2014 Spring Meeting Lille, France – May 26th - 30th

SYMPOSIUM G

Carbon- or nitrogen-containing nanostructured thin films

Symposium Organizers:

Mariana Braic, National Institute for Optoelectronics, Magurele-Bucharest, Romania

Jochen M. Schneider, RWTH Aachen University, Aachen, Germany

Rony Snyders, Mons University, Mons, Belgium

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Carbon- or nitrogen-containing nanostructured thin films

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start at	Subject	Num.
	Functional carbon- or nitrogen-containing nanostructured thin films -I : Mariana BRAIC, Rony SNYDERS	
09:00	**Study of surface properties and wettability of Diamond-Like Carbon Plasma modified cotton fibers** **Authors :** D. Caschera, B. Cortese, R. G. Toro, T. De Caro, C. Riccucci, F. Federici, G. Gigli, G. M. Ingo **Affiliations :** D. Caschera; R. G. Toro; T. De Caro; C. Riccucci; F. Federici; G. M. Ingo Istituto per lo Studio dei Materiali Nanostrutturati, Consiglio Nazionale delle Ricerche, Via Salaria km. 29.300, 00015 Monterotondo Stazione, Rome, Italy B. Cortese National Nanotechnology Laboratory-Institute Nanoscience-CNR (NNL-CNR NANO), via Arnesano, 73100 Lecce, Italy Department of Physiscs, University Sapienza, P.le A. Moro 5, I-00185, Rome, Italy G. Gigli National Nanotechnology Laboratory-Institute Nanoscience-CNR (NNL-CNR NANO), via Arnesano, 73100 Lecce, Italy Department of Mathematics and Physics, University of Salento, Lecce, Italy Center for Biomolecular Nanotechnologies (CNB), Italian Institute of Technology (IIT), Lecce, Italy **Resume :** Wettability is one of the most important parameters influencing textile's performance. The ability to control the wettability of cotton fibers is of increasing awareness in both academic and industrial fields. An interesting strategy is to use plasma treatments to obtain the desired assets in terms of wettability, adhesion promotion, and surface energy improvement. In this work, we show that Plasma Enhanced Chemical Vapour Deposition (PECVD) of DLC coatings on cotton fibers results in a significant increased hydrophobicity of cotton textiles. The advantages of using amorphous carbon based coatings lies in the fact that their properties can be tuned conveniently selecting the appropriate growth parameters. In particular, we demonstrate that the selection of the most appropriate growth parameters permits to optimize both the sp2/sp3 carbon hybridization, from which the mechanical stability of the coating depends, and the surface roughness, which controls the wettability behaviour. Structural, compositional, and morphological characterizations have been performed by Raman, AFM and SEM measurements. Water contact angle (WCA) measurements are carried out to evaluate the variation in the hydrophilic/hydrophobic behaviour of the DLC coated cotton fabrics. Finally, the stability and durability of the coatings have been also evaluated by cyclically washing the DLC modified cotton fibers in a detergent solution.	G.I 1
	add to my program (close full abstract)	
09:15	**DLC Hard Protective Coatings Synthetisized by Pulsed Laser Deposition** **Authors :** C. NİTA, L. DUTA, G.E. STAN*, C POPESCU, V. CRACİUN, M. HUSANU*, B. BİTA**, R. GHİSLENİ***, C. HİMCİNSCHİ****, A. C. POPESCU **Affiliations :** National Institute for Lasers, Plasma and Radiation Physics, Magurele, Romania, * National Institute for Materials Physics, Magurele, Romania, **National Institute for Research and Development in Microtechnologies, Bucharest, Romania ***EMPA, Swiss Federal Laboratories for Materials Science and Technology, Thun, Swizerland **** Institute of Theoretical Physics, TU Bergakademie Freiberg, Freiberg, Germany **Resume :** Hard carbon thin films were synthesized on Si (100) and fused silica substrates by Pulsed La-ser Deposition in vacuum or methane ambient in view of studying their suitability for applica-tions requiring high mechanical resistance to shock and friction in high temperatures and harsh environments. The deposited layers were investigated in terms of surface morphology by AFM	G.I 2

and SEM, crystalline status by XRD, packing and density measurements by XRR and bonding architecture by Raman spectroscopy and XPS. The films adherence was determined by pull-out tests, the surface energy was inferred from contact angle measurements, hardness (H) end elastic modulus (E) were assessed by nanoindentation and wear resistance by nanotribology. The films had a high tendency to exfoliate on fused silica, requiring special optimizations of the deposition process in terms of laser fluence and substrate temperature for stabilization, while being adherent on Si in all deposition conditions. The deposition gas pressure played a crucial role in films thickness, structure and mechanical properties. All films were smooth, amorphous and composed of a mixture of sp3-sp2 carbon, with sp3 content ranging between 50-90%. The load-displacement curves resulted from nanoindentation evidenced that the approximately equal ratios of sp3-sp2 in films content induced a higher hardness (30 GPa vs 5 GPa) and elasticity (E=190 GPa vs E=70 GPa) as compared to structures composed mainly of sp3 bonds (>85%).

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09:30 **Coffee break**

10:00 **Tutorial - Part II**

12:00 **Lunch break**

Polymer based thin films - Applications : Dick HEGEMANN, Thien-Phap NGUYEN

14:00 **Conjugated polymer/TiO2 composites for photo-catalytic applications**

Authors : Yi Dan, Long Jiang
Affiliations : State Key Laboratory of Polymer Materials Engineering of China (Sichuan University) Polymer Research Institute of Sichuan University

Resume : Considering the spectral characteristic and electronic properties of conjugated polymers and the characteristic photo-catalytic properties of TiO2 with anatase crystal structure, the polymer/TiO2 composites have been investigated for photo-catalytic applications aiming at degrading organic pollutants and then for developing new and efficient photo-catalysts. As a part of these studies, we present here poly(3-hexylthiophene)/TiO2 (P3HT/TiO2) composites used for photo-catalyzing the degradation of model pollutant phenol. The composites was prepared by the combination of the monomer polymerization and the organic/inorganic composite techniques and then characterized by FT-IR, 1H-NMR, SEM, XPS, XRD, TGA and BET. The spectral characteristic of the composites was investigated by DRS, while the photo-catalytic activity was evaluated by determining the concentration change of the model pollutant-phenol-during the photo-catalytic experiments under dark and under light. To elucidate the photo-catalytic mechanism, photoluminescence experiments were carried out to study the transfer of photo-induced carriers from the conjugated polymer to the TiO2 nanoparticles. The enhanced photo-catalytic activity of the composites compared to the TiO2 not only under ultraviolet light but also under visible light is attributed to the absorbance of light by the conjugated polymer and hence to the efficient transfer of the photo-induced carrier from the conjugated polymer to the TiO2.

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14:30 **Photoactivity Increment in TiO2/Graphene Nano-composite films Prepared by Sol-Gel Technique**

Authors : Y. Kusumawati (a,c), Th. Pauporté (a), J. Rathousky (b), M. A. Martoprawiro (c)
Affiliations : (a) Laboratoire d'Electrochimie, Chimie des Interfaces et Modélisation pour l'Energie. Ecole Nationale Supérieure de Chimie de Paris, 11 rue P. et M. Curie, 75231 Paris cedex 05, France; (b)J. Heyrovský Institute of Physical Chemistry, v.v.i., Academy of Sciences of the Czech Republic, Dolejskova 3, 18223 Prague 8, Czech Republic; (c) Laboratorium Kimia Fisik dan Anorganik, Faculty of Mathematics and Sciences, Insitut Teknologi Bandung (ITB). Jl. Ganesha 10, Bandung, 40132, Indonesia

Resume : TiO2/Graphene nano-composite has been prepared by sol-gel technique. Single-layer Graphene Oxide (SGO) was used as a resource of graphene. The amount of SGO that was added was varied 0.6; 1.2 and 3

G.II. 2

weight % to the amount of TiO2 nano-particle. The composite was used as photocatalyst and photoelectrode in Dye-Sensitized Solar Cells (DSSC). Its photoactivities, including photodegradation of 4-chlorophenol and cell performance in DSSC, were tested. Incorporation of SGO increased both photodegradation and photovoltaic activities of the composite compared to the pure TiO2. The best activities were showed by composite with SGO composition at 1.2% (TiO2/graphene_1.2). Kinetically, the rate constant for 4-chlorophenol photodegradation TiO2/graphene was higher than for pure TiO2. The DSSC overall conversion efficiency of TiO2 and TiO2/graphene_1.2 was 5.79% and 6.42%, respectively. There was an increasing in the short current density (Jsc) of the composit after graphene incorporation, but the open circuit voltage (Voc) was almost constant. These results were accompanied by the same results of surface area and dye loading for both TiO2 and TiO2/graphene. To clarify the processes at the origin of the solar cell improvement, impedance spectroscopy measurements have been performed and will be presented.

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14:45 **Plasma polymerization of cyclopropylamine for bioapplications**

Authors : Anton Manakhov, Lenka Zajickova, Marek Elias, Jan Cechal, Josef Polcak, Stepanka Bittnerova, David Necas, Adrian Stoica, Petr Klapetek
Affiliations : Masaryk University, Brno, Czech Republic; Masaryk University, Brno, Czech Republic; Masaryk University, Brno, Czech Republic; Brno University of Technology, Brno, Czech Republic; Brno University of Technology, Brno, Czech Republic; Masaryk University, Brno, Czech Republic; Masaryk University, Brno, Czech Republic; Masaryk University, Brno, Czech Republic; Czech Metrology Institute, Brno, Czech Republic

Resume : Amine-rich films prepared by plasma polymerization have a great potential for biomolecule immobilization, microfiltration membranes, enzyme electrodes, adhesion enhancement or biosensor applications. The bioapplications require good stability in water. However, increased plasma polymer cross-linking, leading to improved film stability, is achieved on the expenses of the amine-group density. Cyclopropylamine (CPA) is a promising monomer recently used for the deposition of amine-rich thin films but the stability of CPA plasma polymers in the contact with water was not yet reported. In this work, low pressure capacitively coupled plasma polymerization of CPA is studied with respect to the discharge mode, continuous wave and pulsed, and CPA flow rate. The analyses reveal complex structure of cyclopropylamine plasma polymers containing hydrocarbon chains, primary and secondary amines, nitriles and possibly imines. In pulsed discharges, it is possible to deposit films with the N/C ratio above 0.24 using higher monomer flow rate. At the optimized monomer flow rate the film exhibits only 20 % thickness loss after 48 hours of immersion in water and still contains about 5 at.% of the NHx environment. It is found that immersion in water lead to the formation of complex nano- and microstructures due to a compressive stress induced by the interaction of the layer with water molecules and the mechanism of chemical changes and amine-rich film degradation is reported.

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15:00 **Multilayer coating with optimized properties for corrosion protection of Al**

Authors : F. Khelifa, S. Ershov, M-E. Druart, Y. Habibi, M. Olivier, R. Snyders, Ph. Dubois
Affiliations : University of Mons, Institute of Research in Science and Engineering of Materials, Belgium

Resume : Al and its alloys are widely used in automotive and aeronautic industries. Due to excellent corrosion resistance, conversion layers containing hexavalent chromate Cr(VI) were since long used for applications in aggressive environments. However, because of their toxicity, European Directives forbade the use of Cr (VI). In the current work a protective multilayer system was developed as an alternative to chromate-based coatings and its corrosion properties were evaluated. As the first layer a plasma polymer film (PPF) was selected due to good adhesion and a highly dense cross-linked structure. The careful control of synthesis from an organo-silicon precursor led to deposition of a hybrid organic-inorganic PPF rich in free radicals. The prerequisite for efficient grafting of the second layer, i.e. the surface free radical density evaluation, was addressed by the means of NO chemical derivatization with subsequent X-ray Photoelectron Spectroscopy analysis. Then the surface reactivity was beneficially exploited for initiation of free radical polymerization of an acrylic monomer guaranteeing a better compatibility with the final layer deposited by spin coating. The characterization of each layer and successive

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individual contributions to the corrosion protection enhancement of the entire multilayer system are reported. The improvement of anti-corrosion properties of the multilayer coating by about three orders of magnitude as compared to the uncoated Al substrate is observed.

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15:15 **CNT/PDMS composite membranes for H2 and CH4 gas separation.**

Authors : Kyle Berean, Majid Nour, Sivacarendran Balendhran, Jian Zhen Ou, Johan Du Plessis, Chris McSweeney, Madhu Bhaskaran, Sharath Sriram and Kourosh Kalantar-zadeh

Affiliations : School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia; School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia; School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia; School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia; School of Applied Sciences, RMIT University, Melbourne, Australia; CSIRO Animal Food and Health Sciences, Queensland BioScience Precinct, St Lucia, Australia; School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia; School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia; School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia

Resume : Despite the possibilities that membranes with embedded nanoparticles can offer, their applications for gas separation and purification have rarely been investigated. In this work, polydimethylsiloxane (PDMS) nanocomposite membranes utilizing multi-walled carbon nanotubes (MWCNT) were synthesised and evaluated for the gas permeation properties to low concentrations of H2 and CH4. By increasing the weight amount of MWCNT above 1% the selectivity of the composite material drastically increases by 94.8%. Furthermore, for CH4 concentrations of less than 1%, permeation was almost totally blocked through membranes containing MWCNT concentrations greater than 5%. Vibrational spectroscopy and X-ray photoelectron spectroscopy techniques revealed that upon the incorporation of MWCNT a decrease in the number of available Si?CH3 and Si?O bonds as well as an increase in the formation of Si?C bonds occurred that initiated the reduction in CH4 permeation. This indicates an increased interaction between the polymer and the MWCNT?s to create an efficient molecular sieve. As a result, the developed membranes can be an effective and low cost solution for separating H2 from larger gas molecules such as CH4.

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15:30 **Coffee break**

Carbon- or nitrogen - containing nanostructured thin films -I : Mariana BRAIC, Rony SNYDERS

16:00 **Analytical calculation of the real surfaces of contact and temperatures of the steels pairs during the dry mechanical friction**

Authors : A.ELHADI1 , A. BOUCHOUCHA2

Affiliations : University of M'sila 28000 (Algeria).

Resume : Abstract The work is to determine by the theory of Archard the quantity of heat dissipated and the evaluation of the real contact surface and changing the temperature of the contact of the special non-alloy pairs steels C35/C55and C45/C55 used in the industry as roller-rail by using a tribometer of type pin-disc. The values of coefficient friction are obtained from tests carried out on the pairs quoted before, by varying the sliding speed. Indeed, in a dynamic contact, raising the average temperature at the interface depends on several parameters, in particular the different values of the sliding speed and the coefficient of friction obtained. The heat transfer depends on the thermal properties of materials and the interfacial films generated by friction. Keywords Dynamic contact, real surface of contact, friction, wear, temperature of contact, heat transfer.

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16:00 **Influence of the normal load and heat treatment on the wear pairs special non -alloy steels and the impact on the friction surfaces.**

Authors : A. El Hadi 1, Y. Mouadji 2, A. Bouchoucha 3

Affiliations : University of M'sila

Resume : Abstract The study presented concerns the behavior of two metal pairs used in the industry, at the company ALGAL (processing company

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aluminum) of Msila (Algeria), especially in hoists where the couple C35 and C45 in the delivered condition (roller), and steel C55 treated (rail). During operation, the roller is worn and replacement is costly. Our study is to investigate the wear of the roller, using a tribometer pin-disc type available at the Laboratory of Mechanical Engineering at the University of Constantine. The tests were conducted in ambient air. Wear is studied as a function of the normal load and the heat treatment (hardening and tempering) of the roller. The modifications induced on the surface of contact and structural ones were analyzed by Energy Dispersive Spectroscopy (EDS) and Scanning Electron Microscopy (MEB). Finally, it has resulted in a technical solution that can reduce a remarkable wear roller. Keywords Dynamic contact, hardness, wear, microstructure of steels, hardening, tempering, and oxidation.

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16:00 **Carbon doping in InSbTe alloys for thermal stable phase transformations** G.PI. 3

Authors : Yongtae Kim, Hyun-Soo Kim
Affiliations : Semiconductor Materials & Devices Lab., Korea Institute of Science and Technology, Seoul, Korea

Resume : We have doped carbon atoms in the InSbTe (IST) alloys and investigated phase change mechanism and electrical performance of multi level cell (MLC) phase change random access memory (PRAM). Among Te-based chalcogenide materials, the IST has been already reported as a promising candidate for MLC-PRAM. However, during the phase transformation process migrations of vacancies and atom generate voids and volume change in the IST, which may result in failure of retention and resistance drift. Increasing the C concentration from 0 to 8.4, and 12.5 at.% glass transition temperature increases from 300 to 370, and 440℃, respectively. The activation energy is also increased from 5.138, to 5.278 and 5.398 eV. High resolution transmission electron microscopy shows that the C atoms form C graphite planes, which interrupts inter-diffusion between the the InSb and the InTe planes to form the InSbTe phase since the C atoms prevent the atomic migrations via the vacancy sites while changing the crystal structure from amorphous to metastable FCC structure. Therefore, it is plausible that the phase transformation needs more energy as increasing the C concentration, and volume change of the C doped IST is reduced by about 30 % comparing the undoped IST. In addition, the resistance drift is completely prevented by the C doping, and switching speed of the C doped IST-PRAM is also not sensitive to the C doping. The reason is ascribed to the micro spherical InSb grains distributed along the bottom to the top phase change volume because switching takes place through these 7-15nm size InSb crystalline grains. In this work, we will discuss the atomic lattice image in detail and electrical performance of MLC-PRAM.

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16:00 **Low stress C doped WN diffusion barrier for Cu interconnection** G.PI. 4

Authors : Yong Tae Kim, Young Hwan Kim
Affiliations : Semiconductor Materials and Devices Lab. Korea Institute of Science and Technology P.O.Box 131, Cheongryang, Seoul 130-760, Republic of Korea

Resume : Carbon doped WN (C-WN) thin films have been deposited by atomic layer deposition (ALD) method and the diffusion barrier performance for Cu interconnect has been investigated. the C-WN prepared with WF6-CH4-B2H6-NH3 gas system has very low resistivity of 100 μΩ-cm, which is normally 5~7 times as low as the WN, TiN and other diffusion barrier thin films. Rutherford backscattering spectroscopy and leakage current measurement for the Cu/C-WN/inter layer dielectric (ILD)/Si interconnect structure show excellent thermal stability to prevent the Cu diffusion even at 700℃ for 30 min. Electromigration failure of the Cu interconnect obtained at an acceleration of 102 A/cm2 clearly shows that life time of the Cu/C-WN interconnect is 4 times as long as that of the Cu/TiN. The excellent life time is explained by the low film stress of the Cu interconnect. The stress measurement indicates that the Cu/C-WN/ILD/Si interconnect has the lowest film stress even at the higher annealing temperature. When high current density flows through the Cu interconnect, high tensile film stress causes voiding in the interconnect line and the stress induced voids lead to the open circuit failure. Therefore, it is plausible that the nucleation of void may be sup-pressed by reducing the film stress. We will discuss the ALD mechanism, influences of the film stress and mechanical hardness in detail.

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16:00 **Formation of Silicon nanoparticles embedded in PECVD silicon nitride by rapid thermal annealing** G.PI. 5

Authors : S. Meziani, A. Moussi, F. Antoni, R. Outemzabet, L. Mahiou, A. Guenda
Affiliations : Centre de Recherche en Technologie des Semi-Conducteurs pour l'Energétique (CRTSE), 02 Bd Frantz Fanon, BP 140, 7 Merveilles, Algiers. Algeria; Institut électronique du Solide et des Systèmes (IneSS) UDS-CNRS (UMR 7163). 23 rue du Loess. BP 20-F-67037 Strasbourg. Cedex 2. France; Laboratoire des semi-conducteurs et oxydes métalliques, Université des Sciences et de la Technologie Houari Boumediene. BP 32 El Alia, Bab Ezzouar. Alger. Algérie.
Resume : We have analyzed the effect of rapid thermal annealing RTA (from 600 to 1100°C) on the optical and physico-chemical properties of hydrogenated silicon nitride (SiNx:H or SiNx abbreviated in the text) layers. These films are deposited by PECVD method on the top of multicristalline silicon (mc-Si) substrate. The influence of rapid annealing temperatures on weighted reflectance (Rw) has been investigated. We have found a minimum of Rw = 9% at annealing temperature T= 700°C. The bonding structure and hydrogen content of SiNx thin films have been investigated. The amount of bond hydrogen was calculated from Si-H and N-H infrared absorption bands. An annealing study shows a decrease on Si-H and N-H bond concentration. In the same range, the value of effective lifetime (τeff) of the minority carriers extracted from the decay curve of QSSPC measurement show a larger value τeff = 49.9µs from the samples coated with SiNx and annealed at 600°C. This is probably due that in this temperature, the SiNx film became denser and a considerable part of hydrogen diffuses in the interface and bulk of silicon substrate to passivate various defects and dangling bonds. The effects of RTA on photoluminescence (PL) and Raman spectra in the SiNx/Si structure are studied and show a variation of PL and Raman intensity, respectively. This behavior is predominantly due to the defect states and silicon nanoparticles Si-QDs formed during the annealing temperature.

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16:00 **Hardening of the stainless steel surfaces by forming expanded austenite phases using PIII treatment in ExB fields**

Authors : Samantha de Fátima Magalhães Mariano 1,2, Elver Juan de Díos Mitma Pillaca 1, Mario Ueda 1, Rogério de Moraes Oliveira 1
Affiliations : 1 National Institute for Space Research (INPE), Associated Laboratory of Plasma (LAP), Av. dos Astronautas, P.O. Box 515, São José dos Campos, SP, Brazil; 2 National Institute for Space Research (INPE), Associated Laboratory of Sensors and Materials (LAS), Av. dos Astronautas, P.O. Box 515, São José dos Campos, SP, Brazil
Resume : In this work, the hardening of AISI 304 stainless steel (SS) was achieved by means of nitrogen Plasma Immersion Ion Implantation (PIII) technique in the presence of an external magnetic field to improve plasma confinement. The PIII treatment processes were divided in two main parts: firstly covering the surfaces of flat samples with a nitrogen layer and then modifying the inner surface of a stainless steel cylindrical tube. Afterwards, the morphology and microstructure of the surfaces were analyzed by X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The mechanical properties were evaluated by means of microhardness Vickers test. The outcomes showed that the magnetic field gives rise to some peaks of expanded austenite on flat samples, which in turn provides a slight increase in the hardening of the alloy dependent upon the pulse intensities. On the other hand, a highly hardened surface was achieved inside the tube exhibiting values of microhardness up to 1800 HV owing to the presence of the expanded austenites.

