanomaterials are well coated on the wall surfaces and altered its wettability. Its high oil sorption capacity and positive environmental footprint makes it ecologically friendly sorbent for oil spill cleanups.

Stability of Materials and Interfaces for Perovskite Based Optoelectric Devices

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Hybrid perovskites (HPV) have recently emerged as highly efficient optoelectronic materials and are currently being intensively investigated as alternative active layer materials for photodetectors, light-emitting diodes, laser devices, sensors and X-ray detectors, among others. Since HPV are direct band gap materials with high optical absorption coefficients ($\sim 10^5\text{cm}^{-1}$) the majority of publications have been dedicated to hybrid organic-inorganic solar cells with certified efficiencies over 20%. However the realization of a long-lasting device implies the understanding of chemical and structural stability of HPV materials and their interface with electron and hole transport layers (ETL and HTL, respectively). This presentation will show detailed XPS analyses of the the chemical stability of the transition metal and transition metal oxides with ABX₃ hybrid perovskites for A=MethylAmmonium (MA), B=Pb, and X=Cl, I, and Br. HTL/HPV interface is not trivial as the reactivity of halogen group elements forms an unstable high resistance interlayer at the charge transport layer interface compromising the optimum operation of the device. The electrical characterization and work function measurements will be discussed and correlated to the chemistry and crystalline structure of the materials of interest.

Highly Selective UV Bandpass Filters by Double-Plate Metamaterials

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Metamaterials(MMs), defined as materials which are not existing in nature, are artificial materials providing unobservable characteristics in nature, including negative refraction, perfect absorption and perfect transmission. Especially, optical metamaterials have been shown to offer a number of useful properties, such as enhancement and control of spontaneous emission, chemical- and bio-sensing and nonlinear optical control and manipulation. Recently, the ultraviolet (UV) becomes more important wavelength range for various applications such as astronomy, cosmology, communications, and biological applications. The more interest in UV applications is, the more precision UV optical components are required. Particularly, for imaging and spectroscopy, the development of wavelength-selective filters that can be directly integrated on silicon detectors and operate in the 200–400 nm range is essential.

In this study, we investigated metamaterials for highly selective UV bandpass filters in wide UV range between 100 nm and 400 nm. Numerical simulation shows that three types of UV MM composing of periodic ring pattern on both side of dielectric substrate allow specific wavelength with narrow bandwidth at UV-A, UV-B and UV-C regime, respectively. On the basis of numerical predictions, we fabricated UV filters by nanoimprint lithography. As a result, we found that narrower and sharper bandpass filter at UV regime can be achieved by dual-layered MMs assembled by two pieces of identical MM filter, while a single-layered MM shows relatively broadened transmission peak.

RGB bandpass filters based on optical metamaterials

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Metamaterials (MMs) can be designed to possess remarkable electromagnetic properties including negative, zero/low, and high indices of refraction. These emergent properties, make it possible for independently manipulating the refractive index and the intrinsic impedance, will enable novel optical design strategies with the potential to either greatly improve the performance of existing devices or to introduce entirely new device functionality. Recently, red, green, and blue (RGB) filters are essential for achieving ultra-high-definition(UHD) television utilizing organic and/or quantum dot. One of requirements on getting the RGB filter is to exhibit an extremely steep cutting edge and narrow bandwidth. It is very difficult to achieve the requirements with a conventional multilayered bandpass filter mainly due to high product costs. Alternatively, by introducing metamaterial concept, inexpensive method for realizing highly selective RGB filter could be potentially made because unique properties of metamaterial.

Here, we theoretically and experimentally demonstrated red, green and blue bandpass filter based on optical metamaterials. The MM-based RGB filter is composed of a tri-layer structure consisting of a metallic-dielectric-metallic layer. Each metal layer on dielectric substrate has a lateral periodic open circle structure and the dependence of optical transmission on periodicity and size of the circle was investigated in this study. Furthermore, multiple-stacked MM-based RGB filters is turned out to demonstrate much enhanced performance in terms of full width-half maximum without any change of center wavelength and optical density.

Influence of reduced baking time of Taiwan photon source front-end system on dynamic pressure

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The Taiwan photon source (TPS), a synchrotron accelerator at the National Synchrotron Radiation Research Center in Taiwan, is a third-generation accelerator operating at 3 GeV that was designed to create a high energy photon source. The TPS front-end (FE) systems are located between the storage ring and beamline, which was designed to protect the safety of users as well as control experimental requirements. As the FE vacuum pressure influences the storage ring and beamline vacuum pressures, the FE vacuum systems must maintain a low dynamic pressure. Therefore, at the beginning of FE system construction, each FE vacuum system is baked at 200°C for 24 hours. Next, when the FE systems need to be upgraded or maintained due to vacuum interventions, it must also be baked for 24 hours to recover a low dynamic pressure. However, the 24 hour baking process requires manpower support on-site owing to facility safety in the TPS tunnel. The maintenance of the FE systems takes two duty days. Therefore, reducing baking time is necessary in the TPS facility. The beam cleaning efficiency after reduced baking time has been described in this paper.

FeO on Ag(111): Growth, structure and work function determination

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Noble metals and bulk oxides are well-known catalysts of many industrially-relevant chemical reactions. Recently, much attention has been paid to the studies of ultrathin oxide films grown on noble metal single-crystalline supports. It is well-established that such systems exhibit properties that differ from those of the corresponding bulk materials. We studied the growth and structure of ultrathin iron oxide (FeO) films on Ag(111) using scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and x-ray photoelectron spectroscopy (XPS). The results obtained by us and other groups show that the structure of FeO films on this particular support critically depends on the films' preparation conditions. The performed scanning tunneling spectroscopy (STS) dI/dz measurements indicate that FeO islands have a higher work function than clean Ag(111), which may have implications on the catalytic properties of this system.

Acknowledgements

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2DEG formation in doped polytype InP nanowires: an optical study

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2D electron gasses (2DEG) are common phenomena in electronic components, like High Electron Mobility Transistors (HEMTs) [Sze, 2006]. They are often realized by modulation doping heterostructures, which are often plagued by unwanted side effects, like strain and compositional intermixing [Sze, 2006]. With the realization of crystal phase control in the growth of nanowires [Joyce, 2010], it opens up the possibility to create heterostructures made from the same materials but different crystal phase. These polytype heterostructures are atomically sharp with minimal strain [Panse, 2011]. In many III-V semiconductors, like InP, the hexagonal Wurtzite (WZ) crystal structure forms a type-II band alignment with its bulk form: Zinc-Blende (ZB) [Mattila, 2006].

In the presented work we have investigated InP nanowires with a single WZ-ZB interface. We compared the power-dependent photoluminescence (PL) signal of nanowires with a sulfur(S)-doped WZ segment with the PL of undoped WZ-ZB heterostructured nanowires. The power dependent PL energy shift of the type-II recombination, characteristic for such band structures [Vainorius, 2014], spans a larger energy range for the undoped nanowires compared to the n-doped nanowires. This indicates the formation of a 2DEG in the triangular well at the wz-zb interface, similar to those found in the aforementioned electronic components.

A nano-scale analytical approach to the investigation of the heterogeneous oxidation of thermally aged cross-linked polyethylene insulated cables used in nuclear power plants

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Operational third generation nuclear power plants (NPPs) were engineered foreseeing an average operational lifetime of 40 years. However, given the growing need for sustainable energy sources and the delays in fourth generation commercial reactors deployment, it is now considered necessary to extend their operation up to 60 years (in Europe). Therefore, the potential effects of ageing over core plant structures need to be properly assessed and managed. One of the critical components for safe operation of NPPs is the electrical cabling system. Artificial ageing, by means of thermo-oxidation, of polymeric insulation jackets is routinely performed in order to assess end-of-life materials characteristics. Practical constraints inducing high temperatures/short times ageing treatments lead to strong influence of diffusion-limited oxidation (DLO) mechanisms that cannot be accounted for assuming a simple "Arrhenius-like" behaviour of volume-averaged mechanical and chemical properties. Therefore we propose an experimental approach exploiting analytical techniques capable of resolving chemistry and physical parameters at the length scales relevant for DLO.