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16:00 **Pretreatments for enhancement of DLC films deposition inside AISI304 tubes**

Authors : Samantha de Fátima Magalhães Mariano1,2,a, Valerie Cecile Corcuera 2,b, Elver Juan de Díos Mitma Pillaca1,c, Mario Ueda1,d, Rogério de Moraes Oliveira1,e, Vladimir Jesus Trava-Airoldi 2,f
Affiliations : 1National Institute for Space Research (INPE), Associated Laboratory of Plasma (LAP), Av. dos Astronautas, P.O. Box 515, São José dos Campos, SP, Brazil 2National Institute for Space Research (INPE), Associated Laboratory of Sensors and Materials (LAS), Av. dos Astronautas, P.O. Box 515, São José dos Campos, SP, Brazil *a samanthafmm@outlook.com, b valerie@las.inpe.br, celver.mitma@plasma.inpe.br, d ueda@plasma.inpe.br, e rogerio@plasma.inpe.br, f vladimir@las.inpe.br
Resume : Depositions of protective layers and multifunctional thin films in pipes of oil and chemical industries are generally applied to extend their lifetime. Diamond-like carbon (DLC) films are a good choice to coat the inside of tubes because of their remarkable properties such as wear and corrosion resistance, high hardness, low roughness, and very low friction coefficient. This work is aimed at the study of the adhesion between DLC and the inner wall of

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a cylindrical stainless steel (SS) tube by means of Plasma Immersion Ion Implantation and Deposition (PIII&D) technique carried out in the presence of ExB fields. As hollow cylindrical substrates AISI304 SS tubes (40 mm external diameter, 150 mm length and 2 mm thickness) were used and some polished samples of same material (disks with 15.0 mm diameter and 2.0 mm thick) were properly placed in different positions inside each tube. Firstly, an hybrid treatment was performed, in order to produce a nitrogen enriched layer inside the tube prior to receiving the DLC film deposition, in the following steps: i) nitrogen PIII (20 µs/500 Hz/ 4 kV/60 min) + ii) DLC deposition with methane (20 µs/500 Hz/ 7 kV/20 min) and acetylene plasma (20 µs/500 Hz/ 4 kV/20 min), all steps performed at about 2 Pa. Duplex coatings were analyzed by Raman spectroscopy, Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD). Current results show the presence of DLC films with hydrogen content of up to 20 at.%. Previously, DLC film was peeled off in all samples without nitrogen PIII. XRD patterns revealed the formation of austenite phases which can also be attributed to thermal diffusion during the whole nitrogen treatment (up to 340°C), and methane PIII (when temperature decreased slowly). Additionally, scratching and pin-on-disk tests were also performed to evaluate adhesion and tribological properties of coatings on substrate. Duplex coatings inside the tube showed good DLC film adhesion to SS samples. In order to increase roughness of substrate and improve coating adhesion, diamond seeding was done by ultrasound before film deposition. Diamond (250 nm grain size) suspensions with different solvents and same concentrations of 10 g/L (1wt%) were prepared. Water, hexane, and heptane were used as solvents. Heptylamine was added on heptane for dispersion improvement of diamond particles. Diamond seeded samples were placed inside the tube. DLC film enhancement on tube is discussed based on XRD analysis and correlated with adhesion test. Comparison of adhesion and tribological properties between seeded and not seeded samples will be discussed. Further details will be shown in the presentation.

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16:00 **Corrosion behavior of NiTi shape memory alloy treated by Nitrogen Plasma Based Ion Implantation**

Authors : (1) Silva, M. M., (2) Pichon, L., (3) Mariano S. F. M., (2) Drouet, M., (1) Otubo, J., (3) Ueda, M.
Affiliations : (1)Instituto Tecnológico de Aeronáutica, São José dos Campos – SP. Brasil; (2)Institut Prime, UPR 3346 CNRS-Université de Poitiers-ENSMA, France. (3) Instituto Nacional de Pesquisas Espaciais, São José dos Campos – SP. Brasil

Resume : NiTi shape memory alloys (SMA) have a good corrosion resistance, due to the formation of stable and protective oxide film on this surface. For many applications it is necessary to modify its surface mechanical properties, to improve the wear resistance, to decrease the nickel release (for the medical applications), etc. Plasma Based Ion Implantation (PBII) is one of the most efficient techniques to produce coatings of nitride. This work aims to study and compare the corrosion resistance of NiTi treated by Nitrogen PBII with the untreated one. The samples were implanted at 750° C during 120 minutes , with 15 kV high voltage pulses, repetition rate of 200 Hz and pulse length of 40 µs. The corrosion resistance of the specimens was evaluated by Potentiodynamic polarization curves performed in an electrolytic cell of three electrodes (Ag/AgCl reference electrode, NiTi as working electrode and Pt counter-electrode), in 3.5 wt% NaCl solution in a LabSolutions potentiostat and the corrosion data were estimated by the Tafel method. The corrosion potential (Ecorr) of coated samples are more positive than the untreated NiTi alloy, about 37% (-180.5 and -288.0 mV respectively). The current density (icorr) of the treated specimens (0.067 µA/cm2) is lower than the untreated (0.096 µA/cm2), about 30%. The corrosion rate is almost twice in the treated samples, 2.88 x 10-3mm/year, while the reference samples rate is 5.18 x 10-3mm/year. With these results we can conclude that Nitrogen PBII improved the corrosion resistance of NiTi SMA since its exhibited noblest potentials and lower current densities, that is, making them less susceptible to corrosion in saline environment.The microstructure was analyzed by SEM (Scanning Electron Microscopy) and the martensitic transformation temperatures are being analyzed by DSC (Differential Scanning Calorimetry).

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16:00 **Superficial evaluation of the Ti-6Al-4V alloy submitted to N-PIII treatment in different times of implantation**

Authors : (1) Susana Zepka, (1,2) Danieli Aparecida dos Reis, (1) Maria Margareth da Silva, (3) Mario Ueda, (4) Luc Pichon

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Affiliations : (1) Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil; (2) Universidade Federal de São Paulo - ICT, São José dos Campos, Brazil; (3) Instituto Nacional de Pesquisas Espaciais, São José dos Campos, Brazil; (4) Institut Prime, UPR 3346 CNRS-Université de Poitiers-ENSMA, France.

Resume : The advance of technology leads to the development of new materials improving their tribology properties. It can be notice in different areas like aerospace industry, chemical and oil that need resistant material in high temperatures and aggressive environments. In this case, it is important to think in its tribological properties, like wear, oxidation, toughness, and hardness. An effective mean, economic and with easy application is the Plasma Immersion Ion Implantation (N-PIII), even in difficult shapes to treat, the material was equal treated. In this work, Ti-Al-4V alloy was submitted to N-PIII during 2, 3, 4 and 8 hours. The comparative analysis to determination of which time was more efficient related on tribological improvement measured by GDOES, EDS and wear. The obtained GDOES results showed the nitrites superficial in the alloy. The wear resistant increased accordingly implantation time, because the TiN formation. The N-PIII 8h samples showed higher wear resistance.

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16:00 **EFFECTS OF NITROGEN PLASMA BASED ION IMPLANTATION (PBII) TECHNIQUE IN MECHANICAL AND THERMODYNAMICS PROPERTIES OF NiTi WIRE IMPLANTED SURFACE.**

Authors : Osmar de Sousa Santos, Maria Margareth da Silva, Luc Pichon, Jorge Otubo
Affiliations : Instituto Tecnologico de Aeronautica; Université de Poitiers

Resume : Wires of NiTi shape memory alloys have been widely used as construction materials for a range of actuators due their shape memory and superelastic properties. Despite the fact of these alloys have generally excellent corrosion resistance; there are some applications of NiTi wires which are required Ni-free surface, such as biocompatibility devices and others which require resistance to atomic diffusion, chemical stability, and increasing hardness of surface. Seen the importance of Ni-free surface in wires of NiTi alloy, this work analyzes the effects of nitrogen plasma based ion implantation (PBII) technique on the mechanical and thermodynamics properties of NiTi wire implanted surface. The samples were treated for 60 min at 750 °C, with 16 kV high voltage pulses. Results of the thermomechanical properties of the PBII treated samples shown that the shape memory effect did not change if compared to NiTi samples without PBII treatment, which is desirable for applications addressing both mechanical and Ni-free properties.

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16:00 **Modeling The Effect of Substrate Surface Roughness On The Impact and Flattening Process of plasma sprayed Al2O3–33 wt.% TiO2 coating**

Authors : ILHEM. R. KRIBA1*; K. BENOUMSAAD1; A. DJEBAILI2
Affiliations : 1 Plasma Laboratory - Faculty of Sciences – Department of Physics- University of Batna- Algeria 2 Laboratory of chemistry and environmental chemistry L.C.C.E - University of Batna- Algeria,

Resume : Titanium and titanium alloys have been used in a number of applications in industry ranging from aircraft components, chemical processing facilities to gas turbine engines due to their high strength to weight ratio, high corrosion resistance and relatively high melting temperature. However, further application of titanium and titanium alloys is considerably restricted by their low surface hardness, high friction coefficient and poor wear resistance. Therefore, the surface characteristics of titanium and titanium alloys need to be improved. Thermal spray coating is one of the most common ways to improve the surface characteristics of materials. The plasma-sprayed Al2O3 and Al2O3–TiO2 ceramic coatings have been extensively used in many applications as surface coating to protect components against wear and corrosion due to their thermal, chemical and mechanical stability. Recently, nanostructured Al2O3–13 wt.%TiO2 coating demonstrate novel and attractive properties such as bond strength, toughness, abrasive wear and thermal shock resistance. In this paper, numerical model is developed using the finite volume method, based on Navier-Stokes equations and (VOF) method to simulate the impact, spreading and flattening of the Al2O3–13 wt.%TiO2 droplets impacting onto a solid surface . The model simultaneously takes into account the fluid flow and heat transfer in the liquid particle and the surrounding gas, and the heat transfer in the substrate. To understand the effect of solidification on the droplet impact dynamics and splat morphology, the simulations were run with smoothed and roughened surfaces considering different roughness magnitude. The results show a substantial build up of temperature at the surface and large

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temperature gradients throughout the thickness, which are due to the differences in the melting point, specific heat and latent heat of fusion of alumina and titania, as well as the difference in their particle sizes. Also, the increase in magnitude of the mean substrate roughness promotes splat instability (jetting and/or satellite break-up) and formation of radial fingers. It was also observed that the increase in general surface roughness may result in the lower spreading ratio (Dfinal / Dinitial) of thermally sprayed ceramic particles. The spreading process of a droplet is governed not only by the inertia and viscous forces, but also by the thermal contact resistance in the substrate surface.

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16:00 **The fractal parametrization of interfaces in nanostructured composite materials and coatings**

Authors : Vityaz P. A., Kheifetz M. L., Senyut V. T. Kolmakov A. G.
Affiliations : Joint Institute of Mechanical Engineering of NAS of Belarus, Minsk; SSPA «Center» of NAS of Belarus, Minsk; Baikov institute of metallurgy and material science RAS, Moscow

Resume : Physical and chemical analysis of diagrams - geometrical images of relationships: composition – system property allows to research structures and phases, determine their amount. The analysis base is principles of continuity and conformity formulated by N. S. Kurnakov [1]. Because of non-equilibrium of rapidly progressing processes for materials synthesis and usage in a macro-, meso-, micro- and nanostructural level their phase transformation diagrams has a metastable nature. In this connection, it necessary to combine main principles of analysis of physical and chemical diagrams for studying non-equilibrium processes of structures and material phase formation in different levels with fractal ideas [2, 3]. Principles of fractal transformation on interfaces of structures, phases and layers were used at modeling of nanostructured composite material during applying of coatings on article's relief surface [2]. Analysis of received multifractal information determined a formation mechanisms sequence and the most important structured and operational characteristics of applied nanostructured coatings. References 1. Kurnakov N.S. Introduction in the Physical and Chemical Analysis.—M.-L.: Acad. Sci. of USSR, 1940. - 562 pp. .(in russ.). 2. Technologies of Constructional Nanostructured Materials and Coatings // Ed. P.A. Vityaz and K.A.Solntsev. - Minsk: Belorusskaya Nauka. – 2011. – 283 pp.(in russ.). 3. Berge P, Lomo I, Vidal C. Order in Chaos: On Deterministic Approach to Turbulence .– M.: Mir, 1991. – 368 pp.

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16:00 **The effect of substrate temperature and film thickness on the properties of epitaxial TiC thin films grown on MgO(001) by DC reactive magnetron sputtering**

Authors : N.C. Zoita1, M. Braic1, V. Braic1, M. Danila2, C.E.A. Grigorescu1, C. Logofatu3
Affiliations : 1) National Institute for Research and Development in Optoelectronics, 409 Atomistilor Str., 077125 Magurele, Romania 2) National Institute for Research and Development in Microtechnology, 126A Erou Iancu Nicolae Str., 077190 Bucharest, Romania 3) National Institute for Materials Physics, 105bis Atomistilor Str., 077125 Magurele, Romania

Resume : Titanium carbide (TiC), as a member of the early transition-metal carbides, presents interesting combination of properties which are usually assigned either to metals or to ceramics. Attributes such as high hardness, chemical inertness, high melting point and wear and corrosion resistance in combination with high electric and heat conductivities make TiC very attractive for a wide area of technological applications. In this work, epitaxial TiCx films were fabricated by DC reactive magnetron sputtering of a Ti target in Ar + CH4 atmosphere on MgO(001) substrates. The influence of substrate temperature (150 °C - 800 °C) and film thickness (50 nm – 600 nm) on the structural, electrical and mechanical properties were investigated by AES, XPS, HR-XRD, micro-Raman spectroscopy, AFM, nanoindentation and Hall effect measurements. The epitaxial growth was observed for substrate temperatures as low as 150 °C, and the same epitaxial relationship was preserved over the entire range of film thickness investigated. The films grown at temperatures larger than 400 °C present electrical resistivities comparable with those of slightly substoichiometric bulk TiCx single-crystals, the lowest one, ~160 μΩ•cm, being obtained for the thinnest film deposited at the highest temperature. The films are partially subjected to compressive strain, which

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relaxes with increasing of the film thickness by developing low aspect ratio nanoislands/nanocolumns on their surface.

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16:00 **Low temperature AlN epilayers deposited by HiPIMS on sapphire substrates**

Authors : N. C. Zoita1, V. Braic1, M. Braic1, M. Danila2, A. Kiss1
Affiliations : 1) National Institute for Research and Development in Optoelectronics, 409 Atomistilor Str., 077125 Magurele, Romania 2) National Institute for Research and Development in Microtechnology, 126A Erou Iancu Nicolae Str., 077190 Bucharest, Romania

Resume : Aluminum nitride (AlN), as one of the III-nitride materials, has some outstanding physical properties that have attracted a lot research interests. AlN exhibits interesting optical, thermal, dielectric and acoustic properties that make it suitable for various fields and applications, some of them requiring single-crystal or high crystalline quality material with specific texture. Reactive magnetron sputtering method demonstrated to be a promising candidate for fabricating highly c-axis orientated AlN films at relatively low substrate temperature. The High Power Impulse Magnetron Sputtering (HiPIMS) technique offers the possibility to better control the energy and direction of the sputtered species at the film's growing surface due to its capability to generate high plasma densities with a high ionization degree of the sputtered particles. The film growth is assisted by an intense ion flux resulting in energic adspecies. Therefore, HiPIMS can be beneficial for growing high crystalline quality thin films at low substrate temperature. In this work, the HiPIMS technique was used for deposition of epitaxial AlN thin films on α-Al2O3 substrates in reactive atmosphere (Ar + N2) using an Al target. The effect of sputtering gas pressure (3 – 10 mtorr) and substrate temperature (100 – 600 °C) on the structural, optical and mechanical properties of AlN epilayers are investigated by HR-XRD, Auger electron spectroscopy, optical transmission, nanoindentation and AFM measurements.

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16:00 **Preparation SiN and SiCN films at extremely low working pressure and by using cyclic chemical vapor deposition system**

Authors : Ha Jun Jang1,2, Jae Seok An1, Cheol Young Park1, Jong Ho Lee1, and Bum Ho Choi1*
Affiliations : 1National Center for Nanoprocess and Equipments, Korea Institute of Industrial Technology, Gwangju 500-480, Korea; 2Advanced Chemical & Engineering, Chonnam National University, Gwangju 500-757, Korea

Resume : As the size of each transistor has been reduced to 1x regime, it is strongly required to prepare high density insulator films with few particle and defects since the thickness of insulator becomes thinner along with the size of transistor. One of technology to meet such needs is to deposit the insulator film at extremely low pressure. It is also regained thin film deposition process below to 300℃. In this study, we have prepared and characterized SiN and SiCN layer which was deposited at the temperature of 180℃ and working pressure of 10mtorr by using pulsed plasma enhanced chemical vapor deposition (PE-CVD) system. To obtain high deposition rate without loss of quality of prepared films, pulsed PE-CVD system has been employed in our experiments. Si precursor and reactant was mixed and co-fed into the substrates, followed by plasma treatment and inert gas purge. The ligand was decomposed 2 times by dual plasma system consist of ICP and CCP, result in pure SiN and SiCN layer. The atomic percent of carbon and hydrogen impurities were negligible. XRD measurement result showed the prepared layers are amorphous phase in all deposition conditions. The refractive index measured at 550nm of wavelength of SiN and SiCN layer was 1.60 and 1.51, respectively with the highest density of 1.98(g/cm3). Furthermore the measured non-uniformity in 300mm scale Si wafer was 2%. Although the SiN and SiCN layer was prepared at low temperature, the typical characteristics of prepared layers are comparable to those deposited at higher temperature, which indicate that low temperature thin film deposition process is possible in semiconductor fabrication steps.

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16:00 **3C-SiC Nanocrystals Growth on Differently Oriented Si Substrates**

Authors : Catherine Deville Cavellin (1,2) , Geetanjali Deokar (1,3), Marie D'Angelo (1), Dominique Demaille (1)
Affiliations : 1 INSP, UPMC, CNRS UMR 7588, 4 place Jussieu, Paris, F-75005, France ; 2 Faculté des Sciences et Technologie UPEC, 61 av. De Gaulle, Créteil, F-94010, France ; 3 Currently at IEMN, University Lille-1, CNRS UMR 8520, Lille, France.

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Resume : The properties of SiC nanocrystals can have various interesting applications especially in the field of optoelectronic and memory devices. We have shown that epitaxial 3C-SiC nanocrystals can be synthesized at the SiO2/Si(100) interface by high temperature annealing in CO2 ambient [1, 2]. The importance of silica overlayer for void free SiC nanocrystal growth was demonstrated. Here, we present and discuss the silicon substrate orientation influence. SiC epitaxial growth on Si is demonstrated, by high resolution transmission electron microscopy, for the three Si orientations studied: (100), (110) or (111) but the nanocrystals shape, size and, density are highly dependent on the Si orientation. Larger size nanocrystals form on Si(100) while, higher density of nanocrystals occurs on Si(110). The as-grown epitaxial SiC nanocrystals on Si could be used as nucleation site for homo/hetero-epitaxial growth of SiC, GaN, diamond and graphene growth.

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16:00 **The influence of different formation types of Si and SiC nanocrystals in SiOx matrix on photoluminescence characteristics**

Authors : Spirin D.E.1; Terekhov V.A.1; Turishchev S.Yu.1; Agapov B. L.1; Serbin O.V.1; Soldatenko S.A.2; Minakov D.A.1; Tetelbaum D.I.3; Belov A.I.3; Mikhaylov A.N.3; Ershov A.V.4

Affiliations : 1 Voronezh State Uneversity; 2 Voronezh State Technical Uneversity; 3 Physico-Technical Research Institute, Nizhnii Novgorod State University; 4 Lobachvsky University of Nizhni Novgorod

Resume : Carbon ions implanting in a matrix of non-stoichiometric silicon oxide (SiOx), followed by thermal annealing can significantly enhance photoluminescence characteristics of light emitting structures with embedded silicon nanocrystals. A replacement of thermal annealing by pulsed photon processing will significantly optimize the formation technology of highly luminescent structures in framework on Si-based technology. Presented studies were performed with the use of wide selection of modern and traditional techniques such as: X-ray absorption spectroscopy and ultrasoft X-ray emission spectroscopy, X-ray diffraction, transmission electron microscopy, photoluminescence spectroscopy. Studies showed a noticeable influence of the carbon implantation in SiOx film on the nc-Si:SiO2 structures phase composition and photoluminescence properties. Moreover, the use of a pulsed photon processing in combination with carbon implantation of SiOx structures, leads to the formation of silicon carbide phase inclusions, that is accompanied of visible photoluminescence intensity increasing. The results of our studies showed the prospectivity of pulsed photon annealing application for silicon carbide nanocrystals formation in SiOx films, and for SiO2 matrix structure recovery after carbon implantation.

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16:00 **Effect on Performance of Aluminum Films Deposited on Sintered NdFeB by Different Pretreatment Process**

Authors : Hu Fang,Xu Wei, Dai Mingjiang,Lin Songsheng,Shi Qian

Affiliations : Guangzhou Research Institute of Non-ferrous Metals

Resume : Sintered NdFeB has been widely used in electronic information, metallurgy, communication, medicine and other fields because of its excellent magnetic properties .Generally,Sintered NdFeB required to maintain its dimensions integrity and the stability magnetic properties during the long-term process because of its temperature and media conditions. The surface of NdFeB material will produce a partial destruction of the structure and composition when NdFeB material corrosion, which result in decrease of its magnetic energy, which affect its practical application. The protective coating deposited on sintered NdFeB by physical vapor deposition technique can effectively solve this problem. Aluminum has good corrosion resistance. Al protective coatings deposited on sintered NdFeB by magnetron sputtering technique in this paper. The effect of pickling, polishing and dry blasting pretreatment on performanc of aluminum films. The results indicate that corrosion resistance of Al films testing by potentiodynamic polarization and neutral salt spray test (NSS) revealed that the pickling pretreatment had much better corrosion than polishing and dry blasting pretreatment,but the dry blasting pretreatment had better adhesion strength of al films than pickling and polishing pretreatment. The corrsion behavior and mechanism were further investigated in this paper.

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16:00 **Synthesis of CNx films by fs-PLD for electrochemical detection of pollutants**

Authors : C. Maddi 1, T. Tite 1, A. S. Loir 1, V. Barnier 2, K. Wolski 2, N. Zehani 3, C. Chaix 3, P. Fortang 3, N. Jaffrezic- Renault 3, J. C. Sánchez López 4, T.C. Rojas 4, C.

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Donnet 1, F. Garrelie 1
Affiliations : 1 Université de Lyon, F-69003, Lyon, France, Université de Saint-Étienne, Laboratoire Hubert Curien (UMR 5516 CNRS), 42000 Saint Étienne, France; 2 Laboratoire Georges Friedel, Ecole Nationale Supérieure des Mines de Saint Etienne, France; 3 Université de Lyon, F-69003, Lyon, France, Université Claude Bernard Lyon 1, Institut des Sciences Analytiques (UMR 5280 CNRS), 69100 Villeurbanne, France; 4 Instituto de Ciencia de Materiales de Sevilla (CSIC-US), Avda. Américo Vespucio 49, 41092 Sevilla, Spain
Resume : Nitrogenated amorphous carbon (a-CNx) thin films are a new class of carbon-based electrode materials, with a wide working potential window in aqueous media. The physical, chemical and electrochemical properties depend on the sp2/sp3 bonding ratio and the content of incorporated nitrogen. Therefore, synthesis and electrochemical characterization of these materials have found lot of interest in environmental analytical microsystems. Here we present the synthesis and characterization of a-CNx deposited by femtosecond pulsed laser technique (fs-PLD). The a-CNx thin films have been deposited on silicon and silicon nitride substrates by ablation of graphite targets in high vacuum conditions (10-6 mbar) and in presence of nitrogen residual pressure (0 to 10 Pa). Plasma assistance in nitrogen atmosphere has been also carried out to improve the incorporation of nitrogen in the films. The chemical composition of the films was investigated by multi-wavelength Raman spectroscopy (633 nm, 488 nm, 442 nm and 325 nm), X-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS) measurements. The films were deposited on Si3N4 substrates used as a working electrode by using cyclic voltammetry for electrochemical characterization and for detection of electroactive pollutants (heavy metals, phenols…). Overall, the properties of a-CNx electrodes prepared by fs-PLD are correlated with nitrogen content and structural properties of the materials.

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16:00 **Antibacterial properties of silver containing amorphous diamond like carbon films**

Authors : Tadas Juknius1, Tomas Tamulevičius1, Asta Tamulevičienė1, Irena Klimienė2, Algimantas Petras Matusevičius2, Šarūnas Meškinis1, Sigitas Tamulevičius1
Affiliations : 1Institute of Materials Science, Kaunas University of Technology, Savanoriu Ave 271, LT-50131, Kaunas Lithuania; 2Veterinary Academy, Lithuanian University of Health Sciences, Tilžės g. 18. Kaunas Lithuania
Resume : Silver was known for a long time as antimicrobial metal for preventing infections, healing wounds, inflammatory and was widely used in different forms including silver colloids, silver-polymer composites, etc. Combination of silver with outstanding mechanical, chemical and optical properties of diamond-like carbon (DLC) matrix opens new application possibilities i.e. coatings for medical implants, surgical instruments, etc. In this study, DLC:Ag thin nanocomposite films were deposited on float glass substrates by reactive unbalanced magnetron sputtering of Ag target in acetylene atmosphere. Scanning electron microscopy, energy dispersive x-ray analysis as well as x-ray diffraction were employed to study morphology, composition and structure of the films. The antibacterial properties of such DLC:Ag nanocomposite films were investigated using S.aureus bacteria from animal respiratory paths. As control samples, pure DLC and pure Ag films were also investigated. The bacteria colony forming units (CFU) have been observed on pure DLC and no CFU formation was observed on pure Ag and DLC:Ag thin films. The inhibition zones on the surface of DLC:Ag films were analyzed in dependence on deposition conditions of the films. The obtained results revealed that antibacterial properties of DLC:Ag nanocomposite films depend on concentration and size distribution of the silver nanoparticles that can be easily controlled adjusting ratio of the sputtering (argon) and reactive (acetylene) gases.

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16:00 **Influence of Ni dopping on structure and mechanical properties of nc-TiC/a-C:H coatings**

Authors : J. Daniel (1), P. Souček (1), V. Buršíková (1), O. Caha (2), M. Stupavská (1), L. Zábranský (1) and P. Vašina (1)
Affiliations : (1) Masaryk University, Faculty of Science, Department of Physical Electronics, Kotlarska 2, Brno 611 37, Czech Republic (2) Masaryk University, Faculty of Science, Department of Condensed Matter Physics, Kotlarska 2, Brno 611 37, Czech Republic
Resume : Nanocrystalline titanium carbide embedded in an amorphous (hydrogenated) carbon matrix is a versatile nanocomposite material which,

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being deposited as thin film, combines the properties of hard titanium carbide nanocrystallites and relatively soft hydrogenized carbon matrix. Hybrid PVD-PECVD process of titanium sputtering in a mixture of argon and acetylene at optimized deposition conditions enables us to deposit superhard nc-TiC/a-C:H coating with hardness and Young's modulus over 40 GPa and 400 GPa, respectively with good adhesion on Ti coated HSS and WC and thickness higher than 5 μm. Further mprovement of the mechanical properties of these coatings was tested by adding third, non carbide formig, element by placing small number of nickel evaporation pellets on the racetrack of the magnetron target. Set of samples with different Ti/C ratio was prepared for different Ni doses. Influence of the Ni content on the properties of nc-TiC/a-C:H system was evaluated. XRD was used to determine crystalite size and latice parameter; depth sensing indenter to get hardness and Young modulus. XPS and EDX provided chemical composition of prepared samples. This research has been supported by the CZ.1.05/2.1.00/03.0086 and GACR P205/12/0407 projects.

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16:00 **Synthesis of thin films of Ti3GexSi1-xC2 and Ti2GexSi1-xC MAX phases on SiC substrates by annealing of Ti-Ge thin films deposited by magnetron sputtering**

Authors : M. Alkazaz, M.F. Beaufort, J.F. Barbot, and T. Cabioc'h
Affiliations : Institut Pprime, CNRS - Université de Poitiers - ENSMA - UPR 3346 Département Physique et Mécanique des Matériaux Boulevard Marie et Pierre Curie - BP 30179 86962 FUTUROSCOPE CHASSENEUIL Cedex, France

Resume : Mn+1AXn phases (n=1, 2, 3) are a family of multifunctional, ternary carbides and nitrides, where M is a transition metal, A is an A -group element, and X is C and/or N. These phases combine the best properties of ceramics and metals, that is promising for multiple potential applications. In this study, we present the synthesis of thin films of Ti3GexSi1-xC2 and Ti2GexSi1-xC (312 and 211 MAX phases). TiyGe1-y layers (y=0.8, 0.67, 0.5 and 0.33) were initially deposited onto 4H-SiC (0001) single crystal and 6H-SiC polycrystalline substrates by magnetron sputtering at the room temperature. Subsequent, annealing experiments at 1000 °C were carried out for 10 minutes and for one hour. At this temperature the interdiffusion processes between the TiGe alloy and the SiC substrate occurred leading to the formation of Ti3GexSi1-xC2 and Ti2GexSi1-xC phases depending on the value of y. The structural and chemical characterizations have been studied by XRD, TEM, HRTEM, and EDS. The obtained results testify to the epitaxial layer growth of Ti3GexSi1-xC2 on 4H-SiC (0001) at 1000°C. Moreover, the electrical properties were studied for Ti0.8Ge0.2 and Ti0.67Ge0.33 layers deposited on 4H-SiC, a nearly - ohmic behaviour being obtained after the thermal annealing.

G.PI.22

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16:00 **Investigation of multilayered TiSiC/NiC protective coatings**

Authors : M.Balaceanu, M.Braic, A.Parau, V.Braic, C.Vitelaru, A. Vladescu
Affiliations : National Institute for Optoelectronics, 409 Atomistilor, POBox - MG 05, 077125, Magurele- Bucharest, Romania

Resume : Nanometer – scale multilayer coatings comprising alternating layers made of different metals and metallic compounds revealed a great potential to be used as protective coatings due to their excellent resistance to wear, corrosion and oxidation. In this paper, preparation and characterization of a novel type of carbide based multilayer, namely TiSiC/NiC, is discussed. The layers in the film structure were selected to produce a non-isostructural multilayer. The coatings were prepared by the cathodic arc technique in a CH4 atmosphere. Different bilayer thicknesses, ranging from 6 to 80 nm, were obtained. The multilayers were analyzed for elemental and phase composition, microstructure, morphology, modulation periodicity, mechanical properties (residual stress, hardness, adhesion) and tribological behavior (friction, wear). For comparison, TiSiC single layer coatings were also investigated. The properties of the multilayers were found to significantly depend on the bilayer period. Typical X-ray diffraction patterns for superlattice coatings (a main (111) Bragg peak surrounded by satellite peaks) were recorded for multilayers with low bilayer thicknesses. The best mechanical and tribological characteristics were obtained for the multilayers with bilayer periods of 10-16nm. As compared to the TiSiC monolayer, reduced residual stress and improved adhesion were found for the multilayers, while the highest hardness was measured to be 1.8 time the "rule of mixture" value.

G.P28I.22

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16:00 **Structural and optical properties of Ge1-xCx deposited on Si and quartz by rf magnetron sputtering**

Authors : C.N.Zoita1, M. I. Rusu1, A.E. Kiss1, M. Stchakowsky2, C.E.A.Grigorescu1,
Affiliations : 1. National Institute R&D Optoelectronics INOE 2000, 409 Atomistilor Str, PO Box MG-5, 77125 Magurele, Ilfov, Romania; 2.HoribaHORIBA Jobin Yvon S.A.S. Z.A. de la Vigne aux Loups - 5 Avenue Arago - 91380 Chilly Mazarin - France

Resume : Germanium carbide (Ge1−xCx) films are extremely attractive due to the low stress, low light absorption and good adhesion on many substrates. In addition, these films allow the band gap tunability over a wide range in conjunction with a high thermostability. Some optical, electrical and structural properties have already been reported for the Ge1-xCx films prepared by CVD, ARE, glow discharge and reactive sputtering methods.The aim of this work is to study the influence of carbon content on the properties of germanium carbide films obtained by the RF magnetron sputtering method. The films were obtained on Si(001) and quartz substrates at three deposition temperatures (2000C, 400oC and 7000C) and two substrate bias values (100 V and 300 V). A pure Ge target was used in a deposition atmosphere consisting of a mixture of Ar and CH4, at different partial pressure ratios. The films were analyzed by quantitative AES for the elemental composition, XRD for structural characterisation, AFM for surface morphology, mechanical profilometry for thickness and film stress measurements. Optical investigations (UV-Vis-NIR, FTIR, and Raman spectroscopies as well as spectroscopic ellipsometry) and Hall mobility measurements were also carried out. The films with low Ge content present a reduced crystalline quality, the high deposition temperature promotes growth of larger grains, while higher methane partial pressures determine the reduction of the observed grain size. The ellipsometry measurements show evidence of strong substrate dependency of optical properties of the films. Germanium carbide films with tuned properties can be obtained by a careful selection of combinations of substrates and deposition parameters.

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16:00 **INFLUENCE OF THE NITRIDING PROCESS ON THE BAND-GAP OF TiO2 THIN FILMS WITH PHASE MIXTURE**

Authors : Enrique Camps, V.H. Castrej?n-S?nchez, M.A. Camacho-L?pez, J. G. Qui?ones-Galvan
Affiliations : Enrique Camps, Departamento de F?sica, Instituto Nacional de Investigaciones Nucleares, Apartado postal 18-1027, M?xico D.F., C.P. 11801; V.H. Castrej?n-S?nchez, Facultad de Qu?mica, Universidad Aut?noma del Estado de M?xico, Paseo Col?n y Tollocan, Toluca, M?xico, C.P. 50110; M.A. Camacho-L?pez, Laboratorio de Investigaci?n y Desarrollo de Materiales Avanzados, Facultad de Qu?mica, Universidad Aut?noma del Estado de M?xico, Km 14.5 Carr. Toluca, Atlacomulco, M?xico; J.G. Qui?ones-Galv?n, Departamento de F?sica, Instituto Nacional de Investigaciones Nucleares, Apartado postal 18-1027, M?xico D.F., C.P. 11801

Resume : Titanium dioxide is a semiconductor material that has a large number of applications an also is one of the most widely investigated photocatalyst. Despite of its several advantages, TiO2 only exhibit photocatalytic activity when it is excited using UV radiation. For this reason, actual research has been focused in minimizing the material?s bandgap, allowing excitation with visible light. Titanium dioxide with mixture of phases (anatase rutile) has a lower value of band gap compared with pure anatase TiO2 . In this work it is shown that the nitrogen doping of TiO2 with phase mixture can further reduce the value of the band gap. TiO2 nanostructured thin films with pure anatase phase were deposited by magnetron sputtering. An annealing process was used to induce different quantities of the rutile phase. The anatase/rutile ratio in the films was estimated by Raman spectroscopy. The films with mixture of phases were nitrided in a microwave plasma source. The bad gap of the treated samples was studied by diffuse reflectance, applying the Kubelka-Munk transformation. The results showed that 2.73 eV was the lowest value of band gap, for a nitrided mixture with 30% of anatase

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16:00 **Morphology of graded composite films**

Authors : Stanislav Novak (1), Rudolf Hrach (1, 2), Martin Svec (1)
Affiliations : (1) Department of Physics, Faculty of Science, J. E. Purkinje University, Ceske mladeze 8, 400 96 Usti nad Labem, Czech Republic; (2) Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, V Holesovickach 2, 180 00 Prague 8, Czech Republic

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Resume : The paper presents a novel very efficient tool to research morphological properties of various composite structures. It focuses on the composites/nanocomposites that are created by metal particles (e.g. Ti) in a dielectric (e.g. Carbon-containing) matrix. Nevertheless, the results could be used for other two-phase systems, too. Computer experiments are used for morphological analysis both homogeneous and graded composite/nanocomposite films. The particles are assumed to be more or less randomly distributed in the matrix. A low metal volume fraction is supposed. The hard-sphere method for generation of the composite structures is used. The Voronoi tessellation was chosen as the very efficient method of mathematical morphology to describe the morphology. It is able to describe three-dimensional composite structure morphology using just one two-dimensional section in the given structure. To evaluate the disorder degree of the structure, a scalar measure is introduced. Results for the homogeneous and graded composite/nanocomposite structures are presented. It is shown that the scalar measure gives the possibility to precisely evaluate the disorder degree of the composite structures. The sensitivity of the method is very well and its noise is low. The method developed is section-independent. The computer tool enables a subsequent analysis of electrical properties of the films and their dependence on the morphology.

add to my program (close full abstract)

16:00 **Multi-principal-element (CuSiTiYZr)C coatings for tribological applications**

Authors : M. Braic, M. Balaceanu, A. Vladescu, C.N. Zoita, V. Braic, A.Parau, M. Dinu
Affiliations : National Institute for Optoelectronics, 409 Atomistilor Str., 077125 Magurele-Bucharest, Romania

Resume : Multi-principal-element (CuSiTiYZr)C coatings were prepared by co-sputtering of pure Cu, Si, Ti, Y and Zr targets in an Ar + CH4 atmosphere, for different CH4/(CH4 + Ar) flow rate ratios (0.25; 0.35; 0.50). The films were analyzed for elemental and phase composition, crystalline structure, morphology, mechanical characteristics, corrosion resistance and tribological performance. Ternary (TiZr)C coatings were also examined for comparison. The (CuSiTiYZr)C coatings were found to be amorphous, whatever the CH4/(CH4 + Ar) ratio. For all the coatings, an increase in the carbon content led to an improvement of corrosion resistance, mechanical and tribological film characteristics, mainly due to the formation and development of an amorphous free-carbon phase. The (CuSiTiYZr)C coatings exhibited superior corrosion and wear behaviour, when comparing to (TiZr)C reference coatings with similar carbon content. The highest hardness (29.5 GPa), the lowest friction coefficient (~0.15) and the best wear-corrosion resistance were measured for the (CuSiTiYZr)C coating with carbon/metal ratio of about 1.3 (CH4/(CH4 + Ar) flow rate = 0.50).

G.PI. 26

add to my program (close full abstract)

16:00 **Growth and characterization of arc evaporated TiSiCN-Ni hard coatings**

Authors : M.Balaceanu, M.Braic, C.Vitelaru, A.Parau, A. Vladescu, V.Braic
Affiliations : National Institute for Optoelectronics, 409 Atomistilor, POBox - MG 05, 077125, Magurele- Bucharest, Romania

Resume : Lately, TiSi based nitride, carbide and carbonitride coatings have been received considerable attention due to their remarkable properties such as excellent resistance to oxidation, corrosion, and wear, as well as high thermal stability up to 12000C. The goal of this work was to determine the main characteristics of TiSiCN-Ni coatings prepared by cathodic arc technique. Ni, which is a weak nitride/carbide forming metal, was used as an alloying element for improving the mechanical properties and tribological behaviour of TiSiCN coatings. 3.5-3.8 μm thick coatings were deposited on Si, C45 and 316 L steel substrates in a CH4 +N2 reactive atmosphere, using TiSi alloy and Ni cathodes. Elemental and phase composition, chemical bonds, microstructure, surface and cross-sectional morphologies, mechanical characteristics and tribological performance of the coatings were investigated. The TiSiCN-Ni coatings, with a (N+C)/metal ratio of about 1.2, and N/C ratio of about 0.2 were found to possess a nanocomposite structure, consisting of nanocrystalline FCC solid solution carbonitride and amorphous free-carbon phases. Fine grained surface and dense cross-sectional morphologies were observed. Ni addition to TiSiCN resulted in grain refinement, reduction of stress (from 5.8 to 0.9 GPa) and improved adhesion, while film hardness remained wear rates of 10-6 – 2x10-6 mm3/Nm were measured for the TiSiCN-Ni coatings.

G.PI. 27

add to my program (close full abstract)

16:00 **Deposition and characterisation of (AlCrNbSiTi)C coatings**
Authors : Mariana BRAIC, Mihaela DINU, Iulian PANA, Anca PARAU
Affiliations : National Institute for Optoelectronics, 409 Atomistilor Str., Bucharest, Romania
Resume : Multi-principal-element (AlCrNbSiTi)C coatings were prepared by co -sputtering of pure Al, Cr,Nb,Si and Ti targets in an Ar + CH4 atmosphere, at two different CH4/(CH4 + Ar) flow rate ratios (0.05; 0.1). The films were analyzed for elemental composition, crystalline structure, morphology, mechanical characteristics and tribological performance. Ternary (TiSi)C coatings were also examined for comparison. The (AlCrNbSiTi)C coatings exhibited superior corrosion and wear behaviour, when comparing to (TiSi)C reference coatings with similar carbon content. The highest hardness (22 GPa), the lowest friction coefficient (~0.1) and the best wear-corrosion resistance were measured for the coating with the highest carbon/metal ratio.
G.PI. 29

16:00 **Effect of Si addition on the corrosion resistance, tribological performance and biocompatibility of the TiON, ZrON and TiZrON thin films**
Authors : C.M.Cotrut1, I.Titorencu2, M.Balaceanu3, M.Dinu1,3, C.Vitelaru3, M. Tarcolea1, A.Vladescu3
Affiliations : 1 University Politehnica of Bucharest, 313 Sp.Independentei, Bucharest, Romania 2 Institute of Cellular Biology and. Pathology Nicolae Simionescu, 8 B.P.Hasdeu, PO Box 35 - 14, Bucharest, Romania 3 National Institute for Optoelectronics, 409 Atomistilor, POBox - MG 05, 077125, Magurele- Bucharest, Romania
Resume : Ternary or quaternary coatings based on oxynitrides, oxycarbides or oxycarbonitrides of transition metals have recently attracted increasing interest in biomedical application because of their good biocompatibility and resistance to corrosion. However these coatings present low mechanical strength and the tribological properties which restrict their use as biomaterials in orthopaedy. In this paper we report on the improvement of mechanical and tribological characteristics of TiON, ZrON and TiZrON thin films by Si addition. The 3 μm thick coatings were deposited on Si and CoCrMo alloy substrates by the cathodic arc method in a mixture of nitrogen and oxygen. The coatings were comparatively investigated in terms of the elemental and phase composition, texture, roughness, hardness, adhesion and corrosion behaviour. Biocompatibility investigations consisted in MTT cell viability tests after 1, 3 and 5 days of culture. The results indicated that the films' mechanical properties, tribological performance, corrosion resistance and biocompatibility were improved by Si addition to the basic ternary or quaternary compound (TiON, ZrON and TiZrON). In vitro tests indicated good biocompatibility for all the investigated coatings. A better corrosion resistance, low friction coefficient and higher cell viability were observed for quaternary coatings.
G.PI. 30

16:00 **Structural, morphological and electrical properties of TaxN thin films**
Authors : N.Radić1, K. Salamon2, M. Očko2, I. Bogdanović-Radović1, S. Bernstorff3
Affiliations : 1Rudjer Boskovic Institute, Bijenicka 54, Zagreb, Croatia; 2Institute of Physics, Bijenicka 46, Zagreb, Croatia; 3Elettra, Basovizza, Italy
Resume : Beside being already used in microelectronics, the TaxN thin films hold promise to be applied in certain superconducting devices, as well. The TaxN thin films for that purpose are usually deposited on sapphire, or on SiO2 in order to decrease the cost of a final product. Here we report an interim investigation of the thin TaxN films prepared by reactive magnetron deposition in a wide range of composition deposited on SiO2. Pure tantalum target and Ar + N2 working gas were used. Films (cca 100 nm) were deposited at room temperature and 550 degC, respectively. A selected samples deposited at room temperature were subsequently annealed at intermediate temperatures in a protective atmosphere. The chemical composition of the films was determined by ERDA (0.5
G.PI. 31

16:00 **Structure and mechanical properties of magnetron sputtered quaternary TiZrSiN films**
Authors : G. Abadias1, I.A. Saladukhin2, V.V. Uglov2, S.V. Zlotski2, S.N. Dub3, G. N. Tolmachova4
Affiliations : 1Institut P', Poitiers, France; 2Belarusian State University, Minsk, Belarus; 3Institute for Superhard Materials, Kiev, Ukraine; 4Kharkov Institute of Physics and Technology, Kharkov, Ukraine
G.PI. 32

Resume : The structural and phase state of hard coatings based on transition metal nitrides as well as mechanical properties can be modified by a variation of elemental composition. In the present work we investigate the structural and phase transformations in (Ti,Zr)1-x-ySixNy films depending on Si content and deposition temperature. (Ti,Zr)1-x-ySixNy films have been deposited onto Si (001) wafers by a reactive unbalanced magnetron sputtering method at the temperatures of 270 and 600°C. Ti, Zr and Si targets were co-sputtered under mixed Ar+N2 plasma discharges. Varying the RF power of the Si target from 60 to 200 W resulted in silicon concentration, x, to increase from 0.06 to 0.22 in films. Ti:Zr concentration ratio was kept constant to ~1.0. The synthesized films are the multiphase systems consisting of (Ti,Zr)N nanocrystals surrounded by X-ray amorphous SiNy matrix. When forming at 270°C the (Ti,Zr)N nanocrystals are characterized by (200) preferred orientation. Transformation of nanocrystalline structure of the films into X-ray amorphous state is observed when Si content reaches the value of 0.22. The maximum hardness values, up to 29 GPa, are observed when $0.06 \leq x \leq 0.09$. For (Ti,Zr)1-x-ySixNy films the friction coefficient is less than for TiZrN film and values are in the range of 0.15-0.26. There is a clear tendency of wear resistance increase with x rise up to x=0.11. Correlation of the mechanical properties of the coatings with their structural state is discussed.

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16:00 **Optical performance of nanostructured, decorative Ti-Al-N films using a combinatorial approach**

Authors : N. Pliatsikas1, A. Siozios2, S. Kassavetis2, G. Vourlias1, P. Patsalas1
Affiliations : 1Aristotle University of Thessaloniki, Department of Physics, 54124 Thessaloniki, Greece; 2University of Ioannina, Department of Materials Science and Engineering, 45110 Ioannina, Greece

Resume : The system TiAlN received significant scientific and technological interest due to its exceptional mechanical performance. However, its optoelectronic properties did not receive so much attention, despite of being particularly interesting because of the performance of the constituents (TiN and AlN), which are a conductor and a wide bandgap semiconductor, respectively. In this work we implement a combinatorial approach for the growth of crystalline and amorphous TixAl1-xN films covering the whole x range and forming all the reported crystal phases (rocksalt, wurtzite, mixed, amorphous) by dual cathode sputter deposition. The substrates were not rotating in order to achieve graded composition x over the samples' surfaces. The sputtering power of Ti cathode was changing for each sample; the combination of varying the Ti-power and the graded composition of each sample resulted in a vast number of experimental data. Furthermore, the set of the formed crystal phases (studied by X-Ray Diffraction) was enriched by using two sputtering powers for the Al-cathode that promote the formation of w-AlN and a-AlN, respectively, and studying the addition of Ti in such films. The composition of specific points on the various samples was recorded by topographic X-Ray Photoelectron Spectroscopy (XPS) and associated with the corresponding optical performance recorder by optical reflectance spectroscopy. Thus, we provide detailed color maps based on the composition x of TixAl1-xN.