Commercial cables and reference polymeric materials have been thermally aged in various DLO conditions. Cross sections of aged samples were analysed using a variety of chemical analysis techniques such as Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS), X-ray photoemission Spectroscopy (XPS) and Fourier-transform infrared spectroscopy (FTIR). The cross sections were also analysed by nano indentation to derive the local mechanical properties after ageing. The combination of the 2 approaches with a few micrometer resolution contributes to the understanding of the thermal ageing process and the possible DLO effect.

Microscopic investigation of the lateral distribution of surface potentials

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Due to contamination and crystal orientation of single grains each real metal surface is not an equipotential. If two metal plates are brought close together, these inhomogeneities in the surface potentials can interact with each other and, for example, disturb the linearity of capacitive displacement sensors. This is known as patch effect. The formation and the characteristics of such patch potentials needs to be investigated.

The Kelvin Probe Force Microscopy (KPFM) is used to simultaneously study the topography and distribution of surface potentials. The lateral resolution depends on the KPFM mode selected. Therefore, measurements are first performed on a reference semiconductor heterostructure (BAM, Sample 4-1) in air. The amplitude-modulated mode and the frequency-modulated mode are compared.

In the next step, gold arrays are deposited on aluminum with different widths. The large difference in their work function (Al: 4.06 eV – 4.41 eV, Au: 5.10 eV – 5.47 eV) makes this material combination very suitable for the simulation of the patch effect.

Finally, the surface potentials of ultra-precision diamond-turned electrodes of capacitive sensors are changed by an etching process. The change of the surface potentials as a function of the etching time is investigated.

The study will provide more information about the measurement and change of surface potentials in order to quantitatively determine the influence of the patch effect on capacitive displacement measurements in further experiments.

Correlation between elastic properties and lattice thermal conductivity of GeTe and Ge₂Sb₂Te₅ by surface Brillouin scattering.

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In this work, the correlation between elastic properties and lattice thermal conductivity of the phase-change alloys, GeTe and Ge₂Sb₂Te₅, in the amorphous phase is presented. Films of thicknesses in the range 50-500 nm were prepared by RF magnetron sputtering at room temperature. The structural properties of the as-deposited films were analysed by Rutherford backscattering spectrometry (RBS), x-ray reflectivity (XRR) and Raman scattering. The surface acoustic modes of these alloys were measured by Surface Brillouin Scattering (SBS). Analysis of the phonon dispersion curves from SBS measurements using the least squares fitting procedure and the Green's function method [1], yields two independent elastic constants, C₁₁ and C₄₄. The results suggest that GeTe films are more elastically stiffer than Ge₂Sb₂Te₅ films. The Cahill's Model [2] was used to determine the minimum lattice thermal conductivity which was found to be lower in Ge₂Sb₂Te₅ compared to GeTe. This is desirable for improving thermal management and data retention in phase-change random access memory (PRAM) devices during programming.

Influence of interfacial states on ZnO/GaN based schottky barrier UV photodetectors

MONU MISHRA, GOVIND GUPTA

Gallium Nitride (GaN) and Zinc Oxide (ZnO) are well established wide bandgap semiconductors absorbing the UV-C radiation of the electromagnetic spectrum. ZnO/GaN heterostructures owing low lattice mismatch, high exciton energy and complimentary material properties open new avenues for the future of next generation optoelectronics. Ultraviolet photodetectors based ZnO/GaN heterostructure are expected to yield optimum efficiency however their performance has remained low due to various challenges associated with interfacial properties. Interfacial properties/states such as band offset, fermi level pinning, localized charge density and defect states associated with overlayer (i.e. ZnO) thickness lacks sufficient investigation and led to degradation of device performance. The disparity and anomaly amongst reported values of valence band offset (VBO) at ZnO/GaN interfaces has been an underestimated issue hampering the optimization of photodetector efficiency. Therefore, in the present report, we have fabricated ZnO/GaN heterostructure (with variable ZnO thickness) based schottky barrier photodetectors and investigated the dependence of photosensitivity & other device parameters on interfacial states/properties. We have witnessed a peak responsivity & detectivity and a high speed photoswitching associated with the band offset, barrier height & defect states at the ZnO/GaN heterojunction having ZnO thickness of 8 nm. The underlying scientific phenomenon (e.g. interfacial dipole strength, charge accumulation etc.) leading to perturbations & discontinuities in interfacial/electronic states were discussed in detail.

The DFT study of optical and thermoelectric properties of N-doped TiO₂

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TiO₂ is widely studied for a range of important applications. In this work we focus on photocatalyst and thermoelectric device applications of TiO₂, important because environmental pollution has become a big problem in a number of countries, including Thailand. A huge amount of waste heat and wastewater is released into the environment, resulting in air and water pollution. Using renewable energy is an attractive option for treating these pollutants, i.e. wastewater treatment by photocatalysts, and conversion of heat to electrical energy via thermoelectric materials are very interesting. However, because of its large band gap (E_g), TiO₂ is active only under UV illumination. To enhance its performance under solar light, and make it a visible-light-sensitive photocatalyst, the band gap of TiO₂ should be reduced, which is achievable by its doping with N. It is important to explore how the density of states (DOS), band structure and E_g , all of them affecting the thermoelectric and optical properties, will behave if oxygen atoms are partly substituted by nitrogen. Vienna Ab initio Simulation Package (VASP) and BoltzTraP codes were employed to calculate DOS, band structure and thermoelectric properties of TiO₂ and N-doped TiO₂, under generalized gradient approximation in the scheme of Perdew–Burke–Ernzerh (PBE), with Hubbard parameter U . The results show that N has important effects, enabling one to engineer the DOS and band structure of TiO₂, favorably changing its E_g and thermoelectric properties. Therefore, it is expected that N-doped TiO₂ is a candidate for a good visible-light-sensitive photocatalyst and thermoelectric material.

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Effect of hydrodynamic cavitation and advanced oxidation processes on treatment alkyd resin wastewater for its reuse opportunities

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In recent years, an increase in the pollutant concentration, the presence of suspended particles, and the recalcitrant organic molecules in the liquid effluent, which cannot be removed by the conventional biological treatments. This has resulted in a constraint for the growth & sustainability of the chemical industry. Hence, it is of paramount importance to introduce newer technologies to partially degrade these recalcitrant compounds which can then undergo biological treatment subsequently or can be mineralized completely & the water can either be reused or safely discharged. The current work focuses on the treatment and reuse opportunities of alkyd resin wastewater. Alkyd resin industry produces large volumes of wastewater that comprise bio refractory chemicals like phthalic acid and its esters in very high concentrations. The effect of the combination of hydrodynamic cavitation and advanced oxidation processes on the mineralization behavior of alkyd resin wastewater containing pollutants is studied. Controlling pH played a vital role in tuning the process. The advanced oxidation processes utilized here are ozone and hydrogen peroxide and their combination. The combination treatment technology was assessed on the basis of electrical energy consumption per unit mass of TOC removal (kWh/kg) [EEM] values.

study of Interfacial Reaction and structural Properties of HfSiO/Si Film Gate Dielectric Prepared by RF Sputtering Deposition

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Abstract

Interfacial reactions in HfSiO/Si structures have been studied for as-deposited and annealed films. For this purpose, ultra-thin (~8nm) and 20nm HfSiO films were deposited on Si substrates by radio frequency reactive sputtering in argon-oxygen mixtures. The microstructure of HfSiO films is analyzed by X-ray photoelectron spectroscopy (XPS) with Ar⁺ sputtering, and a careful assessment of chemical states is carried out for their precise identification. The results show that the HfSiO film is a mixture of hafnium silicate and hafnium dioxide, and an interface layer is formed during the deposition process. In addition, SiO₂ and Si-Ox (silicon sub-oxides, x<2) are produced near the Si substrate due to interfacial reactions. After 30 minutes thermal annealing at 600 °C, the decomposition of hafnium silicate is observed on the surface of the ultrathin HfSiO films (~8nm), producing large amount of Si-Ox. However, the decomposition reaction becomes weaker near the Si substrate, and the interfacial layer is thermally stable in direct contact with silicon. Compared with annealing effects on the 20nm HfSiO films, thermal instability of the ultrathin HfSiO films on the surface is influenced by the Si substrate. It is further observed that the migration of silicon at high temperature is likely responsible for the reaction on the surface during thermal annealing process.

Green synthesized silver nanoparticles for deterioration sensing in fruit's post-harvest spoilage

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In the sub-Saharan African countries, post-harvest food spoilage is the main cause of global food shortage, rather than the under-production of food. Tools for the rapid detection of spoilage in fruits like banana (*Musa acuminata*) would help alleviate the losses caused by postharvest deterioration during the storage period. In the present study, silver colloidal nanoparticle (AgNPs) solution synthesized using the wet biomass (cell pellets) of *Bacillus subtilis* was applied as a colorimetric sensor for the compound released during banana deterioration. The green synthesized silver nanoparticles solution was confirmed by UV-Vis Spectrophotometer and characterized by Scanning Electron Microscope (SEM), X-ray Diffractometer (XRD) and Fourier Transmission Infrared (FT-IR). The initial reddish brown colour of the silver nanoparticle solution changed to light brown after four days and finally turned transparent after ten days of exposure to the deteriorating banana. Concurrent analysis of the resulting solution by UV-Vis spectroscopy agrees with our study of AgNPs as a colorimetric biosensing agent which displayed specificity and selectivity for 1,2-Benzenedicarboxylic acid, bis (2-methyl propyl) ester that was released during the period of banana deterioration. The easy detection of crop deterioration for the control of food spoilage will be helped by applying a colorimetric sensor as shown in this study.

Radiation and Thermal Chemistries of Organotin Cluster Based Extreme Ultraviolet Resists

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Our recent efforts to study organotin compounds as extreme ultraviolet (EUV) resists have leveraged surface science approaches, where we have focused on characterizing both radiation and thermal induced processes. A benefit of organotin clusters as EUV resists is that they can incorporate high absorption coefficient elements (e.g., Sn) and radiation sensitive ligands (e.g., butyl groups) to improve photoresist sensitivity while providing high contrast. In this presentation, we are investigating a butyl tin-oxo Keggin cluster-based EUV photoresist. The goal of these studies are to better understand both surface chemistries and patterning mechanisms. The thermal and radiation induced chemistries were initially studied using temperature programmed desorption and electron stimulated desorption. We have found that the butyl ligands are thermally stable up to ~650 K. However, low energy electrons, with energies comparable to the electrons expected during a EUV exposure, lead to the homolytic cleavage of the carbon-tin bond. We have further characterized the clusters using ambient pressure X-ray photoelectron spectroscopy to evaluate processes occurring during exposure to radiation. Studies performed in different ambient conditions, and photon energies, have shown large effects on the radiation induced chemistries, where a significant enhancement in carbon decay was observed for O₂ pressures up to 1 torr. These studies provide a means to better understand radiation induced processes that result in the solubility contrast of these materials, and may guide in the development of improved EUV photoresists for nanolithography.

Sniffer helium leak primary traceability

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The helium sniffer leaks are used for calibration of the helium leak detectors configured for the sniffing mode. In this mode, the leak detector sucks the surrounding air in the probe. Typical flowrate of this suction is 1 ml of gas per second.

To get a traceable reading of the leak detector, the sniffer leak outlet helium flowrate (typically $2E-5$ ml/s) has to be calibrated. This article describes one possible primary method of ensuring this traceability. The described procedure is based on the indirect comparison of helium leaks using the helium leak detector as comparator. The comparison is done by the comparing of the unknown leak rate from the sniffer leak and the known leak rate calculated from the suction flowrate and the inlet helium concentration. The low helium concentration (20 ppm level) is achieved by the three-step gas dilution system in this work.

The article describes the used procedure and components and analyse the main uncertainty sources.

The presented method is not dependent on the concrete gas. In the same above described way, it may be used for helium as well as for hydrogen, SF₆, refrigerants etc.

Few atomic layer MoS₂/InP heterostructure solar cell

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Presently the global warming effect is causing us to seek for the renewable energy alternatives for our everyday life. The huge population around us is stressing to search for the long lasting, clean and affordable energy resources. Solar energy is clean, renewable, abundant in availability and is affordable to the mankind. Now, it is the need of hour to focus our attention towards the solar cells as an energy generators to fulfill the modern tech savvy lifestyle. It is the most promising technologies that directly convert solar light into electricity. In order to be able to apply solar cells to practical applications that should meet the three factors of efficiency, stability and low cost of production. TMD materials are able to absorb up to 5-10% of incident sunlight in less than 1 nm thickness to achieve an order of magnitude higher solar light absorption. Metal organic chemical vapor deposition (MOCVD) was employed to obtain atomic layered MoS₂ on SiO₂/Si substrate which subsequently transferred on InP substrate using a simple transfer protocol. We realized photovoltaic operation in atomically few-layered MoS₂ by forming a type II heterojunction with low doped p-InP, instead of widely used p-Si. The built-in electric field arised due to interface between n-MoS₂ and p-InP heterojunction is beneficial for the photogenerated carrier generation and separation. The solar cell device could achieve a power conversion efficiency of 0.11% with 1.87 mA/cm² current density, first attempt of TMD based solar cell on InP substrate, demonstrating a promising solar cell performance. The obtained results pave the way for the integration of TMD materials with the InP substrate to obtain efficient solar cells.

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study on vacuum leak calibration technology based on static expansion primary vacuum standard

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Constant conductance gas flowmeter is commonly used to generate known gas flow. In general, the inlet pressure of the flowmeter is measured by capacitance diaphragm gauge (CDG) or spinning rotor gauge (SRG). In this work, static expansion primary vacuum standard was applied to generate a standard pressure. This can reduce the uncertainty introduced by the inlet pressure measurement and the combined relative standard uncertainty is 0.88%. A vacuum leak with a leak rate of 10⁻¹⁰ Pa·m³/s (at 23 °C) is calibrated by static commulative comparison method.

Atomically controlled growth of high current interest functional semiconductor systems.

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Growth of GaN films with high quality interfaces to SiC wafers by atomically controlled co-deposition of Ga reacting with atomic N produced by microwave excitation of nitrogen gas is reported.

All the steps and processes involved require very high temperatures (ca. 900 – 1000). To obtain atomic control and high-quality interfaces, depositions at very low deposition rates have been used. This work is focused on surface and interface studies using high-resolution photoelectron spectroscopy with photon energies optimizing the surface sensitivity, and/or the photoelectric cross sections. Thus, maximum of information about as many aspects of the growth processes and structure of the systems, is provided at the new ASTRID II facility (high brilliance and stability). The growth processes are characterized in-situ by photoelectron core-level and valence band spectroscopy).

As is well known, these systems need a buffer layer of Al. However, the focus of this work is to understand the process at the very first atomic layers at all interfaces, initiating the study without using a buffer layer. Results of direct GaN deposition on SiC at very low deposition rate without the AlN buffer will be reported.

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Hard gap hybrid materials for stronger topological superconductivity

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In-situ growth of hybrid semiconductor-superconductor materials have received increasing attention due to their proposed ability to host topological superconductivity in one and two dimensions. To enter the topological regime four main material requirements must be present. Namely, quasi one-dimensional conductance (in for instance a nanowire), strong spin-orbit interaction, large Landé g-factors and induced superconductivity.

In this study we explore new material combinations and crystal phases to find materials with enhanced properties for a variety of quantum transport experiments. We perform electrical transport measurements and investigate induced superconductivity, spin-orbit interaction and reproduce experiments that are believed to indicate the presence of a topologically protected state.