G.PI. 33

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16:00 **Modified TiN-TiO2 composites intended for high-temperature sensors**

Authors : Eva Bartonickova.Petr Ptacek.Radoslav Novotny.Lukas Kalina.Tomas Opravil.Jaromir Havlica
Affiliations : Materials Research Centre, Faculty of Chemistry, Brno University of Technology, Brno Czech Republic

Resume : Nowadays, modified metallic nitrides are industrially widespread due to their advanced anti-corrosive, electrical and mechanical properties. Especially, TiN is greatly suitable material for desirable high temperature applications (i.e. electrocatalysts, contact or sensors). Paper deals the TiN based cermets (modified by Fe, Al or Ni) synthesis via precipitation reactions and/or high-reaction milling that provide demanded industrial costs reduction. Investigation of morphology (SEM), phase and chemical composition (XRD, XPS and Raman study) of prepared TiN-TiO2 composites are discussed as key parameters for understanding of relation between type of synthesis of the particles and required properties. Finally, bulk properties of as-prepared layers and their dense counterparts were determined.

G.PI. 34

add to my program **(close full abstract)**

16:00 **Comparison between TiAlN films deposited by HPPMS and RF magnetron sputtering**

Authors : D. Valerini, D. Lorenzo, L. Tapfer, and A. Rizzo
Affiliations : ENEA - Italian National Agency for New Technologies, Energy and Sustainable Economic Development - Technical Unit for Brindisi Material Technologies, Laboratory of Materials Technology (UTTMATB-TEC), Brindisi Research Center, S.S. 7 Appia km. 706, 72100 Brindisi, Italy

Resume : Recently, high-power pulsed magnetron sputtering (HPPMS) is a widely studied PVD technique, due to its potential benefits over conventional sputtering deposition. The high power of pulses applied to the target material during HPPMS processes results in high plasma densities and increased ionization rates of the sputtered species, thus producing films with high density, low content of defects, strong adhesion, good smoothness and high hardness. As a result, through the proper choice of deposition parameters, HPPMS-deposited films can exhibit enhanced properties with respect to films deposited by conventional sputtering. These properties can be exploited in several applications, like e.g. in the case of nitride films used as protective hard coatings. Here we report the HPPMS deposition of titanium aluminum nitride (TiAlN) films at different process parameters, comparing the film properties with those of TiAlN films deposited by RF magnetron sputtering. The influence of pulse peak power (up to 300 kW) and length (up to 3 ms), on structural, morphological and tribological (hardness and adhesion) properties was analyzed. X-ray diffraction measurements revealed how the different nitride phases inside the films were tuned by changing the pulse parameters, while scanning electron microscopy showed the corresponding variations in surface morphology and film section. Nanoindentation and microscratch measurements were used to evaluate the improvement in tribological responses.

G.PI. 35

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16:00 **Synthesis of reinforced magnesium embedded in carbon matrix by using Thermionic Vacuum Arc (TVA) technology**

Authors : R. Vladoiu, A. Mandes, V. Dinca
Affiliations : Department of Plasma Physics, Faculty of Physics Chemistry Electronics and Oil Technology, Ovidius University, Mamaia 124, Constanţa, 900527, Romania

Resume : With the expanding use of magnesium materials in numerous new applications within the automotive and consumer goods sectors, there is currently growing interest in developing new applications. For this reason, there is a great demand for joining of Mg in composites such as carbon containing nanostructured thin films, giving rise to unique combination of properties. The aim of the present work is to achieve the controlled synthesis of pure magnesium and nanocrystalline magnesium embedded in hydrogen-free amorphous carbon (a-C) matrix. The films with compact structure and extremely smooth are prepared using the Thermionic Vacuum Arc (TVA) method in one electron gun configuration on glass and OLC 45 special substrate, demanded by industrial area. Nanostructured coatings with homogenous and dense surface without any faults (pinholes and cracks) were achieved at low temperatures to not affect the materials properties. The results of deposition conditions on the morphology, composition and wettability of the coatings were investigated in terms of Transmission Electron Microscopy (HRTEM), XPS, AFM, scanning electron microscopy with energy-dispersive X-ray detection (SEM/EDX) and free surface energy (See System). Reports on optimized coatings by a graded structure and adjusting stress level were also discussed.

G.PI. 36

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16:00 **Multifunctional relations between synthesis conditions, material nanostructure and thin films properties of Ti added in carbon matrix**

Authors : VLADOIU Rodica1, DINCA Virginia1, MANDES Aurelia1, PRODAN Gabriel1
Affiliations : 1 Dep. of Plasma Physics, Faculty of Applied Science and Engineering, Ovidius University, Mamaia 124, Constanta, 900527, Romania

Resume : Modern engineering applications demand development of hard coatings with improved wear resistance combined with low friction and high toughness. Titanium carbide is one of the most widely used hard coating materials. Interestingly, its chemical bonding is similar as transition metal showing mixed covalent, metallic and ionic characters. A wide variety of techniques have been used to synthesize TiC metal carbide thin films. Among these, a well-established technique is the Thermionic Vacuum Arc (TVA) method. This method uses an electron beam emitted by an externally heated cathode that will evaporate the anode materials, found inside a crucible. The

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paper reports relations between synthesis conditions, material nanostructure and thin films properties of Ti added in carbon matrix. The surface morphology, wettability and strength of the obtained TiC multifunctional thin films were investigated. The thin films were characterized using: transmission electron microscope (TEM, Phillips CM 120 ST, 100 kV) and SEE SYSTEM contact angle device. Nanocomposite coatings of obtained TiC consisting of crystalline phase embedded into an amorphous matrix constitute a multifunctional coating architecture due to its combination of properties, suitable for emerging applications in metallurgical industry, yielding an enhanced corrosion resistance.

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16:00 **Evaluation of wear resistance of CrB(N) films by sliding-, impact-, and abrasive tests**

Authors : Ph.V. Kiryukhantsev-Korneev1, J.F. Pierson2,3
Affiliations : 1- National University of Science and Technology MISIS,Moscow 119049, Russia 2- Institut Jean Lamour, Université de Lorraine, UMR 7198, Nancy, F-54000, France 3- CNRS, Institut Jean Lamour, UMR 7198, Nancy, F-54000, France

Resume : Nanostructured nc-CrB2 and nanocomposite nc-CrB2/a-BN films were deposited by DC magnetron sputtering of CrB2 target in Ar and Ar+(10, 15, and 25)%N2 gas mixtures. The structure, chemical and phase composition of films were studied before [1]. The films were characterised by scratch-test, micro- and nanoindentation. Behaviour of films in sliding condition was investigated in "pin-on-disk" configuration. Steel and cemented carbide were used as the counter-part materials. The impact wear of films were studied by "ball-on-plate" cyclic impact machine. Three groups of tests with 103, 104, 105 cycles were performed. Abrasive resistance was estimated by calowear-tester. Rotation speed and load were varied in the experiments. Failure zones on the film surface after all tests were investigated by optical profilometry, optical and scanning electron microscopy. Results obtained show that the wear resistance of the films increased significantly with raising of nitrogen content in the films due to strong structure modification. Influence of hardness, plasticity index, resistance to the plastic deformation, adhesion strength, crack resistance on the tribological characteristics are discussed. [1] Ph.V. Kiryukhantsev-Korneev, J.F. Pierson, M.I. Petrzhik et al. Thin Solid Films 517 (2009) 2675

G.PI. 38

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16:00 **Influence of the substrate bias potential on the properties of ta-C coatings deposited using a water-cooled electromagnetic Venetian blind plasma filter**

Authors : V. Zavaleyev, J. Walkowicz
Affiliations : Koszalin University of Technology, Institute of Technology and Education, ul. Sniadeckich 2, 75-453 Koszalin, Poland

Resume : The paper presents the research results on the formation of amorphous ta-C films with a minimum amount of defects, deposited by pulsed vacuum-arc method with the use of a water-cooled electromagnetic Venetian blind plasma filter. The subject of the research was the influence of the substrate bias voltage, in the range of -25 to -200V, on the structural and mechanical properties of ta-C coatings. Dependence of the microstructure and phase composition of ta-C films on the substrate bias voltage were analyzed by Raman and XPS spectroscopy. The results of the structural analysis of coatings showed characteristic changes in the content of the diamond-like sp3 fraction on the substrate potential. Mechanical properties of ta-C films ? roughness, adhesion, hardness and Young's modulus were investigated using a profilometer, the scratch tester and a nanoindenter. The highest content of sp3 bonds, of about 63%, was obtained in the coating deposited at the substrate bias potential of -100V, which also showed the minimum surface roughness and maximum hardness and Young's modulus of 50GPa and 371GPa respectively. Synthesized carbon coating had excellent adhesion ? complete film delamination occurs at the load of 41N. Application of an electromagnetic Venetian blind plasma filter for deposition of thin ta-C coatings with a minimum amount of defects and enhanced properties opens new possibilities for the design and the use of such filters.

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PROGRAM VIEW : 2014 Spring
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Symposium : G

Carbon- or nitrogen-containing nanostructured thin films

26 May 2014 | **27 May 2014** | 28 May 2014 | 29 May 2014 | 30 May 2014

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start at	Subject	Num.
	Recent advances in polymer based thin films : Yi DAN, Lenka ZAJICKOVA	
08:30	**Controlling the Nanostructure and Stability of a-C:H:N Plasma Polymers** **Authors :** Dirk Hegemann **Affiliations :** Empa, Swiss Federal Laboratories for Materials Science and Technology **Resume :** Plasma polymer deposition enables the controlled modification of material's surfaces such as e.g. polymers (including textiles and fibers) at the nanoscale. Industrial applications based on plasma polymer deposition require reliable processes that can be transferred to production-scale reactors. For this purpose, both gas phase and surface processes should be well controlled during plasma polymerization. While gas phase processes are governed by the energy invested per particle (plasma chemistry), surface processes also depend on the energy flux and on the momentum transfer during film growth (plasma physics). For the deposition of a-C:H:N plasma polymers gaseous mixtures of NH3/C2H4 as well as N2/H2/C2H4 are examined using RF discharges both in a batch reactor and in a pilot plant (at low pressure). The gas composition and energy input are found to determine the incorporation of nitrogen into the hydrocarbon network, while ion bombardment during film growth supports the formation of nucleation sites, surface diffusion, chemical bond opening and cross-linking. The amine-functional group density thus depends both on gas phase and surface processes. Moderate energetic conditions favor the formation of voids during film growth due to steric hindrance of incorporated amino groups resulting in a nanoporous film structure. Such a-C:H:N films are used for the attachment of molecules (e.g. thermoresponsive PEGs enabling controlled drug release through membranes) as well as for improved adhesion (e.g. light-weight fiber-reinforced composites). Plasma polymers containing more than 2 at% of amino groups, however, undergo hydrolysis and show leaching of polyamines in aqueous environments which has to be considered for biomedical applications (e.g. tissue engineering). The remnant films (after washing the leachable products) are found to be very stable enabling for example superhydrophilic surfaces due to the remaining nanostructure.	G.III 1
	add to my program (close full abstract)	
09:00	**Experimental and theoretical study of the plasma-surface interaction during the growth of ethyl-lactate plasma polymers** **Authors :** S. Ligot , P. Raynaud , P. Gerbaux , V. Lemaur , R. Snyders **Affiliations :** Chimie des Interactions Plasma-Surface, CIRMAP, Université de Mons, Place du Parc 23, B-7000 Mons, Belgium ; Matériaux et Procédés Plasmas, Université Paul Sabatier, 118, route de Narbonne, F-31062 Toulouse, France ; Groupe de Recherche en Spectrométrie de Masse, Université de Mons, Place du Parc 23, B-7000 Mons, Belgium ; Chimie des Matériaux Nouveaux, CIRMAP, Université de Mons, Place du Parc 23, B-7000 Mons, Belgium ; Chimie des Interactions Plasma-Surface, CIRMAP, Université de Mons, Place du Parc 23, B-7000 Mons, Belgium **Resume :** Polylactic acid (PLA), derived from renewable resources, is a (bio) degradable polymer accepted as a good alternative to conventional polymers for packaging applications. Nevertheless, as for other polymers, it presents too high water and gas permittivity. In order to improve its barrier properties and, as a consequence, its degradation rate, we are developing a cross-linked ethyl lactate-based plasma polymer film (ELPPF). The control of both chemical composition (hydrolysable ester bonds density) and cross-linking degree would allow tuning the degradation rate of the polymer by ester bond hydrolysis [1].	G.III 3

In this work, our objective is to correlate the plasma and film chemistries and, ultimately, to propose a clear picture of the plasma-surface interaction during the process. ELPPF have been synthesized by PECVD using both continuous and pulsed RF power (PRF) through an ICP copper coil (5 W < PRF < 400 W). The ELPPF chemistry, especially the ester function density, has been evaluated by the combination of chemical derivatization and XPS measurements and compared to the plasma phase composition measured by using RGA mass spectrometry and in situ infrared spectroscopy. These plasma diagnostic data are discussed in view of DFT calculations. Our data reveal that the mass spectrometry (MS) data supported by DFT calculations allow proposing a clear fragmentation pattern of the precursor as a function of the experimental conditions [2]. Nevertheless MS, as single diagnostic tool, does not allow evaluating the density of ester groups in the plasma phase. It is therefore necessary to combine MS with in situ infrared spectroscopy. The latter data are understood using synthetic IR spectra generated by DFT calculations. In the defined experimental window, by increasing PRF, the ester content in the ELPPF decreases from 18 at.% to 1.4 at.% which is perfectly correlated to the decrease of the ester density in the plasma phase from 2.2x1015 to 9.1x1012 molecules/cm³. Altogether, this set of data paves the way for a reproducible and controllable synthesis of ELPPF with defined chemical composition. [1] S. Ligot, F. Renaux, L. Denis, D. Cossement, N. Nuns, P. Dubois, R. Snyders, Plasma Process. Polym. 2013, 10.1002/ppap.201300025. [2] S. Ligot, M. Guillaume, P. Gerbaux, D. Thiry, F. Renaux, J. Cornil, P. Dubois, R. Snyders, Accpeted for publication in the Journal of physical chemistry C

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09:15 **Elaboration of plasma-polyaniline nanofibers by discharge power variation**

Authors : Andrii Zaitsev, Fabienne Poncin-Epaillard, Ana Lacoste, Dominique Debarnot
Affiliations : CUE LUNAM, UMR Université du Maine, CNRS 6283, Institut des Molécules et Matériaux du Mans (IMMM), Département Polymères, Colloïdes et Interfaces (PCI), avenue Olivier Messiaen, 72085 Le Mans, France; CUE LUNAM, UMR Université du Maine, CNRS 6283, Institut des Molécules et Matériaux du Mans (IMMM), Département Polymères, Colloïdes et Interfaces (PCI), avenue Olivier Messiaen, 72085 Le Mans, France; Laboratoire de Physique Subatomique et de Cosmologie, Université Joseph Fourier Grenoble 1, CNRS/IN2P3, Institut Polytechnique de Grenoble, 53, Avenue des Martyrs, 38026 Grenoble, France; CUE LUNAM, UMR Université du Maine, CNRS 6283, Institut des Molécules et Matériaux du Mans (IMMM), Département Polymères, Colloïdes et Interfaces (PCI), avenue Olivier Messiaen, 72085 Le Mans, France

Resume : The interest of one-dimensional materials has been demonstrated in a great number of applications due to their high shape factor and sometimes, new properties. The objective of this work is to synthesize polyaniline nanofibers thanks to the plasma technique without using any template. The polymerization of polyaniline is conducted by chemical vapor deposition (PECVD) thanks to a reactor that provides the possibility of PEPVD and PECVD. It uses the multi-dipolar microwave-assisted excitation source that offers uniform plasma at low precursor pressures (0.01 Torr) and low energy supply (60W). Also the advantage of this configuration is that the substrate is situated out of the plasma phase that prevents the polymer from the degradation. In this work, a new process called the step power variation plasma process has been developed that allows obtaining a nanostructured polymer combined with a high retention of the monomer structure. The effects of discharge power and deposition time on the morphology and chemical structure are studied using this new process. The morphology of the polymer is studied by the means of atomic force microscopy (AFM). The chemical structure of the fibers is studied by Fourier transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS). This work was supported by Région Pays de la Loire.

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09:30 **A detailed description of the chemistry of thiol supporting plasma polymer films**

Authors : Damien Thiry (1), Remy Francq (1,2), Maxime Guillaume (3), Jérôme Cornil (3), Rony Snyders (1, 2)
Affiliations : (1) Chimie des Interactions Plasma Surface, CIRMAP, University of Mons, Place du Parc 23, B-7000 Mons, Belgium (2) Materia Nova Research Center, Parc Initialis, Avenue N. Copernic 1, B-7000 Mons, Belgium (3) Service de Chimie des Matériaux Nouveaux, CIRMAP, University of Mons, Place du Parc 23, B-7000 Mons, Belgium

Resume : Plasma polymerization of sulfur-based molecules such as propanethiol is a promising approach to grow thiol (-SH) supporting surfaces that can serve as nucleation centers for gold nanoparticles or for the immobilization of DNA molecules. However, despite the potential of such a kind of thin films, it is still necessary to get a deeper understanding of the plasma

G.III 5

polymerization of sulfur-based precursors. In this work, propanethiol plasma polymers (Pr-PPF) were synthesized varying the mean power (

) dissipated in the discharge in pulsed and continuous modes. The –SH density ([SH]) is measured by means of XPS combined with a recently developed derivatization method. As a function of

, nearly constant values of [SH] of the Pr-PPF are observed. This peculiar behavior is explained considering (i) mass spectrometry data revealing a similar relative concentration of condensable SH-bearing species in the plasma and (ii) similar energetic conditions at the growing film/plasma interface. On the other hand, it has been observed that the low

synthesized Pr-PPF are not chemically stable in aqueous solutions likely due to the release of trapped sulfur-based species supported by mass spectrometry measurements. In addition, DFT calculations have been employed to assist the interpretation of the experimental data. The whole set of our data allows drawing a clear picture of the growth mechanism of Pr-PPF which is essential in view of the optimization of the layers properties.

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09:45 **New way to deposition of phosphorus nitride film on InP: phosphazene like film**

Authors : C.Njel, D.Aureau, A-M Gonçalves*, A.Etcheberry
Affiliations : Institut Lavoisier de Versailles ILV - UMR- CNRS 8180 (http://www.ilv.uvsq.fr) UVSQ, 45, Avenue des Etats-Unis 78000 Versailles Cedex-France. *Fax/Tel: + 33 (0) 1 39 25 44 19/18 - E-mail: anne-marie.goncalves@uvsq.fr

Resume : This paper deals with a novel nitrogenated III-V passivation route, which involves a self-limited nanoscale process. Film properties have shown extreme chemical resistance and no ageing of surface properties when exposed to ambient air over 18 months, as confirmed by XPS analysis. The beginnings of phosphazene science can be traced back more than 180 years to the discovery by Liebig[1]. This polymer differs from others because the unsaturated phosphorus nitrogen bonds are not organic. Phosphorus nitride insulating films as passivation layers on InP seem to be very attractive to realize MISFETs with high channel electron mobilities and low interface state densities. This is mainly due to the presence of the common P element in the film and the substrate; this increases the adhesion of the PN passivating film. The deposition of phosphorus nitride on InP by several methods and the dielectric properties have been described by different authors[2-3].This paper presents an original electroless approach for the formation of this polyphosphazene film on InP in liquid ammonia (-55 °C). The electroless mode is attractive to the industry since it avoids any electrical (potential and current) control of the interface. As a result, an ultra thin film which structures the interface at a nanometer scales has been obtained. In this work, the electrochemical tools (open circuit potential, capacitance measurements) and XPS analysis are used to characterize the formation of the passivated film.

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10:00 **Coffee break**

Recent advances in transition metal nitrides-I : Christian MITTERER, JF PIERSON

10:30 **Control of Micro- and Nanostructure in Transition Metal Nitrides: Recent Advances**

Authors : Ivan Petrov
Affiliations : University of Illinois, USA and Linköping University, Sweden

Resume : Polycrystalline TiN and related transition-metal nitride (TMN) thin films are typically deposited by reactive magnetron sputter deposition and employed as diffusion barriers in microelectronics as well as hard, wear-, and corrosion-resistant coatings in mechanical and optical applications. We use a combination of HR-XRD, TEM, HR-XTEM, AFM, and STM analyses to characterize micro- and nanostructures. We will review the fundamental film growth processes - nucleation, coalescence, competitive growth, and recrystallization - and their role in thin film microstructure evolution as a function of substrate temperature. Special attention will paid to in-situ substrate treatment by ion-

G.IV. 1

irradiation and its effect on film microstructure and adhesion. Using spontaneous natural patterning processes, we show that self-organized nanostructures consisting of commensurate nanolamellae, nanocolumns, nanospheres, and nanopipes can be synthesized to further extend the range of achievable properties. All of these structures are a result of kinetic limitations and require low growth temperatures combined with low-energy (less than the lattice atom displacement potential), very high flux, ion irradiation during deposition. Quantitative information of adatom transport and surface site energies required for the models are obtained from in-situ high-temperature STM and LEEM analyses. In addition, we use classical molecular dynamics and the modified embedded atom method formalism to investigate the dynamics of atomic-scale transport and film growth on a low-index model compound surface, TiN(001). This approach allows us to gain insight in kinetics of the pathways of Ti, N, and TiNx (x = 1 – 3) adspecies on terraces and single-atom-high TiN(001) in the picosecond regime which are not accessible by state of the art atomistic experimental techniques or by static DFT calculations. We will also review recent advances in the selective use of metal ions during HIPIMS co-sputtering to extend the attainable structures and properties in metastable TMN with examples of Ti(1-x)AlxN, Ti(1-x)SixN, ad Ti(1-x)TaxN.

add to my program (close full abstract)

11:00 **Elastic properties of ternary nitride hard coatings: experimental and computational approaches**

Authors : G. Abadias (1), Ph. Djemia (2), L. Belliard (3)
Affiliations : 1. Institut P', CNRS-UPR 3346, Université de Poitiers, France; 2. LSPM, CNRS-UPR 3407, Université Paris 13, Sorbonne Paris Cité, France; 3. INSP, CNRS-UMR 7788, Université Pierre et Marie Curie, France

Resume : Since the pioneering materials selection concept of Holleck [1] to design multi-component hard coatings, efforts have been made to synthesize new ternary or multinary transition metal nitride (TMN)-based alloys, which offer the possibility of fine tuning the mechanical and physical properties by an appropriate choice of metal or non-metal alloying elements and by optimizing deposition process parameters. Recent ab initio calculations by Sangiovanni et al. [2] have shown that Mo and W alloying into TiN decisively induced a ductile behaviour, which corresponds to a shear modulus to bulk modulus (G/B) ratio lower than 0.5, while retaining high hardness. However, there exists little experimental evidence of such improved ductility, as the elastic properties of such metastable compounds are scarcely studied. In an effort to address this issue, we have carried out a thorough investigation of the elastic properties of various ternary TMN systems, by combining thin film growth experiments and computational modeling. Three systems will be comparatively reviewed, TiZrN, TiTaN and TaZrN, for which the valence electron concentration spans the region of interest from 9 to 10 and which corresponds as well as to iso- and non-isostructural cases. All ternary films were obtained by reactive magnetron co-sputtering in Ar+N2 atmosphere, with the composition covering the whole range from binary counterparts. The transverse and longitudinal sound velocities were determined by Brillouin Light scattering (BLS) and picoseconds acoustics (PA), while the hardness was measured by nanoindentation. The evolution with composition of polycrystalline (effective) elastic constants , deduced from BLS and PA, will be compared to that of single-crystal elastic constants cij derived from ab initio calculations (on ordered and disordered alloys with cubic structure). The influence of phase composition, crystal structure, preferred orientation and film morphology on the elastic and mechanical properties will be discussed. Rather complex variations of and elastic constants with alloy composition are reported for both TiTaN and TaZrN systems. First, the evolution of and does not reflect in a direct way the evolution of sound velocities due to the large increase in mass density as TaN fraction increases. Another important contribution arises from the change in texture and phase composition observed for TaN-rich films. Interestingly, for TaN atomic fractions ranging from 0.5 to 0.8, the formation of a nanocomposite structure, with cubic and hexagonal grains, results in enhanced hardness (>30 GPa). [1] H. Holleck, J. Vac. Sci. Technol. A 4, 2661 (1986) [2] D. G. Sangiovanni, L. Hultman, V. Chirita, Acta Mater. 59, 2121 (2011)

G.IV.2

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11:15 **Nanostructured tantalum nitride thin films for diffusion barriers**

Authors : L. Boulat, R. Viennois, M. Dadras, D. Ravot, N. Fréty
Affiliations : Université Montpellier 2, Institut Charles Gerhardt, UMR 5253 CNRS-UM2-ENSCM-UM1, cc 1504, Place E. Bataillon, 34095 Montpellier Cedex 5, France ; Université Montpellier 2, Institut Charles Gerhardt, UMR 5253 CNRS-UM2-ENSCM-UM1, cc 1504,

G.IV.3

Place E. Bataillon, 34095 Montpellier Cedex 5, France ; Centre Suisse d'Electronique et de Microtechnique SA, Jaquet-Droz 1, Case Postal, CH-2002 Neuchâtel, Switzerland ; Université Montpellier 2, Institut Charles Gerhardt, UMR 5253 CNRS-UM2-ENSCM-UM1, cc 1504, Place E. Bataillon, 34095 Montpellier Cedex 5, France ; Université Montpellier 2, Institut Charles Gerhardt, UMR 5253 CNRS-UM2-ENSCM-UM1, cc 1504, Place E. Bataillon, 34095 Montpellier Cedex 5, France

Resume : Tantalum nitride thin films have received particular interest during the past three decades due to the unique properties of this material such as low electrical resistivity and good thermal stability. These thin films have been widely used as diffusion barriers for microelectronic applications. In this work nanostructured tantalum nitride thin films have been developed to study their potentiality as diffusion barriers for thermoelectric devices. The tantalum nitride barrier was deposited by radio-frequency sputtering process between the CeFe4Sb12 skutterudite substrate and the Cu electrode. The thermal stability of the nitride layer was investigated using X-ray diffraction (XRD), Secondary Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The as-deposited thin layers are made of nanocrystalline grains, with a size of about 5 nm, embedded in an oxynitride amorphous phase. The barrier efficiency of these tantalum nitride-based layers was investigated from CeFe4Sb12/TaN/Cu samples annealed at 673 K. Results showed that the formation of the Cu2Sb and CeCu2 intermetallic phases due to the interdiffusion of Sb, Ce and Cu elements can be inhibited with a tantalum nitride interlayer. Consequently nanostructured tantalum nitride-based films appear as promising diffusion barriers for thermoelectric energy systems made of CeFe4Sb12/Cu couples.

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11:30 **The Effect of Microstructure on the Thermal Conductivity of Nanoscale Polycrystalline AlN Thin-Films**

Authors : Juliana Jaramillo; Wassim Kassem; Yann Chalopin; Emmanuel Ollier; Sebastian Volz
Affiliations : Laboratoire des Composants pour la Conversion de l'Energie, CEA; Laboratoire d'Energétique Moléculaire et Macroscopique, CNRS, Ecole Centrale Paris; Laboratoire d'Energétique Moléculaire et Macroscopique, CNRS, Ecole Centrale Paris; Laboratoire des Composants pour la Conversion de l'Energie, CEA; Laboratoire d'Energétique Moléculaire et Macroscopique, CNRS, Ecole Centrale Paris

Resume : In the process of understanding and developing a structured material permitting the modulation of phonon transport, we investigated how growth parameters influence microstructure and thermal conductivity of aluminum nitride (AlN) thin-films. Wurtzite AlN thin films were deposited by reactive RF and DC sputtering on Si(100) and Al2O3(0001) substrates. The influences of chamber pressure, N2 flow rate, applied power and substrate nature on deposition rate, crystalline structure and morphology of polycrystalline AlN thin-films were studied. The microstructure and texture of the films were characterized by X-ray diffraction and scanning electron microscopy. The experimental results showed that sputtering at a lower pressure leads to a higher deposition rate and a sufficiently high ion energy to form a textured AlN film with (002) preferred orientation. (002) crystallographic orientation is also enhanced with the increase in nitrogen (N2) concentration when maintaining a moderate applied power. Strong influence of the substrate on the growth mechanism of the AlN films was observed. The thermal conductivity was found to increase for strong fiber texture depending on the microstructure and growing conditions. Results regarding the influence of microstructure and preferred orientation on thermal conductivity of the material system are discussed.

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11:45 **Low sheet resistance titanium nitride films by low-temperature plasma-enhanced atomic layer deposition using design of experiments methodology**

Authors : Micheal Burke, Alan Blake, Ian M. Povey, Michael Schmidt, Nikolay Petkov, Patrick Carolan, Aidan Quinn.
Affiliations : Tyndall National Institute

Resume : A design of experiments methodology was used to optimize the sheet resistance of titanium nitride (TiN) films produced by plasma-enhanced atomic layer deposition (PE-ALD) using a tetrakis(dimethylamino)titanium precursor in a N2/H2 plasma at low temperature (250 ?C). At fixed chamber pressure (300 mTorr) and plasma power (300 W), the plasma duration and N2 flow rate were the most significant factors. The lowest sheet resistance values (163 ohms/sq. for a 20 nm TiN film) were obtained using plasma durations ~ 40 s, N2 flow rates > 60 standard cubic centimeters per minute and purge times ~ 60 s. Time of flight secondary ion mass spectroscopy data revealed reduced levels of carbon contaminants in the TiN films with lowest sheet resistance (163

G.IV. 5

ohms/sq.), compared to films with higher sheet resistance (400 to 600 ohms/sq.) while transmission electron microscopy data showed a higher density of nano-crystallites in the low-resistance films. Further significant reductions in sheet resistance, from 163 ohms/sq. to 70 ohms/sq. for a 20 nm TiN film (corresponding resistivity ~ 145 micro-ohm.cm), were achieved by addition of a post-cycle Ar/N2 plasma step in the PE-ALD process.

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12:00 **Lunch break**

Modeling : Valeriu CHIRITA, Stanislav NOVAK

14:00 **Optical Absorption of Carbon-Metal Nanocomposites**

Authors : G. Hadjisavvas1, G. Tritsaris2, C. Mathioudakis1, E. Kaxiras2, and P. C. Kelires1
Affiliations : 1 Research Unit for Nanostructured Materials Systems, Department of Mechanical and Materials Science Engineering, Cyprus University of Technology, P.O. Box 50329, 3603 Lemesos, Cyprus; 2 Department of Physics, Harvard University, Cambridge, Massachusetts02138, USA

Resume : Carbon-based materials, including diamond-like carbon (DLC), have been suggested as promising materials for solar energy harvesting. The properties of DLC may be tuned by the incorporation of transition metal atoms, either dispersed or forming nanoparticles. In a recent work [1], we studied DLC/metal nanocomposites, with metal atoms (Ag, Cu) dispersed in the matrix at substitutional sites. We used 64-atom computational cells and density functional theory (DFT) calculations. We found that metal inclusions enhance the optical absorption in the visible, but lower the sp3 fraction and thus the strength and hardness of the DLC matrix. Here, we extend these studies to the nanoparticle case. We start with metal atoms inserted in the DLC matrix interstitially, which eventually grow into larger nanocrystals. We use larger cells of 512 atoms. The initial DLC networks are generated with tight-binding calculations. The final structures with metals are relaxed with DFT and then properties are calculated. The first results indicate that the reduction of sp3 fraction is less drastic than in the dispersed case, which is beneficial for the mechanical properties. Also, the optical absorption is enhanced. By decomposing the absorption coefficient into site contributions, we aim to identify the strong absorbing atoms in the system, especially in the metal nanocrystals. [1] G. Tritsaris, C. Mathioudakis, P. C. Kelires, and E. Kaxiras, J. Appl. Phys. 112, 103503 (2012).

G.V. 1

add to my program (close full abstract)

14:15 **Crossover from coalescence-controlled to impingement-controlled growth in metal-on-insulator thin film deposition**

Authors : Bo Lü, Viktor Elofsson, Daniel Magnfält, Peter Münger and Kostas Sarakinos
Affiliations : Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83, Linköping, Sweden

Resume : Deposition of metal vapour on insulating substrates commonly proceeds in the so-called Volmer-Weber growth mode, in which isolated islands nucleate, grow in size, coalesce, form an electrically conducting network (percolation) and eventually form a continuous structure. The initial formation stages, i.e., island nucleation, growth and coalescence set characteristic length scales on the growing surface. Therefore, fundamental understanding of the dynamics of those formation stages and of their complex interplay is paramount of knowledge-based design and synthesis of thin films and nanostructures. By establishing the effect of growth conditions on the scaling behaviour of characteristic transition thicknesses, e.g., the percolation transition thickness, theoretical research has suggested the existence of two regimes; one in which growth is dominated by coalescence and a second one in which growth behaviour is determined by island growth and impingement. Here we use kinetic Monte-Carlo growth simulations and analytical expressions to derive the universal condition for the transition from one regime to another as a function of adatom arrival rate, adatom surface diffusivity and coalescence completion rate. Experimental evidence for the existence of both regimes is provided by monitoring in-situ the growth of Ag on SiO2 both by continuous and pulsed vapour fluxes. The implications of our findings for surface science and surface engineering communities are discussed.

G.V. 2

add to my program (close full abstract)

14:30 **Morphological and electrical properties of composite films affected by growth conditions**

Authors : M. Svec1, S. Novak1, R. Hrach1,2
Affiliations : 1Faculty of Science, J. E. Purkinje University, Usti nad Labem, Czech Republic 2Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Resume : Composite films are very interesting materials for their extraordinary physical properties. These properties can be strongly influenced by geometry of inclusions embedded into an amorphous or crystalline matrix. The inclusions are metal particles (e.g. Ti) and the matrix can be an oxide or a polymer in our case. We have dealt with particles of spherical or regular shapes in our previous work. Experimentally observed structures give us information that the particles are often of more general form. In our contribution, we study an influence of inclusion shapes on morphological and transport properties of composite films by help of a self-made simulation and analytical tool. We prepared several sets of model structures with the shape of inclusions close to a general shape (irregular geometry). The shape and distribution of inclusions are strongly affected by growth conditions of the composite structure. Composite structures are prepared by the help of several models where especially the Monte Carlo method is used. Mathematical morphology methods are used for analysis of these structures in both two-dimensional (sections and projections) and three-dimensional cases. Transport properties of such structures are revealed by the theory of percolation, in particular to determinate a percolation threshold in light of electrical conductivity and the geometry of an infinite cluster (backbone, dead -ends, critical bonds). Finally, the morphological and transport results are compared and relationships between the geometry and transport properties in connection with growth conditions are searched.

G.V. 3

add to my program (close full abstract)

14:45 **Doping induced Rashba spin splitting in graphene and BN nanoribbons**

Authors : Andrzej Skierkowski, Mikolaj Sadek, Jacek A. Majewski
Affiliations : Faculty of Physics, University of Warsaw, ul. Hoza 69, PL-00-681 Warszawa, Poland

Resume : Hexagonal, single atom layers of carbon (graphene) and BN have emerged recently not only as a very promising candidate for charge electronics but also for spintronics. However, the very tiny spin-orbit interaction in these systems hinders many potential spintronic applications of graphene and BN. Therefore, as a remedy to this problem, the doping of graphene layers with various atoms has been proposed. Here, we present first-principles studies of the zero field spin splitting of energy bands in graphene and BN layers and nanoribbons functionalized by substitution of Si, Ge, Sn, Pb, and Ca at various concentrations. In contrast to pristine graphene, the BN layers have considerable band gap, so it is interesting to figure out the role of the band gap on the doping induced spin splitting. We perform non-perturbative fully relativistic ab initio calculations in the framework of density functional theory and pseudopotential method. Our calculations reveal that the functionalized graphene layers change considerably their electronic structure (e.g., the fundamental band gap moves from K to Γ k-point) and the linear-k spin splitting of Bychkov-Rashba type appears in the energy spectra. From our ab initio calculations, we determine the magnitude of the constant in the Bychkov-Rashba effective Hamilltonian, and discuss the magnitude of this constant as a function of the adsorbate's type and concentration. We consider also the functionalized graphene and BN nanoribbons, which allows us

G.V. 4

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15:00 **Kinetics of bilayer graphene growth on copper**

Authors : Ning Yang, Kemal Celebi, Hyung Gyu Park
Affiliations : Nanoscience for Energy Technology and Sustainability, Department of Mechanical and Process Engineering, ETH Zurich

Resume : Bilayer graphene has been attracting great interest due to its unique electronic and thermal transport properties. However, scalable synthesis of graphene bilayers remains challenging. Here, we report a systematic study on the kinetics and termination mechanisms of bilayer graphene growth on copper. We find that it is the continuous carbon supply, rather than the initially captured carbon species, which drives the secondary graphene layer enlargement, implying the role of surface diffusion between the top layer graphene and copper surface. Graphene re-growth experiments support selective enlargement of the secondary graphene layers already existing, while re-growth of the top first graphene layer is inhibited, ascribed to the oxidation of the nearby copper surface. Based on these findings, we present strategies for growing large-scale, continuous bilayer graphene synthesis on copper.

G.V. 5

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15:15 **Large scale exfoliation of BN nanosheets by sonication and ball milling**

Authors : Konstantinos Kouroupis-Agalou, Andrea Liscio; Emanuele Treossi; Luca Ortolani; Vittorio Morandi; Nicola Maria Pugno; Vincenzo Palermo
Affiliations : Institute of Organic Synthesis and Photoreactivity, Council of National Research (ISOF-CNR), Bologna, Italy.

Resume : A main advantage for large scale applications of Graphene and related 2-dimensional materials is that they can be produced on large scales by liquid phase exfoliation. The exfoliation process shall be considered as a particular fragmentation process, where the 2-dimensional (2D) character of the exfoliated objects will influence significantly fragmentation dynamics as compared to standard materials. Here, we used automatized image processing of Atomic Force Microscopy (AFM) data to measure, one by one, the exact shape and size of thousands of nanosheets obtained by exfoliation of an important 2D-material, Boron Nitride, and used different statistical functions to model the asymmetric distribution of nanosheets sizes typically obtained. Being the resolution of AFM much larger than the average sheet size, analysis could be performed directly at the nanoscale, and at single sheet level. We find that the size distribution of the sheets at a given time follows a log-normal distribution, indicating that the exfoliation process has a "typical" scale length that changes with time and that exfoliation proceeds through the formation of a distribution of random cracks that follow Poisson statistics.

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15:30 **Dynamic Electronic Response of Metal-Coated Graphene: A First Principle Study**

Authors : Deng Tianqi [1 2], SU Haibin [1 2], Dominique BAILLARGEAT [2]
Affiliations : 1. School of Materials Science and Engineering, Nanyang Technological University, Singapore; 2. CNRS International NTU THALES Research Alliance, Nanyang Technological University, Singapore

Resume : With exotic electronic properties and low dimensional structures, graphene thin films and carbon nanotubes seem quite suited for nanoscale electronic devices and therefore attract numerous theoretical and experimental studies. Although free-standing graphene and carbon nanotubes are reasonable models in many cases, the role of environment including electrode and metal gate is fundamental in real devices. To eliminate the effect of metal-graphene contact in such electronic devices, a first principle study is conducted on the dynamic response of metal-coated graphene. Random phase approximation is employed together with density functional theory to simulate the frequency dependent dielectric function and optical conductivity. A variety of metals with different metal-graphene interaction types, from traditional electrode materials like Cu, Ag and Au, to some other important metals including Ti, Pt, Pd, Co etc, are compared. The bond type and doping effect between metal and graphene are proved critical to device performance and a reasonable choice of material is therefore essential in design. This work helps understanding the importance of metal composite in metal-carbon matrices and provides a reference for designing carbon-based AC nano-devices.

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15:45 **Coffee break**

Functional carbon- or nitrogen-containing nanostructured thin films -II : Brigitte BOUCHET-FABRE, Tomas POLCAR

16:30 **Recent innovative coatings developments for aerospace, biomedical and oil & gas industries at Tecvac**

Authors : Sarah Banfield Jonathan Housden
Affiliations : Research Manager

Resume : Tecvac has been involved in developing and supplying advanced wear resistant coatings for over 30 years. The coatings, which include amongst others, TiN, CrN, TiAlN, CrAlN, DLC and WCC are usually deposited by PVD or CVD techniques for use in a wide range of industries. In recent years, research into innovative coating development at Tecvac has centred on three main industries namely aerospace, biomedical and oil and gas. In the aerospace sector for example, this has led to the development of multilayer erosion-resistant PVD coatings for application on aero-engine turbine blades to improve efficiency and extend the life of aircraft engines. Also in the aerospace industry, Tecvac was recently involved in the development and optimisation of a duplex

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treatment and coating process on titanium alloy aircraft landing gear bearings, enabling the switch of substrate material from steel to lighter titanium, thereby reducing aircraft weight, fuel consumption and CO2 emission. Tecvac's main research in the biomedical sector has revolved around finding new wear-resistant and antimicrobial coatings for hip and knee prostheses. A Cr-based coating meeting those requirements has been successfully tested on a hip simulator. In the oil and gas industry, Tecvac has been actively involved in trialling Inner Armor, a type of DLC coating, which can be applied on the internal surfaces of pipes and cylinders to provide protection against erosion, corrosion and wear.

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16:45 **Infrared optical properties of ZrC thin films synthesized by pulsed laser deposition**

Authors : V. Craciun1, C. Martin2, G. Socol1, D. Tanner3, and D. Craciun1
Affiliations : 1Lasers Department, National Institute for Lasers, Plasma and Radiation Physics, Magurele-Bucharest, Romania 2Ramapo College of New Jersey, NJ 3Physics Department, University of Florida, Gainesville, FL

Resume : ZrC thin films were grown on Si substrates by the Pulsed Laser Deposition technique. By changing the substrate temperature and ambient gas nature and pressure during deposition, films having a wide range of crystal grain sizes, mass densities and C/Zr ratios were obtained. We investigated the IR optical properties of ZrC films by measuring the optical reflectance from 30 cm-1 (4 meV) to 30 000 cm-1 (4 eV), using a Bruker-113v FTIR spectrometer and a Carl Zeiss microscope photometer. The resistivity values extracted from the optical data were similar to those measured using a four point probe technique. The results indicated that ZrC films exhibited high reflectivity in the mid IR range regardless of the structure and composition. Very low resistivity values of around 5×10-5 □.cm and slightly lower wear rates were measured for films having the highest ratio of C/Zr, while higher hardness values were measured for films having the largest crystal grains. These excellent qualities recommend the ZrC films for applications as thermal radiators working at very high temperatures in the outer space.

G.VI. 2

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17:00 **Silver surface segregation in silver doped diamond like carbon (Ag-DLC) nanocomposite coatings**

Authors : Noora K.Manninen1, Ramón Escobar Galindo2, Sandra Carvalho1,3, Albano Cavaleiro1
Affiliations : 1 - SEG-CEMUC, Mechanical Engineering Department, University of Coimbra, 3030-788 Coimbra, Portugal. 2 - Instituto de Ciencia de Materiales de Madrid (ICMM -CSIC), Cantoblanco, 28049, Madrid, Spain. 3 – GRF, Physics Department, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal.

Resume : DLC coatings have been largely used in different biomedical devices own to their wear protective properties. Still, microbial colonization and consequent infection represent the major limitation of different types of medical devices, being responsible for over half of all nosocomial infections, which drastically reduce the patient´s comfort and safety. Thus, the development of new materials which enable to reduce the implants failure caused by infections represents the future direction in the biomedical field. Ag nanoparticles (Ag-NP´s) have been pointed as one of the most effective antibacterial agents, thus, the surface modification of different biodevices with Ag NP´s has gained a considerable attention over the past years. The incorporation of Ag NP´s in wear protective coatings has been proposed as a promising concept, able to improve the wear resistance (due to the lubricant properties of Ag) and to reduce the infections. Previous works in AgDLC coatings suggested that Ag is not stable in DLC coatings, being found that Ag is able to segregate to coatings surface, which will strongly influence the coatings final properties. AgDLC coatings were deposited by magnetron sputtering and the thermodinamical stability of the coatings at room temperature conditions was evaluated along time. The effect of coatings thickness on the Ag surface segregation was evaluated. Two AgDLC coatings (20 at.% Ag) with thicknesses of 250 nm and 1000 nm were deposited. The in depth distribution of silver along time was evaluated by glow discharge optical emission spectroscopy (GDOES) and the agglomeration of Ag was studied by means of scanning electron microscopy (SEM).

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17:15 **TiSiON thin films as possible candidates in biomedical applications**

Authors : A. Vladescu1, C. Vitelaru1, M. Dinu1,2, T. Petreus3, C.M. Cotrut2
Affiliations : 1 National Institute for Optoelectronics-INOE 2000, 409 Atomistilor Str., Magurele, Romania 2 University Politehnica of Bucharest, 313 Spl. Independentei Str.,

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Bucharest, Romania 3University of Medicine and Pharmacy “Gr. T. Popa”, 16 Universitatii Str., Iasi, Romania

Resume : The goal of the present paper was to prepare and investigate TiSiON coatings as possible candidates to be used in biomedical applications. The coatings were deposited by cathodic arc method at different substrate bias voltages, in a reactive atmosphere consisting of a mixture of N2 and O2 and characterized in terms of microstructural, mechanical, friction, anticorrosive and biological properties. The influence of the substrate bias voltage on coating characteristics has also been evaluated. Particular focus was given to the use of TiSiON coatings in dental restorations for improving the bond strength of ceramic layer to the metallic substrate. The coatings, with (N+O)/(Ti+Si) ratios close to unity, consisted of crystalline solid solutions (FCC structure, (111) texture). A maximum hardness of about 32 GPa was measured for the coatings grown at bias voltages between -100 and -150 V, and the highest adhesion strength was found for a bias of -100 V. The electrochemical tests in artificial saliva with pH =5 indicated that all the coatings improved the corrosion resistance of both alloys, the best corrosion protection being provided by the TiSiON-(100 V bias) and TiSiON-(150 V bias) coatings. The biocompatibility tests revealed that the TiSiON coatings showed a superior biocompatibility compared to those of the bare alloys, only minor differences being observed between the two coated alloys. However, the best cell proliferation was obtained for the TiSiON-(200 V bias) coated CoCr.