We investigate ternary III-V semiconducting materials by magnetoconductance measurements on axial-heterostructures with varied group V flux ratios and find a compositional dependent spin-orbit interaction. Specifically, we show that epitaxial InAsSb/Al interfaces allow for hard induced superconducting gaps and $2e$ transport in Coulomb charging experiments and find measurements consistent with topological phase transitions at low magnetic fields due to large effective g-factors.

The ternary structure allows for control of the spin-orbit interaction based on the Sb/As ratio, which is a parameter

that cannot be controlled in binary nanowires. Finally, new superconducting materials have been tested. We discuss which of these hybrid combinations could provide a new platform for transitioning into the topological regime and thus hosting Majorana zero modes.

Vacuum Leak Location in Spacecraft Structures Based on Acoustic Emission

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With rapid increasing of the space debris, the possibility of orbiting spacecraft collision by space debris grows with time. In order to assess, detect and locate the orbiting spacecraft gas leakage and ensure the safety of astronauts, it is important to study a new method for vacuum leak location in spacecraft structures. In this paper, firstly, the characteristics of acoustic emission signals generated by vacuum leak is introduced. The signals have a wide frequency band between 100Hz and 500kHz and signal parameters are closely related to leakage aperture. As the frequency of pump running noise is below 20 kHz, the acoustic emission signal with frequency between 20 kHz and 500 kHz is used to detect and locate the vacuum leak. Secondly, the reflection and transmission of acoustic emission signals by vertical stiffeners is analyzed. Many stiffening members such as ribs, stringers, and the integral stiffeners are used in spacecraft structures. Different signal models have different stop-bands for transmission. At Last, a new method to locate the leak based on Beam-forming is given, the leak location accuracy is better than $\pm 100\text{mm}$ when the leak rate is more than $1\text{Pa}\cdot\text{m}^3/\text{s}$. This method can meet the needs of leak detection for the spacecraft on orbit.

Surface Science Of Catalysis Research In Nano-X

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Vacuum Interconnected Nanotech Workstation (Nano-X) is an integrated research platform for nanoscience and nanotechnology research, with capabilities for material growth, device fabrication, characterization and test in the same vacuum interconnected workstation. All major facilities in Nano-X are interconnected by ultrahigh vacuum tubes. The transfer and exchange of samples among different facilities can be realized in ultrahigh vacuum (or atmosphere controlled environment) to solve the sample contamination issues.

Comprehensive understanding of catalytic process requires multi-scale research methods. NANO-X is a promising example to illustrate the advantage of integrated or interconnected analytical instruments in catalysis research. As each characterization tool can only provide specific and partial information, while taking advantage of an array of characterization systems interconnected by ultrahigh vacuum tubes, multiple characterization can be performed on a single sample excluding the contamination step through air. And these tools may not all provide in situ characterization, but through vacuum interconnection, together with in situ techniques will drive our understanding of catalysis as it goes.

Nano-X is jointly established by Suzhou Institute of Nano-Tec and Nano-Bionics (SINANO), Chinese Academy of Sciences (CAS) and the local governments in Suzhou, Jiangsu Province. The facilities in NANO-X are fully open to the world, extensive and in-depth collaboration with us are always welcome.

In this presentation, some primary results performed in a NAP-XPS/STM combined system will be introduced, including molecular intercalation at h-BN/Pt(111) interface, structure transformation of iron oxide on Pt(111) under near ambient pressure, and in-situ monitoring the chemical state of zinc oxide in methanol synthesis reaction.

Narrow gap spintronics and electron g-factor engineering

Antonio Ferreira da Silva, Marcelo Alejandro Toloza Sandoval

Narrow gap bulk semiconductors are one of the main trends in semiconductor spintronics, in view of the strong dependence of the electron effective g-factor on the energy gap material [1]. In addition, semiconductor nanostructures provide a fertile ground to tune the effective g-factor, combining bulk properties with mesoscopic quantum confinement effects. We investigate the effective g-factor and its anisotropy for bound electrons in semiconductor nanostructures formed by coupled InSb active nanolayers, with CdTe tunneling barriers, using an accurate analytical multiband envelope-function solution based on the Kane model [2]. With respect to the growth direction, longitudinal and transverse configurations for the external magnetic field are considered and the corresponding effective g-factors obtained in first order perturbation theory. We analyze the diagram for the electron g-factor anisotropy within the space spanned by the two structural parameters, i.e., the CdTe and InSb layer thicknesses. Interesting features are observed for thin active layers in strong interacting regime, as a critical point for which the anisotropy changes the sign and large negative anisotropies in the limit of extreme confinement.

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Tuning magnetic properties of [Co/Ni] multilayers with PtMn thin films and annealing processes

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Spin-orbit torque (SOT) induced magnetization switching that does not require an applied magnetic field has been reported for structures with antiferromagnetic/ferromagnetic (AF/FM) bilayers. This magnetic switching can be achieved by using the exchange bias effect between an AF and a FM multilayer with a perpendicular easy axis. To this end, the interplay of magnetic properties between coupled AF and FM layers play important role for device applications; especially in spintronic devices. In this study, the structures of these multilayers made by different post-deposition field and thermal processes, and the resultant magnetism have been investigated. Ag (8 nm)/[Co (2.5 nm)/Ni (2.5 nm)]₂/PtMn (3 to 32 nm) thin films were prepared on amorphous SiO₂ substrates by using a dual ion-beam sputtering deposition technique [1]. The reference [Co/Ni]₂ multilayers are magnetically soft at room temperature with a coercivity $H_c = 20$ Oe. However, the characteristic of exchange bias between the AF/FM PtMn/[Co/Ni] layers is revealed at 100 K by an enhanced coercivity $H_c = 900$ Oe as well as exchange bias field $H_{ex} = -150$ Oe under field cooling processes. The temperature dependent magnetization indicated that the FM [Co/Ni] moments were influenced by coupling to different PtMn thicknesses.

The results of annealing changed the structural phase ordering of the AF PtMn and influenced the exchange bias as well as tuned the magnetic anisotropy of the FM [Co/Ni] multilayers.

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Growth of millimeter-size cvd graphene single crystals using height-confined reaction cavity

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In conventional chemical vapour deposited (CVD) polycrystalline graphene, adsorptions on grain boundaries introduce severe electron/hole scattering, which degrades the physical properties of the material. Through nucleation density control in a graphite reaction cavity, high-quality graphene single crystals can be grown over large areas. The graphite reaction cavity mimics the Cu-enclosed configuration [1] where sublimated Cu atoms are effectively trapped, thus increasing the Cu vapour pressure inside the cavity. In this way the roughness of the growth substrate is reduced by Cu re-deposition. Contrary to the Cu-enclosed configuration, our approach does not damage the catalyst substrate and allows upscaling graphene growth on flat Cu foils of arbitrary size. We used a secondary height-controlled sapphire cavity to accommodate the substrate inside the primary graphite cavity and release trace amounts of oxygen that oxidize the Cu substrate and reduce the nucleation density [2]. The oxygen concentration at the Cu surface was further controlled by ex-situ pre-oxidation of the substrate. Using e-beam lithography multiple graphene transistors are patterned and measured sequentially within a single mm-sized crystal. A detailed map of the electronic properties of the single crystal is thus obtained with sub-micrometre resolution. The structure of the graphene single crystal is further elucidated by atomic resolution Transmission Electron Microscopy measurements.