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17:30 **Luminescent organic nanocomposite thin films deposited by remote plasma assisted vacuum deposition for photonics applications**

Authors : M. Alcaire, F.J. Aparicio, L. Cerdán, F. Lahoz, A. Borras, I.García-Moreno, A. Costela, A.R. González-Elipe, A. Barranco.
Affiliations : M. Alcaire; F.J. Aparicio; A. Borras; A.R. Gonzalez-Elipe; A. Barranco, nstituto de Ciencia de Materiales de Sevilla (CSIC-Universidad de Sevilla). c/Américo Vespucio 49, 41092 Sevilla, Spain. L. Cerdán; I. García-Moreno; A. Costela, Instituto de Química Física Rocasolano, (CSIC),c/ Serrano 119, 28006 Madrid. Spain. F. Lahoz, Dpto. Física Fundamental y Experimental, Electrónica y Sistemas, Universidad de La Laguna. C/ Astrofísico Francisco Sanchez s/n, 38206 La Laguna.Santa Cruz de Tenerife, Spain

Resume : Remote plasma assisted vacuum deposition is a novel a versatile deposition methodology, which permits the fabrication of organic films from non -chemically polymerizable organic or organometallic molecules.[1-3] The technique is based in the effective control of the interaction between the sublimated precursor molecules and a remote glow discharge. Thus, the technique has some similarities with the vacuum deposition and the plasma polymerization processes. Once formed, the films are solid cross-linked organic structures typically insoluble in organic solvents and thermally stable at temperatures higher than the sublimation temperatures of the precursor molecules. The technique also permits the direct fabrication of microstructures and low dimensional nanostructures. The optical properties of the films (light absorption, luminescence, sensor response, etc) depend on the precursor molecules and on the particular thin film nanostructures and final composition. Examples of multifunctional films and microstructures deposited from laser dyes and other relatively complex molecules for the fabrication of photonic structures, gas sensors, optical films, lasing media and optoelectronic components will be presented and studied. [1] A. Barranco, P. Groening, Langmuir 22 (2006) 6719. [2] I. Blaszczyk-Lezak et al. J. Phys. Chem. 113 (2009) 431. [3] F.J. Aparicio et al. Adv. Mater. 23 (2011) 761.

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17:45 **Study of plasma treatment effect on low temperature metalorganic chemical vapor deposition (MOCVD) deposition of TiN as a barrier layer for copper diffusion in high aspect ratio through silicon vias**

Authors : Larissa Djomeni a, Thierry Mourier a, Stéphane Minoret a, Sabrina Fadloun c, Steve Burgess b, Andrew Price b , Laurent Vandroux a, Daniel Mathiot d
Affiliations : a CEA, LETI, MINATEC Campus, 17 rue des Martyrs, Grenoble Cedex 9, 38054, France; b SPTS, Ringland Way, Newport, Gwent , NP18 2TA, UK; c SPTS SAS, Inovallée - Bat B 445, rue Lavoisier, Montbonnot, 38330, France; d ICube Laboratory Université de Strasbourg and CNRS) 23 rue du Loess, Strasbourg cedex 2, B.P. 20, 67037,

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Resume : In order to overcome the performances, dimensions and cost limit beyond the 22 nm technology node, three-dimensional (3-D) integration with through-silicon-vias (TSVs) has emerged as an effective solution. Another potential of the TSVs is their promises in enabling advanced multi-level chips, integrating heterogeneous CMOS technologies with emerging technologies such

as MEMS and bio-chips. TSV Metallization, particularly barrier and seed layer deposition, has become a critical process step of the integration. In a previous work, the investigation of a low temperature (200°C) MOCVD of TiN film as a barrier layer to prevent copper diffusion was studied. From these studies, it comes out the plasma treatment have a great effect on the result TiN film. The resistivity of the film is lowered by two orders of magnitude. The film microstructure changes from amorphous to 7 nm crystal size. The carbon contain of the film is lowered from 4% to less than 1% of the composition of the film. In order to understand the effect of the plasma on the film, Fourier Transform Infrared spectroscopy (FTIR) of the film at different plasma condition were used to study the chemical bond in the TiN. It comes out that the plasma frequency and ammonia flow have a great impact on the film. High plasma frequency compared to lower one breaks T-N-C-H bond thereby enabling a pure TiN carbon free film. The study was compared to the reference TiN film deposited with ionized physical vapour deposition.

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PROGRAM VIEW : 2014 Spring
MY PROGRAM : 2014 Spring

Symposium : G

Carbon- or nitrogen-containing nanostructured thin films

26 May 2014 | 27 May 2014 | **28 May 2014** | 29 May 2014 | 30 May 2014

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start at	Subject	Num.
	Recent advances in transition metal nitrides-II : Panos PATSALAS, Nikola RADIC	
08:30	**Knowledge-based design of TiAlN-based hard coatings** **Authors :** Christian Mitterer **Affiliations :** Department of Physical Metallurgy and Materials Chemistry, Montanuniversitaet Leoben, Austria **Resume :** TiAlN-based hard coatings deposited by plasma-assisted vapor deposition are widely used to reduce friction and wear of cutting tools. The excellent performance of these coatings at elevated temperatures is based on formation of stable Al2O3 scales and self-hardening by spinodal decomposition of the metastable Ti1−xAlxN solid solution into cubic AlN and cubic TiN. Transformation of the cubic into wurtzite AlN results in deterioration of coating properties. Tailoring of oxidation and decomposition behavior is thus a key for further optimization. More volume-consuming cubic TiN domains leading to a more pronounced hardness increase are formed by decomposition of coatings with tensile stress, while compressive stress promotes formation of smaller cubic AlN [1]. Impurities like Fe reduce the onset temperature of coating oxidation and increase the wear rate [2]. Droplets in coatings grown by cathodic arc evaporation also contribute to coating degradation by providing nucleation sites for shear cracks and by the release of abrasive fragments in sliding contacts [3]. On the other hand, formation of dense grain boundaries has been shown to shift the detrimental formation of wurtzite AlN to higher temperatures [4]. 1 N. Schalk et al., Surf. Coat. Technol. 209 (2012) 190 2 M. Muehlbacher et al., Surf. Coat. Technol. 215 (2013) 96 3 M. Tkadletz et al., Surf. Coat. Technol., in press 4 T. Weirather et al., submitted for publication	G.VII.1
	add to my program (close full abstract)	
09:00	**Lattice Ordering Effects on Toughness Enhancement in TiN and VN Thin Films Alloys** **Authors :** D. Edstr?m, D.G. Sangiovanni, V. Chirita and L. Hultman **Affiliations :** Thin Film Physics, IFM, Link?ping University, Sweden **Resume :** Enhanced toughness in hard and superhard thin films is a primary requirement for present day ceramic hard coatings, known to be prone to brittle failure during in-use conditions, in modern applications. In our previous Density Functional Theory (DFT) investigations, we predicted significant improvements in the hardness/ductility ratio of several pseudobinary B1 NaCl structure transition-metal nitride alloys, obtained by alloying TiN or VN with NbN, TaN, MoN and WN [1, 2]. The initial calculations, which were carried out on model, highly ordered configurations with Cu-Pt ordering on the cation sublattice, reveal that the electronic mechanism responsible for toughness enhancement stems from the high valence electron concentration (VEC) of these alloys, and ultimately allows a selective response to tetragonal and trigonal deformations. Recently, these results have been validated experimentally. Single-crystal V0.5Mo0.5N/MgO(001) [3] and V0.6W0.4N/MgO (001) [4] alloys, were grown by dual-target reactive magnetron sputtering, together with VN/MgO(001) and TiN/MgO(001) reference samples. The V0.5Mo0.5N films exhibit hardness >50% higher than that of VN, and, in contrast to nanoindented VN and TiN reference samples, which suffer from severe cracking, the V0.5Mo0.5N films do not crack. No ordering on the cation sublattice is observed in the V0.5Mo0.5N films, however, the onset of W ordering on adjacent {111} planes of the metal sublattice, is observed in	G.VII.2

V0.6W0.4N alloys. Here we present new DFT results, which address the issue of lattice ordering effects on the mechanical properties of these pseudobinary alloys. Our investigations concentrate on V0.5Mo0.5N, V0.5W0.5N, Ti0.5Mo0.5N and Ti0.5W0.5N alloys obtained by alloying TiN and VN with WN and MoN. Our calculations, carried out for structures with increasing levels of disorder, reveal that while the degree of electronic structure layering, i.e. the formation of alternating layers of high and low charge density upon shearing, becomes less pronounced in disordered configurations, the overall VEC effect is not affected. The essential feature in the disordered alloys, as initially predicted for highly ordered configurations, remains the increased occupancy of electronic d-t2g metallic states, which allows the selective response to tensile/shearing stresses, and explains the enhanced toughness confirmed experimentally for V0.5Mo0.5N films. [1] D. G. Sangiovanni et. al. Phys. Rev. B 81 (2010) 104107. [2] D. G. Sangiovanni et. al. Acta Mater. 59 (2011) 2121. [3] H. Kindlund et. al. Appl. Phys. Lett. Materials, 1 (2013) 000000. [4] H. Kindlun et. al. J. Vac. Sci. Technol. A 31 (2013) 040602.

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09:15 **Synthesis and microstructure of layered-ternary TiAlN thin films**

Authors : A. Rizzo, L. Mirenghi, D. Valerini, R. Terzi, L. Tapfer
Affiliations : ENEA - Italian National Agency for New Technologies, Energy and Sustainable Economic Development - Technical Unit for Brindisi Material Technologies, Laboratory of Materials Technology (UTTMATB-TEC), Brindisi Research Center, S.S. 7 Appia km. 706, 72100 Brindisi, Italy

Resume : A comprehensive study on the influence of the Al content on TiAlN coating microstructure and related mechanical and tribological properties are presented. A layered structure of TiAlN and AlN is obtained applying an average power density of 2.468 W/cm2 and 1.234 W/cm2 to a TiAl and Al target respectively, by the RF modulated pulse power. X-ray diffraction reveals fcc single-phase coatings at low Al contents and dual-phase or hcp phase at higher Al contents. As-deposited TiAlN and TiAlN/AlN film compositions are determined by X-ray Photoelectron Spectroscopy (XPS). The single TixAl1-xN film has x = 0.36 which remains unchanged even in the multilayer. The Ti 2p 3/2 peak can be fitted with two components, whose relative areas vary along the sample depth, and are ascribed to the fcc and hcp phase of the ternary compound. The peak at lower B.E. is shifted respect to the TiN peak at about 455.3 eV. The second peak is associated to a ternary structure like hcp-TiAlN. The presence of two different chemical states on Ti 2p does not induce any variation on Al 2p and N 1s spectra. Hardness measurements show high values for x=0.36, decreasing with increasing Al to values of 17 GPa at x=0.76. Friction coefficients are around 1.5 at room temperature but decrease significantly at higher temperatures to 0.88 at 700 °C. This investigation clearly shows the relations between coating composition and the resulting structure explains their mechanical and tribological properties.

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09:30 **Residual stress distribution and thermal stability of the Cr/CrN multilayer coatings**

Authors : P. Wieciński (1), R. Dobosz (1), J. Jaroszewicz (1), J. Smolik (2), H. Garbacz (1), K.J. Kurzydłowski (1)
Affiliations : (1) Faculty of Materials Science, Warsaw University of Technology, 141 Woloska Str., 02-507 Warsaw, POLAND (2) Institute for Sustainable Technology – National Research Institute, 6/10 Pulaskiego, 26-600 Radom, POLAND

Resume : The aim of this work was to investigate the residual stress and thermal stability of the Cr/CrN multilayer coatings. For this purpose, multilayer Cr/CrN coatings were deposited on titanium alloy Ti6Al4V using the PVD vacuum arc method. The residual stress distribution was analyzed using x-Ray synchrotron source at ESRF (European Synchrotron Radiation Facility) in Grenoble. Because of potential application of the coatings, thermal stability in temperature range of 300-500°C as well as corrosion resistant in salt fog test were also determined. The investigations of stress distribution in multilayers Cr/CrN coatings revealed the presence of compressive residual stresses in CrN constituent layers. The stresses were the highest in first CrN layers and became smaller in layers localized closer to the substrate material. In case of Cr layers, tensile residual stresses were localized in the layers located close to the substrate material. In external layers compressive residual stresses were observed. The thickness ratio of the Cr and CrN layers did not affect the character of stress distribution but had a small influence on the values of measured stresses. The results also showed that microstructure of Cr/CrN multilayer coating was stable up to 400°C. Annealing at temperature of 500°C

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changed the microstructure and increased the hardness of Cr/CrN coating. XPS analysis revealed the presence of the CrO3 and Cr2O3 on the surface after annealing. The multilayer Cr/CrN coatings exhibit excellent corrosion resistance during salt fog test.

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09:45 **Defect structure and surface chemistry of transition metal aluminum nitride thin films alloyed with oxygen**

Authors : K. P. Shaha a, H. Rueß a, S. Rotert a, M. to Baben a, D. Music a, Ch. Kunze b, G. Grundmeier b and J. M. Schneider a
Affiliations : a Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany b Technical and Macromolecular Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

Resume : The influence of oxygen concentration on the structure and mechanical properties of V0.5 Al0.5 Ox N1-x thin films was investigated. The unexpected experimental lattice parameter decrease with increasing oxygen concentration can be understood based on ab initio data: The oxygen incorporation induced formation of metal vacancies reduces the equilibrium volume and stabilizes the metastable solid solutions. Charge balancing is identified as the underlying physical mechanism by Bader decomposition analysis. Hence, property predictions for these oxynitrides are only meaningful if the defect structure is described. Furthermore, oxygen chemisorption on transition metal aluminum nitride surfaces is discussed by theory and experiment. Both the experimental and theoretical data imply that Ti and not Al determines the oxygen chemisorption process. Dissociative adsorption of oxygen is followed by upward movements of Ti, generating vacancies in the TiAlN interface and the formation of Ti-O-Ti bridges with Ti2O3-like bonding passivating the surface.

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10:00 Coffee break

Nanocarbons from metal/carbon nanocomposite thin films : Pantelis KELIRES, Sigitas TAMULEVICIUS

10:30 **Metal-carbon nanocomposite thin films: a way to synthesize nanocarbons**

Authors : P.Y. Tessier, A.A. El Mel, N. Bouts
Affiliations : Institute of Materials Jean Rouxel - IMN, University of Nantes, CNRS, France

Resume : Metal/carbon thin films can be deposited by cosputtering of metal and graphite targets or by plasma enhanced chemical vapor deposition using hydrocarbon gas combining with magnetron sputtering of a metal target. The shape and size of the metal nanoparticles in the composite and the organization of the carbon matrix can be controlled by the deposition conditions. Moreover the deposition of thin films on template surface broadens the possibility to elaborate complex carbon nanoobject. It appears to be an interesting way to create nanocarbon objects such as nanotubes and nanocarbon electrodes.

G.VIII.1

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11:00 **Single-Walled Carbon Nanotube Networks for Ethanol Vapor Sensing Application**

Authors : Albert G. Nasibulin1, Ilya V. Anoshkin1, Prasantha R. Mudimela1, Maoshuai He1, Vladimir Ermolov2, Oleg Tolochko3 and Esko I. Kauppinen1
Affiliations : 1 Aalto University School of Science, P.O. Box 15100, Espoo, FI-00076 AALTO, Finland (albert.nasibulin@aalto.fi) 2 Nokia Research Center, Helsinki, Finland 3 Saint-Petersburg Polytechnic State University, Russia

Resume : FIlms of pristine high quality single walled carbon nanotubes (SWNTs), the SWNTs after Ar-plasma treatment (from 2 to 12 min) and carbon nanobuds (CNBs) have been tested for ethanol vapor sensing. It was found that the pristine high quality SWNTs do not exhibit any ethanol sensitivity, while the defect introduction in the tubes results in the appearance of the ethanol sensitivity. The CNB network showed the ethanol sensitivity without plasma treatment. Both CNB and low defective (after 3 min treatment) SWNT networks exhibit significant drift in the resistance baseline, while heavily plasma-treated (9 min) SWNTs exhibited high ethanol vapor sensitivity without the baseline change. The mechanisms of the ethanol sensitivity and stability after the plasma irradiation are attributed to the formation of sensitive dangling bonds in

G.VIII.2

the SWNTs and formation of defect channels facilitating an access of the ethanol vapor to all parts of the bundled nanotubes.

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11:15 **Carbon nanotubes patterned electrodes for photovoltaic applications**

Authors : C. Ciceroni, G. Mincuzzi, G. Ulisse, A. Di Carlo, F. Brunetti
Affiliations : University of Rome "Tor Vergata"

Resume : Nowadays the replacement of Indium Tin Oxide (ITO) for the production of transparent and conductive electrodes is a critical issue in the organic photovoltaic field. Carbon based semitransparent electrodes, using graphene or carbon nanotubes (CNTs) as conductive materials, are some of the most promising technologies for ITO replacement [1-2]. We report the production of semitransparent electrodes based on patterned CNTs. Through a laser etching process we realized a micrometric patterning of the metal catalyst, in stripes with different dimensions. Then, using a "double-zone" chemical vapor deposition technique (CVD) it was possible to synthesize CNTs directly on glass substrates. Scanning electrons microscopy images and Raman spectroscopy analysis have been performed. The samples were characterized in terms of Sheet-Resistance (SR) and Optical Transparency (OT). A correlation between the catalyst stripes width and the SR/OT ratio is shown. The reported technique is an initial step towards the realization of ITO free contacts for organic solar cells. [1] ACSNano 2010, VOL. 4, NO. 5, 2865–2873 [2] Adv. Mater. 2009, 21, 3210–3216

G.VIII.3

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11:30 **Photoemission Response and Annealing Effects of Nitrogen Plasma Functionalized Carbon Nanotubes**

Authors : M. Scardamaglia 1, F.J. Aparicio Rebollo 1, C. Struzzi 2, P. Mudimela 4, J.-F. Colomer 4, L. Gregoratti 2, L. Petaccia 2, R. Snyders 1, and C. Bittencourt 1
Affiliations : 1 Chemistry of Interaction Plasma Surface (ChIPS), University of Mons, Belgium; 2 Elettra Sincrotrone Trieste S.C.p.A., AREA Science Park, Italy; 3 Institut des Mat?riaux Jean Rouxel, Universit? de Nantes, CNRS, Nantes, France; 4 Research Centre in Physics of Matter and Radiation, University of Namur, Belgium;

Resume : The electronic properties of sp2 carbon nanostructures are very sensitive to local perturbations, such as surface charges and adsorbed gas molecules, so that the grafting of functional groups in a controllable way has been proposed as a feasible reproducible solution for band gap engineering and controllable doping, in order to exploit and tailor the extraordinary properties of these materials. Plasma-based functionalization methods have the advantage to be solvent-free, time efficient and flexible. Within this context, we will discuss the functionalization of vertical aligned carbon nanotubes (v-CNTs) via nitrogen plasma treatment. Valence band (UPS) and scanning X-ray photoelectron spectromicroscopy (SPEM) measurements were performed at ELETTRA Synchrotron. The creation of defects induced by ions drives the grafting of nitrogen species (pyridinic, pyrrolic and graphitic) on the CNTs. A depth of functionalization up to 4 μm was evaluated by SPEM, beyond which the properties of the v-CNTs remain unperturbed. Furthermore, an intriguing different behavior of the grafting at the CNT tips with respect to the sidewalls was observed. This indicates a different reactivity of the CNT tip, where the presence of natural defects may be involved in different bonding formations between carbon and nitrogen. The effect of the temperature has been evaluated both during the plasma treatment and with post synthesis annealing, showing variations in the ratio between the nitrogen species.

G.VIII.4

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11:45 **Study of nanometrically thin pyrolytic carbon films for explosive electron emission cathode in high-voltage planar diode**

Authors : Vladimir Baryshevsky 1, Nikolai Belous 1, Alexandra Gurinovich 1, Evgeny Gurnevich 1, Polina Kuzhir 1, Sergey Maksimenko 1, Pavel Molchanov 1, Mikhail Shuba 1, Tommi Kaplas 2, Yuri Svirko 2
Affiliations : 1 Research Institute for Nuclear Problems, Belarusian State University 2 University of Eastern Finland

Resume : We report high current density explosive electron emission from a copper cathode with diameter of 50 mm with pre-deposited pyrolytic carbon (PyC) films being from 70 to 150 nm thick. In the diode configuration, we demonstrate the current density as high as 300A/cm2 under applied voltage below 400 kV. The Raman measurements reveal that the PyC film survives after 7 shots. In order to study the cathode degradation we compared optical microscope images of the cathode before and after shots. We observed that the pre-deposited PyC film cathode prevents copper evaporation and oxidation. This property ensures a higher explosion emission stability and longer lifetime

G.VIII.5

of the PyC/Cu-cathodes in comparison with conventional graphitic/Cu ones. Our results show that PyC/Cu cathodes are most promising for applications that require electric field strengths from 50 to 60 kV/cm.

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12:00 **Lunch break**

13:30 **Carbon Nanotubes as Transparent Electrodes For Organic Solar Cells**

Authors : Osman Urper, Elif Arici, Nilgun K.yavuz
Affiliations : Osman Urper (MSc) Nilgun K.yavuz (Prof.Dr) Elif Arici (Assoc.Prof.Dr) Department of Energy, Istanbul Technical University, Istanbul, Turkey

Resume : One of the key parameter for the efficiency of the solar cell is the light harvesting. Hereby, together with the absorbance properties of the active layer, the optical transmittance of the front-electrode plays an important role. Indiun tin oxide (ITO) is the mostly used electrode material for organic solar cells. In long term, because of the rarity of Indium as source material, there is a need to replace ITO by alternatives. Indium tin oxide (ITO) is not only expensive in fabrication but also mechanically brittle, which increases the fabrication cost and also limits the flexibility of solar cell devices. In recent years, several transparent electrode materials are tested to replace ITO. Among these materials, carbon nanotubes (CNTs), seems to be a promising alternative having its unique features such as optical transmissions not only in visible but also in IR range of the sun light together with its electrical and flexibility properties. In this poster, we will introduce the synthesis methods of single wall carbon nanotubes, and present the fabrication methods of transparent CNT layers from solution. We will characterize the transparency, electrical properties of the layers and discuss its advantages for photovoltaic applications.

G.PII. 1

add to my program (close full abstract)

13:30 **Au-GaAs PHOTOVOLTAIC STRUCTURES WITH SINGLE-WALL CARBON NANOTUBES ON THE MICRORELIEF INTERFACE**

Authors : N.L. Dmitruk1, O.Yu. Borkovskaya1, S.V. Mamykin1, T.S. Havrylenko1, I.B. Mamontova1, N.V. Kotova1, E.V. Basiuk2
Affiliations : 1V. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Kyiv 03028, Ukraine, dmitruk@isp.kiev.ua; 2Centro de Ciencias Aplicadas y Desarrollo Tecnológico Universidad Nacional Autónoma de México, Circuito Exterior C. U., 04510 México D.F., Mexico

Resume : Carbon based nanomaterials attracted great interest in optoelectronics and photovoltaics due to their unique properties. This work is devoted to the study of the surface barrier heterostructures Au-n-GaAs with single wall carbon nanotubes (SWCNTs) on the flat and microrelief interfaces. N -type (100) GaAs single crystal with ~10*16 cm-3 doping level have been used. Microreliefs of quasigrating and dendrite type have been prepared by anisotropic etching. Highly purified SWCNTs were prepared by the arc-discharge method. Well-sonicated SWCNT-ethanol mixture was used to deposit the SWCNTs onto GaAs substrates modified with poly (vinil pyridine) (PVP). Optical, photoelectric and electrical properties of Au-n-GaAs structures have been studied. The short-circuit photocurrent were measured in the 0.4-0.9 μm spectral range. The light (AMO conditions) and dark current-voltage characteristics were measured. The enhancement of the photocurrent especially in the long-wave range was found for structures with SWCNTs and its mechanism was analyzed with taking into account optical and electrical characteristics of structures. It is surprise that the greatest effect of the photocurrent enhancement was observed for structures with SWNTs deposited on the flat substrates. Therefore we conclude that effect of the photocurrent enhancement is essentially determined by optical properties of SWCNT/PVP/GaAs structure (light trapping), dependent on SWNT nanolayer thickness and its homogeneity.

G.PII. 2

add to my program (close full abstract)

13:30 **Diameter control of vertically aligned, single-walled carbon nanotubes via chemical treatment of a catalyst support**

Authors : Ning Yang, Seul Ki Youn, Hyung Gyu Park
Affiliations : Nanoscience for Energy Technology and Sustainability, Department of Mechanical and Process Engineering, ETH Zurich

Resume : Understanding the interaction and size matching behavior between catalyst and its support is a key to modulate the individual and collective properties of vertically aligned (VA) single-walled carbon nanotubes (SWCNTs).

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We examine the combinational influence of catalyst support asperity and its chemical state on the diameter distribution and population properties (number and mass density, alignment) of SWCNTs. After different physical or chemical etching processes, catalyst support evolves into different surface roughness and chemical states, resulting in a variety of ensembles of catalyst nanoparticles with distinct catalytic activities. Specifically, an acid treated catalyst support creates higher surface roughness and acidity, leading to unique SWCNT diameter distribution as well as modification of the alignment and density of resultant nanotubes. This method of controlled etching of the catalyst support could offer a route to accurate SWCNT diameter control below a nanometer scale while preserving uniformity at a macro scale, which can potentially alleviate current hurdles faced by mass production of SWCNT forests.

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13:30 **Activation energy variation in the chemical vapor deposition of carbon nanotubes under temperature gradient**

Authors : Ning Yang, Seul Ki Youn, Hyung Gyu Park
Affiliations : Nanoscience for Energy Technology and Sustainability, Department of Mechanical and Process Engineering, ETH Zurich

Resume : The growth of vertically aligned carbon nanotubes (VA-CNTs) via chemical vapor deposition (CVD) is commonly understood by a kinetic model of a single rate-determining step, assigning one value of activation energy often independent of partial pressure of a carbon precursor. Interestingly, we observed that the activation energy increases monotonically with respect to the acetylene partial pressure, especially when feedstock gases are pre-heated at high temperature. We attribute this observation to complex thermal rearrangement of the precursor that is dependent on the initial acetylene pressure. A resulting mixture of various carbonaceous precursors is assumed to have different probabilities and rates for catalytic conversion from precursor to CNT. Based on the observation, we propose an analytical model with multiple parallel reaction pathways which can relate the acetylene pyrolysis products and surface reaction processes, thereby explaining the diversifying Arrhenius slopes of the CNT growth rate.

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13:30 **Surface property modification of carbon nanotube carpet by plasma**

Authors : Thibault Labbaye(1), Mireille Gaillard(1), Eva Kovacevic(1), Thomas Lecas(1), Julien Simonneau(1), Aurélien Canizarès(2), Mohamed-Ramzi Ammar(2), Thomas Strunkus(3), Christian Kübel(4), Nadjib Semmar(1), Nicole Raimboux, Patrick Simon, Chantal Boulmer-Leborgne(1)
Affiliations : 1 GREMI, Université-CNRS, BP6744, 45067 Orléans cedex 2, France 2 CEMHTI, CNRS, 45071 Orléans cedex 2, France 3 Karlsruhe Institute of Technology KIT, Germany 4 Christian-Albrechts-University of Kiel, Institute for Material Science, Kiel, Germany

Resume : Carbon nanotubes (CNT) are important building blocks for novel applications in science and technology. They can be used for example for chemical or biological sensors as interconnection microelectronics devices. In this contribution we report on experiments performed in low-pressure capacitively coupled RF plasma with C2H4 in H2 or NH3 mixtures. This process is used to grow densely packed vertically aligned CNTs on different sets of substrates and catalysts. For CNT growth, metal catalyst thin films (9 nm in thickness) were deposited at room temperature on different substrates by pulsed laser deposition. Films were then heated up to 550 – 700°C under vacuum and maintained in a hydrogen atmosphere during a period where the film morphology is transformed into nanoparticles. Important parameter for the future applications and development concerns the surface modification of these materials, which can result in controllable changes of their electronic or chemical properties. Of interest are here in particular nitrogen containing functional groups. We focus on first results dealing with the controlled functionalization of CNT carpets by means of low temperature nitrogen containing plasmas. CNT are observed by SEM and TEM and the effect of the plasma is analyzed by means of in situ Raman, NEXAFS and HR-XPS to evidence C-N bonds. Additional information about the effect of the plasma treatment on the surface properties of the materials are obtained by means of contact angle measurements.

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13:30 **Nitrogen and Carbon Doped TiO2 Nanotubes: Fabrication and Gas Sensing Properties**

Authors : Erdem SENNIK1, Necmettin KILINC1, Zafer Ziya OZTURK1,2

G.PII. 6

Affiliations : 1Gebze Institute of Technology, Department of Physics, Kocaeli 41400, Turkey; 2 TUBITAK Marmara Research Center, Material Institute, Kocaeli 41700, Turkey
Resume : TiO2 nanotube arrays have been used a wide range of applications in areas such as photoelectrochemical materials, solar cells, gas sensors, bio-sensing and biomedical applications. TiO2 nanotubes were doped with various elements such as carbon, nitrogen, boron, fluorine etc. especially for DSSC applications. Besides it?s known that the gas sensing properties of TiO2 nanomaterials could be developed by doping. TiO2 nanomaterials were doped by several methods such as hydrothermal, CVD, wet processing. In this study, nitrogen (N) and carbon (C) doped TiO2 nanotubes (TiO2 NTs) were fabricated by wet processing. For N doped TiO2 nanotubes, firstly TiO2 NTs on Ti foil were synthesized by anodization method, and then these samples were dipped in doping solution (containing nitrogen). In order to achieve C doped TiO2 nanotubes, TiO2 NTs were fabricated and doped in doping solution (containing carbon) by anodization method at the same time. We will investigate these samples for investigating gas sensing properties depending on concentration and temperature. Acknowledgement: This study was supported by Scientific and Technological Research Council of Turkey (TUBITAK) with Project Number: 111M261.

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13:30 **SYNTHESIS OF CARBON NANOSTRUCTURED THIN FILMS NEAR ROOM TEMPERATURE USING PECVD ASSISTED BY MICROWAVE**

Authors : Flavio Carvalho (1), Alfredo A. Vaz (2), Mário A. Bica de Moraes (2), Stanislav A. Moshkalev (2), Rogério V. Gelamo (1)
Affiliations : (1) Universidade Federal de Triangulo Mineiro - UFTM, Uberaba, MG, Brazil; (2) Universidade Estadual de Campinas - UNICAMP, Campinas, SP, Brazil
Resume : In this work we present and discuss results related to obtained carbon nanostructured thin films synthesized onto Si (001) substrates using plasma enhanced chemical vapor deposition (PECVD) from C2H2-Ar mixtures. The plasma was activated by a microwave generator and various nanostructures were grown at low substrate temperatures (about 120 ºC) on top of previously deposited catalytic Ni and Cu films of 3 nm thickness. No treatment of the films was made prior to the deposition of the carbon nanostructures. Nanoholes, nanospheres and nanofibers were obtained, depending on acetylene partial pressure used during depositions. Atomic force microscopy (AFM) and scanning electron spectroscopy (SEM) were employed for the morphological characterization of the catalytic films, in an attempt to investigate carbon nanostructures growth mechanisms. Raman spectroscopy was used to investigate carbon hybridization states. Nanofibers of 300 to 400 nm length were observed for some plasma conditions (pressure and microwave power), while a mixture of sp2 and sp3 hybridizations as revealed by the Raman spectra. The results shown herein indicate a promising simple and low cost technique for the production of conductive carbon nanofibers grown directly over Si wafers.

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13:30 **The effect of TiSiN interlayers on bond strength of dental ceramic to Ni-Cr and Co-Cr alloys**

Authors : M.Tarcolea1, C.M.Cotrut1, M.Dinu1,2, C.Vitelaru2, F.Baciu1, A.Vladescu2
Affiliations : 1University Politehnica of Bucharest, Romania 2National Institute for Optoelectronics, Magurele, Romania
Resume : TiSiN coatings were prepared to enhance the bond strength between metal and dental ceramic in the systems used in prosthetic restorations. The coatings were deposited on NiCr and CoCr dental alloys by the cathodic arc technique at various substrate bias voltages and characterized in terms of elemental composition, crystalline structure, mechanical properties, surface roughness and contact angle. The bond strength of the metal-ceramic system, with and without TiSiN interlayers, was evaluated by a three-point bending test. The coatings consisted of nanocrystalline solid solutions (grain sizes of 3.6 ¬ 4.3 nm), with FCC structures. The film hardness, ranging from about 21 to 38 GPa, was found to increase with increasing substrate bias, while the best adhesion (critical loads of ~ 54 N) was obtained for a bias voltage of -100 V, irrespective of the substrate type. The deposition of the TiSiN coatings resulted in a roughness decrease of the NiCr and CoCr alloys. The contact angle measurements indicated a hydrophobic character for the films deposited for bias voltages ranging from -50 to -150 V and a hydrophilic character for a bias of -200 V. The experimental results demonstrated that the use of the TiSiN coatings improved the bond strength of metal–porcelain systems in the case of NiCr substrates.

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13:30 **Optical Properties of Transition Metal Doped AlN Nanowires**

Authors : A. Aghdaie 1, H. Haratizadeh 1, S.H. Mousavi 1,2
Affiliations : 1. Physics Department, Shahrood University of Technology, Shahrood, Iran 2. INM– Leibniz Institute for New Materials, 66123 Saarbrücken, Germany

Resume : Undoped, Cu and Mn doped aluminium nitride (AlN) nanostructures were synthesized using a chemical vapour condensation (CVC) method. The raw materials were a mixture of Al and NH4Cl powder with different weight ratios and Cu and Mn powders, which were used as a dopant. Field emission scanning electron microscopy (FE-SEM) results showed different nanostructures, including nanowires and nanoparticles of different sizes. Photoluminescence (PL) spectroscopy of as-prepared samples show intense peaks in red, blue-green and blue regions in the Mn doped, Cu doped and undoped samples, respectively. These results are important for optoelectronical applications.

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Carbon- or nitrogen-containing nanostructured thin films - II : Thien-Phap NGUYEN, Jochen SCHNEIDER

13:30 **Novel biomimetic nanocomposites based on nanohydroxyapatite/vertically-aligned/polymeric nanofibers produced by electrospinning to bone tissue regeneration**

Authors : Patricia O. Andrade 1 Joao Vitor da Silva Moreira 2 Ana Maria do Espirito Santo 1 Anderson Oliveira Lobo 2
Affiliations : 1 Universidade Federal de Sao Paulo, Department of Materials Science and Engineering, Sao Jose dos Campos, SP, Brazil 2 Laboratory of Biomedical Nanotechnology, Development Research Institute (IP&D), Universidade do Vale do Paraiba (Univap), Av. Shishima Hifumi, 2911 - Sao Jose dos Campos, 12244-000, SP, Brazil

Resume : Biomimetic biomaterials are promising to bone tissue engineering due to similarities of natural components of extracellular matrix (ECM). The potential applications of polymeric nanofibers have attracted the attention for several investigations because they usually show low toxicity and they are biocompatible and biodegradable. However, polymeric nanofibers present unappropriated mechanical properties for bone tissue regeneration. For this reason, incorporated ceramic nanoparticles are largely used. Vertically aligned carbon nanotubes (VCNT) are used also as scaffolds in cellular growth in vitro improving the tenacity of the implanted material [3]. The combination of these materials to the development of new biomaterial is very attractive for many applications. In this issue, the current Project aims the production of new hibrid material by multi layers of i) hydrophilic VCNT produced by plasma assisted vapor deposition, ii) hydroxyapatite nanocrystals produced by electrodeposition and simulated body fluid immersion, and iii) Poly-acid lactic (PLA) or Poly (butylene adipate-co-terephthalate) (PBAT) nanofibers.Scanning electron microscopy and wide-angle x-ray diffraction were used to morphology and structure analyses, respectively. Differential scanning calorimetry, thermal gravimetric and dynamic mechanical thermal analyses performed the thermal properties. We succeed to obtain nHA/VAMWCNT-O2/PLA and nHA/VAMWCNT-O2/PBAT hybrid nanocomposites.

G.PII. 10

add to my program (close full abstract)

13:30 **Light emitting and photoresponse of n-ZnO/graphene heterojunctions**

Authors : Feng Wei, Geming Wu, Hongbin Zhao, Yan Zhang, Du Jun
Affiliations : Advanced Electronic Materials Institute, General Research Institute for Nonferrous Metals, Beijing, P.R. China;

Resume : Recently, the two dimensional material graphene, with the merit of high mobility and high optical transparency have been stimulated a lot of research interest in new and diverse application. Especially, the hybridization of graphene with ZnO has been reported for various devices, such as gas sensors and solar cells. Furthermore, the feasibility of transferring chemical vapor deposition (CVD)-grown graphene would enable the fabrication of vertical-geometry devices with low threading dislocation densities by a simple process, which provides many attractive advantages, including flexibility, light weight, and transparency. In this report, the electroluminescence from n-ZnO/graphene heterojunctions light-emitting diodes at room-temperature is investigated. The devices with the structure of n+-Si/n-ZnO/graphene/Au show a clear rectifying behavior, indicating a Schottky barrier at the n-ZnO/graphene

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contact interface. By modifying the defects in ZnO thin film who determine the transition between the oxygen defects energy level and conduction band of the ZnO, green and white electroluminescence are acquired respectively. We demonstrate that graphene layer plays an enhancement role on the injection of the holes into ZnO thin film and consequently improve the recombination of electrons from n-ZnO and holes from the acceptor level of graphene. By further modulating the defects in ZnO film, the emission of the n-ZnO/thin film will benefit in developing graphene-based multicolor display and optoelectronic integration in future. In addition, the photoresponse properties based on the heterojunction as a representative system show significantly enhanced conductivity and steady photoresponse with a fast response time. It reveals that the n-ZnO/graphene heterojunction has potential applications in the high-speed and high-sensitivity photodetectors and photoelectronic switches.

add to my program (close full abstract)

13:30 **Nitrogen ion casting of suspended graphene flakes: temperature effects and selectivity of sp2 nitrogen species**

Authors : M. Scardamaglia 1, B. Aleman 2, M. Amati 2, C. Ewels 3, P. Pochet 4, N. Reckinger 5, J.-F. Colomer 5, T. Skaltsas 6, N. Tagmatarchis 6, R. Snyders 1, L. Gregoratti 2, and C. Bittencourt 1 and C. Bittencourt 1

Affiliations : 1 Chemistry of Interaction Plasma Surface (ChIPS), University of Mons, Belgium; 2 Elettra Sincrotrone Trieste S.C.p.A., AREA Science Park, Italy; 3 Institut des Matériaux Jean Rouxel, Université de Nantes, CNRS, Nantes, France; 4 Laboratoire de simulation atomistique (L_Sim), SP2M, INAC, CEA-UJF, Grenoble F-38054, France; 5 Research Centre in Physics of Matter and Radiation, University of Namur, Belgium; 6 Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constaninou Avenue, 116 35Athens, Greece;

Resume : Achive the fine tuning of the graphene electronic properties is one of the main challenges for optimal fabrication of graphene-based nano-devices. Notably the low carrier density in pristine graphene at the Fermi level means that charge carrier doping is very attractive for nanoelectronics applications. Among these, the introduction of nitrogen atoms into the hexagonal carbon lattice of graphene has attracted interest in the recent years. Within this context, we present an experimental report that combines scanning photoemission microscopy analysis with in-situ nitrogen ion casting on suspended graphene. Nitrogen doping was performed by N2 ions bombardment in ultra-high vacuum. Inclusion of up to 20 at. % nitrogen can be reached through this clean technique with absence of oxygen species in the final product, while maintaining a largely sp2-carbon network. The inclusion was observed by scanning X-ray photoelectron microscopy which can be used to follow the evolution of nitrogen species: pyridinic, graphitic, and pyrrolic, at different doping stages and annealing temperatures. Variations in the ratio between sp2 nitrogen species was observed for increasing treatment time; annealing results in quenching of the sp3 component, suggesting graphitic nitrogen as the most thermal stable species. The occurrence of graphitic species together with the absence of pyrrolic is indicative of N-incorporation into a hexagonal graphene-based lattice.

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add to my program (close full abstract)

13:30 **Graphene-Au nanoparticle hybrid structure by DNA assisted self-assembly**

Authors : Tae Geun Kim 1,3, Jae Hyun Hur 2, Un Jeong Kim 2, Yeonsang Park 2, Kyuhyun Im 2, Chang-Won Lee 2, Nokyoung Park 2, Sungwoo Hwang 1,2, and Sangsig Kim 3

Affiliations : 1 Research center for Time-domain Nano-functional Device, Samsung Advanced Institute of Technology, Yong-In, Gyeonggi 446-712, South Korea; 2 Nano-Electronics Lab, Samsung Advanced Institute of Technology (SAIT), P. O. Box 111, Suwon 440-600, South Korea; 3 Department of Electrical Engineering, Korea University, Anam-dong, Seongbuk-gu, Seoul 136-713, South Korea

Resume : Au nano particles of approximately 12 nm in diameter capped with single strand DNA are successfully self-assembled on graphene. Hydrophobicity of graphene surface needs to be modulated to form uniformly self-assembled DNA capped Au nano particles, which is dissolved in water. By optimizing UV-ozone treatment time, agglomeration of DNA capped Au nano particles is avoided. Surface morphologies of DNA capped Au nanoparticle superlattice on graphene are observed by scanning electron microscopy and transmission electron microscopy. Field effect transistors are formed with Graphene-Au nanoparticle hybrid structure to characterize its electrical properties. N-doping effect on graphene is observed due to negatively charged DNA. In the future, by utilizing surface plasmon enhancement from Au nano particles, Graphene-Au nano particle hybrid structure can be applied for opto-electronic device.

G.PII. 13

add to my program (close full abstract)

13:30 **Raman studies of Graphene-Metal Interface**

Authors : Un Jeong Kim, Yeonsang Park, Chang-Won Lee, Sungwoo Hwang
Affiliations : Nano-Electronics Lab, Samsung Advanced Institute of Technology (SAIT), P. O. Box 111, Suwon 440-600, Republic of Korea

Resume : High quality graphene has been synthesized on copper foil by chemical vapor deposition (CVD) at 985 ℃. Graphene was transferred on quartz substrate by conventional method. Various metals such as Au, Ag, Cu, Cr, Ti are formed as a thin film of 50 nm on graphene surface by e-beam evaporation. Through quartz substrate, interface of graphene and metal thin film was investigated by Raman spectroscopy. Degree of chemical bindings with graphene and metal thin film can be observed through D-band enhancement behavior for certain materials. Theoretical calculation by first principle is consistent with the results from Raman scattering. This is very important step to understand graphene-metal interaction since these metals can be electrode materials for various device applications.

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add to my program (close full abstract)

13:30 **Raman mapping of G band: Implication of local strain due to inherent structural twist and folding in free-standing GO fiber alphabets**

Authors : Rajarshi Roy†, Nilesh Mazumder†, Gundam S. kumar‡, Hitesh Mamgain§, Uttam K. Ghorai‡, Dipayan Sen†, Kalyan K. Chattopadhyay†,‡
Affiliations : †Thin Film and Nanoscience Laboratory, Dept. of Physics, Jadavpur University,Kolkata-700032, India; ‡ School of Materials Science and Nanotechnology, Jadavpur University,Kolkata-700032, India; §WITec GmbH, Lise-Meitner-Strasse, 6 D-89081 Ulm, Germany.

Resume : Recently synthesis of graphene oxide (GO) fibers has gathered quite a bit of attention due to their superlative properties exhibiting high mechanical strength and robustness. With large scale processing yield now being realized, this next generation material is hailed as an important tool for integration of flexible macroscopic electronic devices and in other multi functional applications like smart clothing, flexible paper etc. In this work, we report in-situ self-assembly of GO fibers resembling the shape of some known English alphabets collected over Si Substrate. Raman spectroscopy for these graphene based analogues revealed some interesting anomaly in the G band due to inherent local structural folding and twists. Furthermore, Raman imaging of G band using width filter for the structures suggested generation of compressive and tensile strain being developed at the junction where folding is encountered with subtle changes in FHWM parameter.

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add to my program (close full abstract)

13:30 **Ultrathin graphene membrane for selective gas separation**

Authors : Nak-Kwan Chung, Yong-hyun Shin, Myung-ho Bae
Affiliations : Division of Industrial Metrology, Korea Research Institute of Standards and Science, Daejeon, Korea; 1 Division of Convergence Technology, Korea Research Institute of Standards and Science, Daejeon, Korea

Resume : Graphene has enormous potential as a promising materials for gas separation and energy storage because because of ultimate thinness, mechanical strength, and good stability. We prepared the layer-by-layer graphene on the polymer film, and conducted gas permeation study with gas molecules such as hydrogen, nitrogen, and oxygen. We demonstrated the the layered graphene films exhibit a good gas separation characteristics.

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add to my program (close full abstract)

13:30 **Enhanced SERS Stability and Reproducibility of Ag Substrates with a Monolayer Graphene Barrier**

Authors : Yuda Zhao, Yang Chai
Affiliations : Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Hong Kong.