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probing intermolecular and molecule-substrate interactions at angstrom scale by ultrahigh vacuum tip-enhanced raman spectroscopy

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Conventional spectroscopic techniques are limited by the optical diffraction limit to about half wavelength and therefore offers about 200 nm X 200 nm microscopic zone for working in the visible light range. Tip-enhanced Raman spectroscopy (TERS) emerges as an advanced analytical technique, where the plasmonically active probe is not only used to detect the tunneling current but also to interrogate the local chemical environment of surface adsorbed molecules with angstrom scale precision. In TERS, the incident laser irradiation is focused at the tip apex which excites localized surface plasmon (LSP) polaritons and causes the electromagnetic enhancement at the tip-sample junction. In this work, we report a topological and chemical analysis of two porphodilactone regioisomers (positional isomers) by scanning tunneling microscopy (STM), ultrahigh vacuum (UHV) TERS on Ag (100) with the spatial resolution down to 8 Å, which has wide range of applications in various field of surface science & nanotechnology such as regioselective catalysis reaction, chemical reactions, molecular electronics etc. We have shown, it is possible to distinguish these two structurally very similar forms with high accuracy & precision. Furthermore, these new class of porphyrinoids i.e. porphodilactones have been studied on different single crystals to probe the surface sensitive interactions. This work demonstrates STM combined TERS is a complementary technique to characterize a system completely at the angstrom scale.

LABEL FREE OPTICAL DETECTION OF DNA USING MICROFLUIDIC PLATFORM

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The combination of the unique optical properties of gold nanoparticles (GNP) with their high stability, high surface area-to-volume ratio and facility for biomolecules conjugation resulted in the development of label free DNA detection platforms. An important key factor when using GNP immobilization on substrates is to maintain their optical features. GNP can be immobilized based on: direct formation of GNP on the surface or deposition of pre-formed GNP onto the surface. The latter offers an inexpensive alternative for deposition of GNP. High surface densities without aggregation are tricky to obtain and for low surface coverage the extinction peak can be too low and the peak sharpness might compromise sensing suitability. Therefore, in order to intensify the optical signal a microfluidic cell was designed to assembly multiple substrate/GNP simultaneously, for DNA detection.

GNP (spheres and nanorods) were electrostatically and covalent immobilized on a glass substrates. GNP/Glass, showed a maximum extinction peak at 532 ± 1.8 and 633 ± 8.3 nm, in buffer. The thiol modified DNA was introduced in the flow cell containing the GNP/Glass at a flow rate of 1 μ L/sec. DNA binds to the GNP causing a change in the refractive index of the surrounding media inducing a red peak shift. To track the DNA hybridization events the shift of the maximum extinction peak is monitored in real time. The simultaneous measurement of up to four GNP/Glass substrates increases 4-fold signal intensity.

This microfluidic platform allows fast analysis, low sample, label-free and great potential for achieving high throughput DNA hybridization detections.

Surface Science Of Catalysis Research In Nano-X

Yi Cui

Vacuum Interconnected Nanotech Workstation (Nano-X) is an integrated research platform for nanoscience and nanotechnology research, with capabilities for material growth, device fabrication, characterization and test in the same vacuum interconnected workstation. All major facilities in Nano-X are interconnected by ultrahigh vacuum tubes (10^{-8} Pa in main tubes). The transfer and exchange of samples among different facilities can be realized in ultrahigh vacuum (or atmosphere controlled environment) to solve the sample contamination issues.

Comprehensive understanding of catalytic process requires multi-scale research methods. NANO-X is a promising example to illustrate the advantage of integrated or interconnected analytical instruments in catalysis research. As each characterization tool can only provide specific and partial information, while taking advantage of an array of characterization systems interconnected by ultrahigh vacuum tubes, multiple characterization can be performed on a single sample excluding the contamination step through air. And these tools may not all provide in situ characterization, but through vacuum interconnection, together with in situ techniques will drive our understanding of catalysis as it goes.

In this presentation, some model catalysis' results performed in Nano-X will be introduced, including molecular intercalation at h-BN/Pt(111) interface, structure transformation of iron oxide on Pt(111) under near ambient pressure, and in-situ monitoring the chemical state of zinc oxide in methanol synthesis reaction.

Field emission properties of carbon nanotube cathode grown on different substrates

Detian Li, Huzhong Zhang, Xiaoqiang Pei, Yongjun Wang, Yongjun Cheng

In this work, field emission characteristics of carbon nanotube films grown on different substrates, including stainless steel, silicon and stainless steel both coated by catalyst layer, by chemical vapor deposition were investigated. The results show that the carbon nanotube films grown on substrates having catalyst layer are vertically aligned to the substrate surfaces with extremely high density, uniform height, together with small diameter. However, the carbon nanotube films directly grown on stainless steel substrate have a random orientation, and the resultant carbon nanotubes have large diameter. The present carbon nanotube films grown on different substrates exhibited excellent field emission properties, including low turn on and threshold fields, high emission stability and repeatability, especially for the ones grown on stainless steel with and without catalyst layer. What is more important is that the carbon nanotube films directly grown on stainless steel substrate have remarkable long-term stability with ~3.4% fluctuation over 50 h continuous measurement under high current density, ~10 mA/cm², which are mainly ascribed to low contact resistance and high adhered strength between emitters and substrate as well as good thermal conductivity and electrical conductivity of the substrate, which is conducive to promoting heat dissipation during field emission period, and hence minimizing the damage to emitters caused by Joule heating. The superior field emission properties of the as-grown carbon nanotubes are very promising for vacuum electric device application.

2838-A-1902

Nanostructure Si/SiO₂ by the magnetron sputtering

Toshio TAKEUCHI, Yoshiji Horikoshi

Nanostructured Ga₂O₃/SiO₂ by magnetron sputtering

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Ultrahigh vacuum radio frequency magnetron sputtering is a kind of qualified physical vapor deposition methods i.e.; a molecular beam epitaxial method and a pulsed laser deposition method. Gallium oxide based layered thin films and solid solution films are deposited by the ultrahigh vacuum radio frequency magnetron sputtering. Deposition parameters are substrates crystallinity, substrate temperatures, sputtering gas compositions, Basic properties are characterized by the optical properties and high-resolution photoelectron spectroscopy. Single layer Ga₂O₃ on the MgO substrate is discussed on the crystallinity and optical stoichiometry. Solid solution Ga_{2-x}Cu_xO₃ layer are discussed on the optical absorption edge energy. Nanostructured Ga₂O₃ and SiO₂ films are characterized with high-resolution photoelectron spectroscopy. The sputter depth profile of Si2p, Ga3d, Ga2p, O1s spectra with low accelerating voltage and with neutralizing beam indicated the preparation of nanostructured oxide films. The Ga3d and Ga2p spectra are most suitable and the can be used under the thickness of 20 angstrom. Nanostructured Si/SiO₂ quantum well films are prepared referring to the Ga₂O₃/SiO₂ film preparations

Nanodefects formation on graphene via oxygen/argon plasma treatment

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Graphene-based materials have recently become a promising candidate material in membrane technology due to its unique set of properties such as its 2D structure, high mechanical strength, and chemical reactivity, which allow modification processes to induce desired properties. In this work, we explore the effects of plasma treatment methods in creating nanopores in graphene. The materials studied were as-received commercial graphene on copper (graphene-Cu) and transferred graphene on polyethersulfone substrates (graphene-PES). A custom-built 13.56 MHz radio-frequency inductively-coupled plasma (RF-ICP) system was used to treat the graphene-Cu and graphene-PES samples. Using a remote plasma configuration, the samples were exposed to 1:10 O₂:Ar ratio gas admixture with operating parameters of 250 and 300 W RF powers and 3 and 5 sec exposure times. The Raman spectra of the samples allowed the determination of both the quality of the transfer process and plasma-treatment of graphene. Scanning and transmission electron microscopy (SEM/TEM) imaging were also performed to visualize and evaluate the porous graphene produced by plasma exposure. Raman spectra of graphene-Cu show that after plasma-treatment defects formed in the surface of the graphene. Raman spectral mapping found that defects are formed either only on a few or almost all regions depending on the plasma parameters used. Raman spectra of graphene-PES show successful transfer of graphene, and the spectra exhibited different graphene profiles. High-resolution imaging showed the pore size of the defects formed on the graphene to be in the nanometer range, and thus offer the possibility of use for nanofiltration and desalination applications.

analysis on the effect of polyaniline and Lactic acid concentration on the Polyaniline-Chitosan film flexibility

Bianca Rae Pasela, Acelle Pearl Castillo, Doebner von Tumacder, Ma. Roxan Abiquibil, Haidee Mana-Ay, Rhys Montecillo, Kathrina Lois Taaca

Flexible biosensors for point-of-care testing are advancing because of the powerful tools towards the monitoring and diagnosis of personal healthcare parameters. Polymer composites became a central part of polymer science and engineering as these have properties unattainable with homopolymers and statistical copolymers. Polymer composites have shown excellent mechanical function after being modified with reinforcements. In this study, a composite comprising of polyaniline (PAni), a conducting polymer and chitosan (Cs), a natural biopolymer, were synthesized via solution casting method with varying polyaniline and lactic acid concentration. The synthesized PAni-Cs films were characterized via Fourier Transform Infrared Spectroscopy (FTIR) and Universal Testing Machine (UTM). Characteristic peak of Cs was observed at around 3310 cm^{-1} and 2880 cm^{-1} corresponding to the stretching vibrations of NH_2 associated in primary amines and the stretching vibrations of C-H bond in the pyranose ring. The stretching vibrations in amide I, II, and II respectively is also observed in the spectra at 1400 cm^{-1} . The characteristic peaks of PAni were also observed in the PAni-Cs films. The C=N stretching vibration of the quinonoid ring and C=C stretching vibrations of the benzenoid ring at absorption peaks 1560 cm^{-1} and 1500 cm^{-1} were observed in the spectra of the composite films. The flexibility of the films showed that the tensile strengths at break of the films decreases and percent elongations increases when the lactic acid concentration was increased, however, increasing PAni content influences the films to brittle. Cell viability and effect of radiation exposure will be further evaluated to determine effect on developing composite-based biosensors.

Mesoporous NiO@TiO₂ Composite Nanostructures with Improved Durability against Electrochemical Degradation

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Nickel oxide (NiO) is the most exhaustively investigated transition metal oxide due to its high electrochromic (EC) efficiency, good cyclic reversibility, and low material cost.

The EC properties of materials are closely related to their morphologies and sizes. Therefore, there are many approaches about fabrication of NiO films having various morphologies. Among them, chemical bath deposition (CBD) method can produce hierarchical networked NiO films with high surface area. In addition, the n-type titanium dioxide (TiO₂) core/p-type NiO shell composite structure can enhance the separation of electron and proton.

In this study, meso/macro double-structured EC thin film based on hierarchically porous NiO and macroscopic TiO₂ nanobowl arrays was successfully prepared on ITO glass by CBD and polystyrene (PS) spheres monolayer assisted solution process. Obtained film exhibits a 2 dimensional honeycomb structures with highly porous NiO layer. Compared to the NiO nano flake film, NiO/TiO₂ nanobowl composite shows better EC performance with larger optical modulation, high coloration efficiency as well as improved durability against number of on/off cycling. In addition, effect on the EC performance according to the pattern size of TiO₂ nanobowl arrays was investigated by controlling the diameter of PS sphere. Smaller pattern size represents the high surface area which allows the electrolyte to penetrate easily and shortens the diffusion paths resulted in faster response time.

2852-A-1902

Transition of excitations and interlayer relaxation in two-dimensional synthesis CuxS/MoS2 heterostructure

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Transition of excitations and interlayer relaxation in two-dimensional synthesis CuxS/MoS2 heterostructure

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The stacking of dissimilar 2D materials introduces new functionalities in material engineering to produce novel structures with specialized properties. In this work, the vertical heterostructure of CuxS and MoS2 nanosheets is synthesized by sulfurization of pre-deposited metal films, which prevails interlayer coupling effect in phonon, photon, and electrons-holes pairs. Bandgap alignment of CuxS with MoS2 is tunable with staggered symmetry. PL intensity of monolayer MoS2 from direct band gap is quenched due to excitons radiative transfer to the indirect band gap of CuxS. Photoexcited electrons and holes pairs are transferred to low energy states by interlayer relaxation. In heterojunction area, Raman shift in phonon vibration modes of MoS2 affirms interlayer coupling effect. Our synthesized CuxS/MoS2 heterostructure is well-defined over a large area with controllable thickness and a scalable position, which can be useful for application in optoelectronics multifunctional devices such as photovoltaics, solar cells, photodetectors, optical modulators, and photocatalysts.

STM and conduction experiments with single helical molecules

Thi Ngoc Ha Nguyen, Diana Slawig, Yossi Paltiel, Christoph Tegenkamp

Polyalanine (PA) has an alpha-helix conformation, which has gathered recently a lot of interest as the propagation of electrons along the helical backbone structure comes along with spin polarization of the transmitted electrons. It was shown, that this class of molecules is indeed suitable for new spintronic devices [1]. However, detailed information of the structure of the molecules are unknown to date. Self-assembly of PA molecules on different substrates (HOPG and Au(111)) form a well-ordered closed package structure, which is governed by the interdigitating between adjacent PA molecules due to the formation of additional hydrogen bonds from their helical back-bones[2]. The ordering within helical film refers to new ordering mechanism and can most likely explain the coherence in the electronic transport and high efficiency for the current induced spin selectivity (CISS) effect[3]. Moreover, we performed DC-transport experiment through single PA molecules by means of mechanically controlled break Au-junctions. The molecule length- and temperature-dependence suggest electron tunneling being the dominant transport mechanism across the molecules.

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Testing the activation temperature of non-evaporable Ti-Zr-Hf-V getter films by XPS

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Developing new non-evaporable getter (NEG) films with low activation temperature is the key of developing next

generation high-energy particle accelerators with an ultimate vacuum degree of the chamber. Here, a new quaternary alloy Ti-Zr-Hf-V getter film with a uniform thickness of 1.64 μm is fabricated by DC magnetron sputtering. The activation temperature of Ti-Zr-Hf-V getter film has been detected by measuring the binding energy of Ti, Zr, Hf and V at different temperatures through in-situ synchrotron radiation based X-ray photoelectron spectroscopy. The Ti-Zr-Hf-V getter films have been activated at 150 $^{\circ}\text{C}$. In addition, the binding energy of Hf 4f at 130 $^{\circ}\text{C}$ is basically the same as that at 300 $^{\circ}\text{C}$. It is the presence of Hf element which greatly reduce the activation temperature of the obtained films.

2863-A-1902

testing the activation temperature of non-evaporable Ti-Zr-Hf-V getter films by X-ray photoelectron spectroscopy

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Developing new type of non-evaporable getter (NEG) films with low activation temperature is key of developing next generation high-energy particle accelerators with an ultimate vacuum degree of the chamber. Here, a new quaternary alloy Ti-Zr-Hf-V getter film with a uniform thickness of 1.64 μm is fabricated by direct current magnetron sputtering. The activation temperature of Ti-Zr-Hf-V getter film has been detected by measuring the binding energy of Ti, Zr, Hf and V at different temperatures through in situ synchrotron radiation based X-ray photoelectron spectroscopy (SRXPS). The Ti-Zr-Hf-V getter films have been activated at 150 °C. In addition, the binding energy of Hf 4f at 130 °C is basically the same as that at 300 °C. It is the presence of Hf element which greatly reduce the activation temperature of the obtained films.

2867-A-1902

Study about improvement of hole distortion and side wall slope in HAR etching using RF pulse and frequency control

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HAR(High Aspect Ratio) Etching is one of the greatest challenges in 1x,1y-nm DRAM manufacturing.

It should guarantee various types of characteristics, such as slope(bottom/top ratio, verticality), distortion(length/width ratio), in wafer uniformity and productivity(wafers per unit time).

In this paper, a brief methode to increase distortion and slope at the same time is suggested.

At the start of the process, high freq. pulse is effective to increase hole distortion, while low freq & high bias power is helpful for increasing side wall slope at the end of the process.

It has confirmed that two conflicting characters, distortion and slope, are increased simultaneously, using high frequency pulsing(2khz to 7khz) and high bias rf power(over 10kW). It suggests that advanced rf system is necessary to overcome the limitation of HAR etching process.

2872-A-1902

Post-thermal induced recrystallization in GaAs/Al_{0.3}Ga_{0.7}As quantum dots grown by droplet epitaxy with near-unity stoichiometry

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We investigate the stoichiometry control of GaAs/Al_{0.3}Ga_{0.7}As droplet epitaxy (DE) quantum dots (QDs). Few tens of core nonstoichiometries in the Ga(As) atomic percent are revealed in as-grown strain-free QDs using state-of-the-art atomic scale energy-dispersive X-ray spectroscopy (EDS) based on transmission electron microscopy (TEM). Precise systematic analyses demonstrate a successful quenching of the nonstoichiometry below 2%. The control of the chemical reactions with well-controlled ex-situ annealing sheds light on the engineering of a novel single-photon source of "strain-free" DE QDs free of defects.

A Sample Environment for Neutron Scattering Studies under Mechanical Confinement and Shear

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The study of soft materials confined between surfaces is central to understand interactions that lead to adhesion, lubrication and colloidal stability. Force measurements have long been able to describe the potential that exists between coated surfaces, but it is only more recently that scattering techniques have permitted detailed structural studies of thin and soft surface layers under confinement. Specifically, the recent development of a confinement cell that consists of a solid surface confined by an expanding flexible film has been able to address key factors that have hampered these investigations for a long time by achieving parallelism and good contact over a large area. These advances have enabled new fields of research for studying surfaces under confinement using neutron reflectometry. Within the framework of projects funded by the Swedish Research Council and Nordforsk, researchers from Malmö University and the collaborative team behind the development of this cell will work with researchers at ILL, ESS and ISIS to build on this success towards a next-generation surface confinement apparatus. The key deliverable will be to develop a sample environment capable of applying shear under confinement that can be integrated with GI-SANS and reflectometry geometries. In this work, advances on how the decoupling of the normal load from the rotational/linear movement of the sample as well as the implementation of the high accuracy motor control for the shear application are analyzed. Experiments in different geometries with the previous confinement cell performed at ILL beamlines (Figaro, D17 and SuperADAM) will be presented.

The Etching property of AlN Thin Film in the Film Bulk Acoustic Resonator Fabrication using a Inductively Coupled Plasma

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Recently, Aluminum nitride has a number of interesting properties such as high thermal conductivity, high electrical insulation and chemical stability. The piezoelectric properties and the high acoustic velocity make AlN very suitable for many applications in MEMS especially in electro-acoustic devices. In FBAR fabrication, the etching of the piezoelectric film is a key step because a number of electro-acoustic properties of FBAR device may be affected by the etch process, i.e., insertion loss, coupling coefficient and the quality factor. Until now, in recent research has been done that shows the dependences of the AlN etch rate on the operating conditions using some gas plasmas, but it does not discuss the etch mechanisms or the relationships between the process parameters, or the and chemistry involved. And, there are only a few studies relating to AlN dry etching using the high density plasma sources favored by modern microelectronic technology. As a result, the influence of the process parameters on the AlN etch rate is not explored in detail and the AlN etch mechanism is not quite clear. In this work, we investigated the etching characteristics and mechanisms of AlN thin films using the gas mixtures in high density plasma system. The chemical reaction on the surface of the etched AlN thin film was investigated with XPS. The patterns of the AlN thin film were investigated using the FE-SEM.

Mechanism of the phase transition process of the polycrystalline copper surface and Single crystal graphene growth

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Chemical vapor deposition (CVD) method on Cu film has been attracted as a promising technique for realizing high-quality and large-scale graphene films, which can be scaled up to meter in size by employing roll-to-roll method.

However, CVD-grown graphene films on a polycrystalline copper film are usually polycrystalline and consist of numerous grains with grain boundaries, which remarkably degrade their electrical and mechanical properties.

In the meantime, many research efforts to reduce grain boundaries have revealed that monocrystalline graphene films have been synthesized on single crystal catalyst surfaces.

In other words, preparation of well-ordered Cu substrates such as single crystal copper is important for well-aligned graphene and rapid growth.

Various efforts have been made to obtain well-ordered substrates, including the use of expensive monocrystalline Cu (111). The thermal recrystallization method of commercial polycrystalline Cu has attracted much attention because of its large area and low cost. However, due to the lack of understanding of the mechanism of the phase transition process of the polycrystalline copper surface, the copper surface could not be controlled consistently with (100) or (111) orientation.

In this study, we successfully recrystallized the copper surface to (100) or (111) by appropriately setting the thermal crystallization process. At the same time, monocrystalline graphene was synthesized.

STRUCTURAL, OPTICAL AND ELECTRICAL PROPERTIES OF TiO_xN_y SOLAR ABSORBER COATINGS PREPARED BY ELECTRON BEAM EVAPORATION

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We report on the structural, optical and electrical properties of titanium oxynitride (TiO_xN_y) solar absorber coatings deposited onto copper, silicon and glass substrates at room temperature by electron beam evaporation technique. The microstructure, composition, surface morphology, optical properties and electrical properties of these films have been investigated as a function of oxygen gas partial pressure in the range of 7.5×10^{-6} - 7.5×10^{-5} Torr. The microstructure, composition elements, surface morphology and surface roughness of TiO_xN_y solar absorber coatings were studied using X-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and atomic force microscopy (AFM), respectively. The optical constants (n and k) of the TiO_xN_y solar absorber coatings were determined using the ellipsometry spectroscopy. The optical properties were measured using UV-Vis-NIR spectrophotometer in the solar spectrum region (300 – 2500 nm) and FT-IR spectrophotometer in the infrared region (3000 – 20000 nm). The resistivity was investigated by four point probe technology. The coating at oxygen partial pressure of 7.5×10^{-5} Torr exhibited high solar absorptance of 0.94 in the solar spectrum region and low thermal emittance of 0.05 in the infrared region. One can conclude that this coating can be a potential candidate as selective solar absorber coatings.

Etching properties of cobalt oxide thin films by inductively coupled plasma

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Cobalt oxides have been investigated extensively as sensitive materials in gas sensors, electrodes in electro-catalytic process, and selective absorbing layers in solar thermal energy collectors. Cobalt oxide thin films have traditionally been prepared by sputtering, pulsed laser deposition, chemical vapor deposition, and sol-gel process. As a result of these efforts, the growth mechanism of the cobalt oxide film has been studied extensively, but the research on the etching process is insufficient. Integrated processes such as dry etch processes must be developed for electronic device applications.

In recent years, the majority of the dry etching for dielectric materials has been carried out using an inductively coupled plasma (ICP) etching system because of relatively low electron temperature and the easy control of ion flux and ion bombardment energy. However, there is no report on the characteristics and mechanism of cobalt oxides thin films during etching process.

In this study, ICP etching system was used for cobalt oxide thin films etching. Cobalt oxides thin films were etched with ICP etching system by varying the etching parameters such as gas mixing ratio, RF power, and process pressure. Chemical effects during cobalt oxide etching were investigated using x-ray photoelectron spectroscopy (XPS) to determine the elemental composition of the etched surface. The etching profile was investigated by scanning electron microscopy (SEM).

Effect of specific structure of MWCNT-Sn composite anode on initial reversibility and cycle behavior

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An anode composite for Li secondary battery in which a Sn compound was inserted into a multi-wall carbon nanotube (MWCNT) was prepared by a simple thermal hydrothermal synthesis method. From the results of X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), surface scanning microscopy (SEM) and high-resolution transmission electron microscopy (HR-TEM) analysis, the tin compounds produced in MWCNT were Sn, SnO and SnO₂. In particular, TEM images showed that no tin compound was coated on the outer wall of MWCNT. The reason why the tin compound exists only in the MWCNT is due to the following steps. Channel-like defects (CLD) were formed on the surface of MWCNT by acid treatment, and Sn precursor penetrated into MWCNT through this CLD. The Sn-based compound is formed inside the MWCNT by the subsequent heat treatment, and at the same time, the CLD disappears due to the annealing effect. The volumetric expansion of the Sn compound during charge and discharge is suppressed by the binding effect of MWCNT, and oxidation reaction in which irreversible Li₂O is generated by initial oxidation of Li is minimized, resulting in an increase of reversible capacity. The initial discharge capacity and the discharge capacity after 80 cycles were 730 mAh / g and 680 mAh / g, respectively. Therefore, it is suggested that Sn compound located only inside the MWCNT can be one of the anode materials for a high-stability power source which can be applied to a wearable device which is difficult to use a metal Li anode.

Selective Epitaxial Growth of Si Using Atmospheric Pressure Plasma-Enhanced Chemical Vapor Deposition

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Plasma-enhanced chemical vapor deposition (PECVD) has advantages applying thin film deposition into very-large-scale integration (VLSI) manufacturing at lower temperature. However, the wide ion energy distribution in a low-pressure PECVD (LP-PECVD) can cause non-uniform film properties such as film roughening or defects in the film caused by ion bombardments. Atmospheric pressure PECVD (AP-PECVD) can reduce the ion energy distribution comparing to LP-PECVD due to the much shorter mean-free-path of the reactive particles in a plasma [1]. Recently even epitaxial growth of Si has successfully demonstrated using AP-PECVD where the porous carbon electrode is used to supply gases of SiH₄, H₂ and He [2]. We have found that Si epitaxial layer is selectively grown on Si, not on SiO₂ using a conventional capacitively coupled plasma (CCP) electrode at atmospheric pressure by modulating gas flow static during plasma ignition. In contrast to the previous demonstrations of Si epitaxy using AP-PECVD and ultra-high vacuum CVD, we used a vacuum process chamber pumping with a dry pump only [2, 3, 4]. The selective epitaxial growth (SEG) of Si was verified by high-resolution transmission electron microscopy (HR-TEM) and explored process window varying the process conditions.

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2962-A-1902

Controlled Growth of Titanium Oxide Thin Films with a different oxygen flow and discharge current in Reactive DC Magnetron Sputtering

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We have grown titanium oxide (TiO_x) thin films with a metallic Ti metal target under the constant current mode in reactive DC magnetron sputtering methods. The oxidation (poisoning) of target is known to have a critical influence on the crystal structure and oxygen contents of the as-grown TiO_x thin films. With this in mind, the reactive oxygen gas flow was adjusted along with the plasma discharge current, in order to achieve wide range of the target impedance which is a good indicator of the target poisoning. We then paid attention to the change of the crystal phases of the TiO_x thin films having different oxygen contents ($0 < x < 2$) with alteration of the target surface, from the metallic to the poisoned mode, via the transition mode. With a comparative analysis, we were able to identify enable formation process of TiO_x thin films with different target conditions. We also found the evolution of the target poisoning are responsible for the change in growth pressure and growth rate. In the presentation, we will report the experimental details and their comprehensive analysis.

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Fabrication and characterization of transparent conductive BaSnO₃ oxide based conductive fibers

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Wearable devices composed of attachable electronic devices have recently been gradually replaced with clothes having the same function. In other words, it is the final goal that the garment itself is made to have both the function of clothes and the function of electronic devices, not the way of combining clothes and devices separately. One of the most important technologies, along with the development of electronic devices, is the development of yarns with appropriate electrical conduction. Until now, the main method is the hybridization of yarn with metal or carbon nanotube. However, metals and carbon nanotubes have limitations in terms of wearing comfort and color. The purpose of this study is to synthesize transparent conductive oxide (TCO) powders with controlled electrical conductivity at the nano level and to fabricate conductive hybrid yarns or fabrics using them. From the analysis results, we propose that TCO based conductive fibers may overcome the disadvantages of metal or carbon-based conductive fibers. The analysis method will focus on suggesting changes in electrical resistance after repeated mechanical expansion and contraction.

Conductance of aromatic and antiaromatic molecules

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Aromatic and antiaromatic molecules are cyclic, planar and conjugated systems. According to Hückel's rule, a molecule is aromatic if it has $4n+2$ electrons and antiaromatic if it has $4n$ electrons contributing to the molecular pi system.

Antiaromatic systems were long predicted to be more conducting [1]. However, due to the challenging synthesis of stable antiaromatic compounds, this relationship was limited to aromatic and non-aromatic molecules. Recently, a stable antiaromatic compound was synthesized and its conducting properties studied for the first time [2]. The conductance of antiaromatic molecule was found to be 20 times higher than the aromatic counterpart. I will describe our study on the electronic structure and conductance of aromatic and antiaromatic molecular junctions. We use DFT and NEGF methods to calculate the transmission spectra of a pair of structurally similar aromatic and antiaromatic molecules. The higher conductance of the antiaromatic molecule is due to the LUMO-derived resonance closer to the Fermi level.

Finally, we extend our analysis to a series of aromatic-antiaromatic molecules. Our comparison shows that antiaromaticity corresponds to p-doping of the aromatic electronic structure. From our analysis, we establish a relationship between the chemical structure of conjugated systems, quantum interference and electronic transport, which helps in the design of single-molecule circuits.

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Study of the photoreflectance of thin films of gan grown on gaas (001) substrates using the mbe technique.

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Using the MBE technique, thin films of cubic phase of gallium nitride (c-GaN) were grown on GaAs substrates (001). The influence of a GaN nucleation layer on the purity of the cubic phase of the GaN film grown was studied by means of the photoreflectance technique. As a modulator of the reflectivity, an UV emitting photodiode at 285 nm and 50 mW power was used. Photoreflectance spectra were obtained in the temperature range from 300K to 14 K, and the fundamental energy gap of the material was determined. This energy gap shifts 30 meV when the temperature passes from 300 to 14 K. The spectra show oscillations due optical interference, these oscillations are due to the thickness of the thin films is of the same order of magnitude of the range of the spectra.

Reduction of molecular tritium flow in the KATRIN beam line

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The objective of the Karlsruhe TRitium Neutrino Experiment (KATRIN) is to determine the absolute neutrino mass with a sensitivity of 0.2 eV/c² (90% CL) after reaching the projected systematic and statistic sensitivity [1]. To achieve this, KATRIN precisely measures the shape of the tritium beta spectrum near its kinematic endpoint. This comprises about three full years of data taking plus the required measurements for evaluating systematic effects. During this time KATRIN will make use of the Windowless Gaseous Tritium Source (WGTS), which is part of the inner tritium Loop. Molecular tritium gas of high isotopic purity (> 95%) is injected from a temperature stabilized buffer vessel into the center of the beam tube of the WGTS magnet cryostat, forming a density profile of nearly triangular shape with a source column density of $5 \cdot 10^{17}$ molecules/cm². The tritium gas is then pumped out by turbo molecular pumps, purified, and refilled into the buffer vessel. This unique closed tritium cycle has a throughput of about 40 g per day.

The decay electrons have to reach the spectrometer and detector section (SDS) without losing energy. To facilitate this, the source is open to the transport section which is in between the source and the SDS. Hence, tritium could reach the KATRIN spectrometers, leading to an increased background rate. Therefore, the transport section has to ensure an adiabatic transport of the electrons from the source to the SDS and reduce the amount of tritium transported to the entrance of the SDS by 14 orders of magnitude with respect to the tritium injection rate in the source [2]. This is an at least five orders of magnitude more stringent limit than given by radiation safety regulations.

The design of the KATRIN beam line addresses both, neutral tritium (molecules) reduction and tritium ion reduction with the differential pumping section (DPS) and the cryogenic pumping section (CPS) and their instrumentation.

KATRIN has started operation with tritium in May 2018. This contribution shows the realization of neutral tritium molecule reduction in the KATRIN beam line as well as the results obtained during the first KATRIN runs with tritium.

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