Resume : Ag thin film is an efficient surface enhanced Raman spectroscopy (SERS) substrate because its quality factor of localized surface plasmon resonance (LSPR) is much larger than other materials, e.g., 10 times larger than that of Au at the wavelength of 500 nm. However, the chemical instability of Ag in ambient environment significantly degrades the SERS properties, and hinders the practical applications. Although conventional protective structures (e.g., silica and alumina barrier) can inhibit the Ag corrosion in ambient, they usually have large light absorption and reduce the plasmonic enhancement. In this work, we transfer monolayer graphene onto Ag SERS substrate, on one hand, to protect Ag from corrosion, and on the other hand, to prevent the photo-induced damages (photocarbonization, photobleaching and metal-

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catalyzed reaction) on the probed molecules. Firstly, we comparatively study morphological characteristic of the Ag SERS substrates with and without graphene protective barrier, revealing high corrosion-resistance of monolayer graphene to the oxidizing gas and liquid. We further demonstrate the graphene coated Ag thin films as stable SERS substrate. After 35-day exposure in air, the graphene coated Ag thin film maintains high SERS sensitivity. Secondly, we systematically study the resistance to photo-induced damages with graphene barrier. Our results show that Ag SERS substrate with graphene coating significantly improves the SERS reproducibility, and simultaneously inhibits metal-catalyzed reaction. In addition, the graphene layer can form strong interaction with the probed R6G molecules through π-π bonding stack, reducing the possibility of photo-induced desorption. In summary, our results show that graphene coating on Ag substrate effectively enhances the resistance to the corrosion and photo-induced damages.

add to my program (close full abstract)

13:30 **Reduced graphene oxide functionalized with metal nanoparticles: Fabrication, structure, and sensing properties**

Authors : Han Gil Na, Hong Yeon Cho, Yong Jung Kwon, Hyoun Woo Kim*
Affiliations : Department of Materials Science and Engineering, Hanyang University, 222 Wangsimni-ro, Seongdong-Gu, Seoul, 133-791, Korea

Resume : We have fabricated reduced graphene oxide (RGO) and functionalized them with metal nanoparticls. To obtain uniform metal-RGO sheets, the supernatant was centrifuged to remove small graphene pieces and water-soluble by product, repeatedly washed with distilled water until the pH = 7. Due to their outstanding physical and chemical properties, graphene and its derivatives have attracted tremendous attention for both fundamental science and possible technological applications. RGO can be efficiently prepared by reducing (i.e. annealing) graphene oxides. Although RGO has irreversible defects, disorder and residual functional groups, it exhibits a sufficient conductivity. Transmission electron microscopy results exhibited the deposition of metal nanoparticles on RGOs. The NO2 gas sensing test was carried out to demonstrate the ability of the metal functionalization to attain the higher sensitivity than bare RGO sheet. We have discussed the possible mechanisms for improvement of the sensing properties by metal-functionalization. We suppose that spillover effect induced by metal nanopartitcles play a significant role in enhancing the sensing properties.

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13:30 **Impact of the hydrocarbon precursor type on the generation and concentration of free radicals in a plasma polymer**

Authors : S. Ershov(1), F. Khelifa (2), Ph. Dubois (2,3), R. Snyders(1,3)
Affiliations : (1) Chimie des Interactions Plasma-Surfaces, Center of Innovation and Research in Materials and Polymers (CIRMAP), University of Mons UMONS, Place du Parc 23, 7000 Mons, Belgium; (2) Laboratory of Polymeric and Composite Materials, Center of Innovation and Research in Materials and Polymers (CIRMAP), University of Mons UMONS, Place du Parc 23, 7000 Mons, Belgium; (3) Materia Nova Research Center, Parc Initialis, Avenue N. Copernic 1, 7000 Mons, Belgium

Resume : Plasma Polymerized Films (PPF) synthesized by Plasma Enhanced Chemical Vapor Deposition (PECVD) differ in many ways from conventional polymers. One of their specifics is the high reactivity of the surface rich in free radicals arising from deposition mechanism. Though generally leading to ageing of PPF, it can be beneficially employed for grafting of a specific functionality. The quantitative evaluation of surface radical density and understanding of radical formation mechanisms are thus mandatory for a successful surface modification. The aim of the work is to compare the free radical formation and concentration in PPF synthesized from a saturated cyclic precursor and its resonant isomer in order to evaluate the impact of aromaticity on radical generation. The surface radical densities of the isopropanol-, benzene- and cyclohexane-based PPF were quantitatively determined by a combination of NO chemical derivatization and X-Ray Photoelectron Spectroscopy (XPS). Once the procedure was optimized on the isopropanol-based PPF, the radical density, derived from XPS-determined at.% N, was evaluated and compared for the benzene- and cyclohexane-based PPF as a function of input power. The former exhibits an increase of the radical density in the entire power range while for the latter a plateau of the radical density above 200 W is observed. It can be explained by differences in radical formation mechanisms and structure of plasma polymers addressed by a set of analytical techniques.

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13:30 **Interfacial charge transfer in P3HT/TiO2 nanocomposites by photoluminescence investigations**

Authors : Long Jiang1, Jianling Zhang1, Haigang Yang1, Thien Phap Nguyen2, Yi Dan1
Affiliations : 1 State Key Laboratory of Polymer Materials Engineering of China (Sichuan University), Polymer Research Institute of Sichuan University, Chengdu 610065, China 2Institut des Matériaux Jean Rouxel, University of Nantes, CNRS, 2 rue de la Houssinière, 44322 Nantes, France

Resume : Incorporation of TiO2 nanoparticles into conjugated polymers (CPs) has received intense interest in areas such as photocatalysis and photo-energy storage for the outstanding photo-physical and photo-chemical properties derived from the synergy between the inorganic semiconductor and organic CPs. CPs/TiO2-based hybrid photocatalysis system has been previously studied [1,2] and the results revealed that the photo-responding range of the hybrid photocatalytic materials was extended to visible part of the solar spectrum with the use of CPs. Meanwhile, conjugated polymers will improve the photocatalytic performance by their photo-conversion efficiency, which is better than that achieved with pristine TiO2. However, the photo-induced charges transfer between CPs and TiO2 in the hybrid photocatalytic materials and the influence of the TiO2 nanocrystals on the optical-properties of conjugated polymers have not been well elucidated so far. Here, we chose P3HT/TiO2 (anatase, of size ~25nm) in chlorobenzene solution as a model system to gain fundamental understanding of the energy and charge s transfer mechanisms between CPs and TiO2 using steady-state luminescence and UV-vis absorption spectroscopy analyses methods. Emission spectra of the P3HT/TiO2 solutions with various TiO2 fractions excited at 275nm, whose energy is higher than that of the bandgap of TiO2, are shown in Figure 1 (a). The PL emission increases initially in the presence of 10-20 wt% TiO2, and then decreases as the nanoparticles concentration is increased. The PL emission enhancement with 10-20 wt% TiO2 is attributed to the efficient transfer of energy from TiO2 nanoparticles to P3HT. Further increasing TiO2 concentration may lead to inorganic particle aggregation in organic solution, resulting in a reduction of the contact area with P3HT as well as the PL emission. Emission spectra of the P3HT/TiO2 solution excited at 400 nm are shown in Figure 1 (b). It can be seen that exposure of P3HT/TiO2 to 400 nm laser does not show PL enhancement effect as observed with the 275 nm laser. This result can be explained as follows: as the energy of 400 nm laser is smaller than the TiO2 bandgap, no electron-hole pairs in TiO2 nanoparticle were generated, resulting in no energy transfer from TiO2 to P3HT. On the other hand, when excited at 400 nm, the PL emission was gradually quenched with the increase of TiO2 concentration. This suggests that the charge transfer occurs from P3HT to TiO2.

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add to my program (close full abstract)

13:30 **New Self-Assembled Supramolecular System based Triphenylene Imidazolim Derivative.**

Authors : Sunjung Jo, Jaemee Kim, K. M. K. Swamy, Jun Yin.
Affiliations : Juyoung Yoon* Korea

Resume : We synthesized a new triphenylene imidazolium derivative, which has triangular shape. Triphenylene is a type of polycyclic aromatic hydrocarbon (PAH) on planar structure. The compound contains two parts. For one thing is rigid, planar core that genarates π-π stacking system, for the other is flexible alkyl chains. The triangle shaped poly-N-Heterocyclic carbene (NHC) ligands have an advantage of formation of polymers. By adding anion, the NHCs interact with ion salt. It?s because the intermolecular π-π interaction induces polymers to stack one sheet by one. Through charges interaction, these forms assembled structure and resulting properties. The self-assembled structure makes charges transfer easily in one plane. The ionic interaction of planar cation receptors and anion salts induce various supramolcular assemblies. The highly arrangement of charged material induce unique properties. In conclusion, the result of this material forms self-assembly structure and nano particle. The imidazoium acted receptor have various characteristic, generate self-assembly nano system. Since the self-assembly structure is used as electron transfer channels, the material is applicable to photovoltaic cell, OFETs, OLEDs, etc. References 1. Zhaochao Xu, Sook Kyung Kim Juyoung Yoon*, Chem. Soc. Rev. 2010, 39(5), 1457-1466.

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13:30 **POLY-(PYRROLE-THIOPHENE-ANILINE)-1,4-DICHLORO-2-BUTYNE STRUCTURES DEPOSITED BY PLASMA POLYMERIZATION**

Authors : S. M. Iordache, A.-M. Iordache, A. Balan, L. Popovici, Ioan Stamatin*
Affiliations : University of Bucharest, Faculty of Physics, 3Nano-SAE Research Center,

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Atomistilor 405, P.O. Box 38, Bucharest-Magurele, Romania, 077125 *Corresponding author: istarom@3nanosae.org

Resume : We report the codeposition of three conjugated polymers, with π molecular orbitals delocalized along the polymer chain, (polyaniline, polypyrrole, polythiophene) and poly-1,4-dichloro-2-butyne from suitable monomers on silicon substrate by plasma polymerization that is aiming to identify the range of negative differential resistance (NDR) behavior in I-V characteristics and their correlation with the conduction mechanisms and space charge distribution. The deposited thin films were characterized by UV-VIS (e.g. band gap), FT-IR-Raman (e.g. structural identification of the structural units) spectroscopy and AFM/STM topography. The polyaniline-poly-1,4-dichloro-2-butyne and polythiophene-poly-1,4-dichloro-2-butyne systems show NDR ranged in 0.5 – 1 V, values that are close to requirements in designing of smart card devices based on tunnel diodes.

add to my program (close full abstract)

13:30 **PREPARATION AND CHARACTERIZATION OF POLYLACTIDE/CHITOSAN NANOCOMPOSITES THIN FILMS**

Authors : W. W. Wang1,2, P. Le Rendu1, Y. Dan2, T. P. Nguyen1*
Affiliations : 1Institut des Matériaux Jean Rouxel, University of Nantes, CNRS, 2 rue de la Houssinière, 44322 Nantes, France 2State Key Laboratory of Polymer Materials Engineering of China (Sichuan University), Polymer Research Institute of Sichuan University, Chengdu 610065, China

Resume : Composites made by polymer blending is an attractive alternative to produce materials with tailored properties intended to industrial applications. Chitosan and polylactide (PLA) are both biodegradable and biocompatible polymers with potential use in medical applications. Their combination to provide new materials with controllable composition and properties is very interesting and promising for specific applications in the medical field. In this work, we present the synthesis of the blends for fabrication of nanocomposite thin films and their characterization by optical spectroscopies. Because of their different polarities, the polymers need to be dissolved in a solvent blends in defined conditions for obtaining a homogeneous solution. We have successfully established a ternary phase diagram using chloroform, acetic acid and water and defined the conditions for obtaining controlled compositions of PLA/chitosan composites. Analysis of the optical spectra of PLA, chitosan and their composites shows that the structure of the polymers is preserved in their blends. This observation suggests that chitosan is fully incorporated to PLA without significant interactions. Degradation study of the blends under prolonged UV irradiation reveals that chitosan is more stable in composites but is decomposed before PLA .

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13:30 **Influence of nozzle geometry on the properties of CNW synthesized in a plasma jet**

Authors : S.D. Stoica, S. Vizireanu, C.R. Luculescu, B. Mitu, G. Dinescu
Affiliations : National Institute for Laser, Plasma and Radiation Physics, Magurele, 077125, Romania

Resume : Nanostructured carbon materials based on graphene are among the most studied materials nowadays, due to interesting properties which allow their utilization in various applications. Previously, we have developed a method for carbon nanowalls (CNW) growth based on downstream deposition from an expanding radiofrequency argon plasma beam discharge injected with acetylene in the presence of hydrogen. So-called ?standard? conditions were defined as: RF power = 300 W, Ar:H2:C2H2 = 1050:25:1 sccm, pressure = 1 mbar, distance from the injection = 5 cm, substrate temperature = 700 ?C. The present study aims to investigate the effect of the nozzle geometry (diameter 2-16 mm) on the material characteristics and to correlate them with the plasma species present during the synthesis process. The main investigation technique was Scanning Electron Microscopy (SEM) for revealing the obtained morphologies and structures, in combination with statistical processing of SEM images for determination of specific length/width ratio of individual CNW. The plasma process was analyzed regarding the excited species by Optical Emission Spectroscopy (OES) performed both at the injection level and on the deposition level. We show that either CNW, or combined nanofibers/nanowalls architectures with various aspect ratios can be obtained, and the OES technique may provide information which allows a correlation between the material characteristics and the internal plasma parameters.

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13:30 **Polyethylene glycol-silver nanocomposite material for antimicrobial applications**

Authors : V. Satulu(1), B. Mitu (1), V. Ion(1), I. Sarbu(2), D. Pelinescu (2), G. Dinescu (1)
Affiliations : (1) National Institute for Laser, Plasma and Radiation Physics, Magurele, 077125, Romania (2) University of Bucharest, Centre for Research, Education and Consulting in Microbiology, Genetics and Biotechnology (MICROGEN),, Bucharest, Romania

Resume : Organic-inorganic nanocomposites have found extensive range of application in various fields, from energy storage to catalysis or biomedical materials. In particular, metallic nanoparticles embedded in polymeric matrices are of high interest for biomedicine. Plasma polymerized polyethylene glycol films present antifouling properties and low water solubility, while the silver particles are well known for their antimicrobial effect as well as for generation of plasmon resonance effect. This work proposes the deposition of polyethylene glycol ?silver (PEG-Ag) nanocomposites with tunable composition by using low pressure RF plasma system. The study aims the obtainment of a synergistic effect by means of proper control of the composition and density of each component through experimental parameters. The morphology, chemical composition and optical properties of the material were determined by means of Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and Spectroscopic ellipsometry, respectively. The antimicrobial effect against various strains as S. aureus, E. coli and C. albicans was demonstrated.

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13:30 **Properties of hybrid composites made of plasma-chemical deposited organosilicon layer on electrospun polymer nanofibers**

Authors : Eva Kedronova1, Lenka Zajickova2, Dirk Hegemann3, Miroslav Michlicek2, Anton Manakhov2, Milos Klima2, Eliska Mikmekova4
Affiliations : 1 Department of chemistry, Faculty of Science, Masaryk University Brno, Czech Republic; 2 Department of Physical Electronics, Faculty of Science, Masaryk University Brno, Czech Republic; 3 EMPA St. Gallen, Switzerland; 4 Institute of Scientific Instruments, Academy of Sciences of the Czech Republic, Brno, Czech Republic

Resume : Electrospinning is commonly used for preparation of polymer nanofibers but the application of the nanofibers usually requires an additional surface treatment. Plasma enhanced chemical vapor deposition (PECVD) is a versatile technique used for surface modification and it is interesting to test it also for highly porous materials such as electrospun nanofibers. Organic/inorganic composites were prepared by PECVD of organosilicon plasma polymers deposited on PVA and PA6 electrospun nanofibers from HMDSO/Ar mixtures. Low pressure RF discharges with capacitive coupling and by cold RF plasma multi-jet working at atmospheric pressure were used. Deposition conditions were varied to get samples with different structure and wettability and their influences on chemical composition of the resulting layers were investigated by IR spectroscopy and the XPS. The values of the WCA were strongly influenced by both chemical composition of deposited layers and overall surface structure. Significant variations in microstructure of resulting composites were revealed by AFM and SEM analysis of composites prepared by different plasma sources.

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add to my program (close full abstract)

13:30 **Stark effect in GaNAsBi/GaAs quantum wells operating at 1.55 µm**

Authors : C. Bilel*, M. M. Habchi, A. Rebey, and B. El Jani
Affiliations : University of Monastir, Faculty of Sciences Unité de Recherche sur les Hétéro-Epitaxies et Applications (URHEA), 5019 Monastir, Tunisia E-mail: * chakroun_bilel01@yahoo.fr

Resume : The effect of an applied stationary electric field on the band structures of GaNAsBi/GaAs quantum wells has been investigated using self-consistent calculations. Such study based on the optimization of N and Bi contents can be useful to improve physical proprieties of emitters or photodetectors devices operating at 1.55 µm. We have examined the quantum confined Stark effect on the shape of the confining potential, the Fermi level, the subband energies and their corresponding wave functions as well as their occupations, and the charge density distributions. We have also determined the oscillator strength and the absorption coefficient of the inter-subband transitions and their dependences on the applied perturbation. Keywords: Stark effect; GaNAsBi/GaAs QWs; band structures; self-consistent calculations.

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13:30 **Composition control PECVD SiCxNy films deposited from new organosilicon precursor**

Authors : E. Ermakova, M. Kosinova, Yu. Rumyantsev
Affiliations : Nikolaev Institute of Inorganic Chemistry SB RAS

Resume : Silicon carbonitride SiCxNy as non-stoichiometric compounds combine a wide range of functional properties in dependence on chemical and phase composition. Their high temperature stability, transmittance and hardness make them a promising material for production of different types of coatings. Use of organosilicon precursors in PECVD processes appeared to be a useful technique for synthesis of SiCxNy films of various composition. In this work phenyltrimethylsilane PhSiMe3 was characterized as a CVD precursor. Its vapour pressure temperature dependence and thermal stability were investigated. High-temperature SiCxNy films were synthesized by PECVD technique using PhSiMe3. Influence of additional gas type (helium, ammonia) on films' structure and properties was investigated. It was shown that structure and functional properties of SiCxNy films depend significantly on synthesis conditions. Ammonia addition into reactive mixture led to deposition of films with different nitrogen and carbon content with change in composition from SiCx and SiCxNy to SiNy (FTIR, EDX). It was shown by Raman spectroscopy that high-temperature SiCx and SiCxNy films contain nanocrystals of graphite phase. Such functional properties as hardness and transmittance were measured. It was shown that both hardness and transmittance depend on the films composition and chemical binding.

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13:30 **EPR study of paramagnetic centers in SiO2:C adsorbent**

Authors : D.V. Savchenko(1),(2), B.D. Shanina(1), E.N. Kalabukhova(1), A.A. Sitnikov (1), V.S. Lysenko(1), V.A. Tertykh(3)
Affiliations : (1)V.E. Lashkaryov Institute of Semiconductor Physics, NASU, Kyiv, 03028, Ukraine (2)Institute of Physics, AS CR, Praha 8, 18221, Czech Republic (3)A.A. Chuiko Institute of Surface Chemistry, NASU, Kyiv, 03164, Ukraine

Resume : Fumed silica A-300 was carbonized by means of pyrolysis of CH2Cl2. The obtained initial SiO2:C nanopowders of black color (d~14-16 nm, carbon concentration 7 wt%) subjected to the oxidation and passivation treatment were studied by electron paramagnetic resonance (EPR) at 4.2-400 K. Two EPR signals of Lorentzian lineshape with nearly equal g-factors and different linewidth were observed in all samples. The two-component EPR spectrum was explained by the presence of the C clusters of different sizes resulting in EPR line of different linewidth due to the spin exchange interaction between paramagnetic centers. The intensive narrow EPR signal was attributed to the carbon related defect (CRD) with non-localized electron hopping between neighboring C-dangling bonds. From the temperature dependence of resonance field position of the CRD EPR signal, caused by exchange interaction between conduction electrons and localized spin system, the parameters of the localized spin system has been determined in oxidized and passivated samples. It was supposed that the conduction electrons are coupled with electrons localized at interface defect. The observed peaks in temperature dependence of the conduction electron EPR signal integral intensity at 200-440 K was explained by ejection of electrons from the confinement energy levels of carbon quantum dots when the temperature become comparable with the confinement energy. The work supported by STCU №5513 and SAFMAT CZ.2.16/3.1.00/22132 projects.

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13:30 **Microanalytical detection and microstructural role of C impurities in ZnO-porous silicon nanostructured composite films.**

Authors : D. Gallach1,2, L. Le Brizoual3, N. Gautier4, M.D. Ynsa Alcalá1,5, V Torres Costa1,2, JP Landesmann6, M Manso Silván1,2
Affiliations : 1 Departamento de Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain 2 Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain 3 Institut d'Electronique et de Télécommunications de Rennes - UMR 6164. Université de Rennes 1.35042 Rennes, France. 4 Institut de Materiaux de Nantes, UMR 6502, Nantes , France. 5 Centro de Microanálisis de Materiales, Universidad Autónoma de Madrid, Madrid, Spain. 6 Institut de Physique de Rennes, UMR 6251, Rennes , France.

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Resume : ZnO- porous Silicon (ZnO-PSi) nanostructured composite films have been prepared exploiting the low wettability of freshly prepared anodized porous silicon towards ZnO sols based on zinc acetate. Upon thermal annealing the ZnO sols diffuse through the columnar PSi and give rise, as evidenced by transmission electron microscopy, to a surface decorated by hexagonal ZnO

crystallites. Relevantly, at temperatures as high as 800ºC the crystallites become void presumably as an effect of C impurities. In fact, X-ray photoelectron spectroscopy and C-resonant Rutherford backscattering spectroscopy show that Integrated C species are observed to continuously diminish for increasing annealing temperatures. The so formed structures present relevant optical properties as derived from ellipsometry measurements, which could be useful for the design of optical filters and other interferential or angular dependent optical devices.

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13:30 **Thin film encapsulation of organic light emitting diodes with multi inorganic layer prepared by cyclic chemical vapor deposition system**

Authors : Jae Seok An1, Ha Jun Jang1,2, Cheol Young Park1, Jong Ho Lee1, and Bum Ho Choi1*
Affiliations : 1National Center for Nanoprocess and Equipments, Korea Institute of Industrial Technology, Gwangju 500-480, Korea; 2Advanced Chemical & Engineering, Chonnam National University, Gwangju 500-757, Korea

Resume : One of the challenging issues in organic light emitting diodes (OLEDs) is long life-time. Since active organic layer is vulnerable to water vapor and oxygen, it is essential to prevent water vapor and oxygen from diffusing into the organic layer by introducing water vapor permeation barrier layer. In this presentation, we have investigated water vapor permeation barrier properties of cyclic chemical vapor deposition (C-CVD) grown SiN/SiCN/SiN multi inorganic layer by the method of Ca-test. The thickness of each layer is 10nm. For Ca-test, 60nm thick Ca layer was evaporated onto the flexible PEN substrate, followed by inorganic preparing SiN/SiCN/SiN passivation layer. For the Ca-test was performed at 85 ℃ 85% relative humidity accelerated conditions with aging factor of 240hrs. The transmittance of Ca-layer was measured with time and those measured at 550nm was used to calculate water vapor transmission rate (WVTR). The WVTR value of 3.2x10-5g/m2/day was maintained until 30,000hrs, which exceeds to industrial requirement. However, WVTR value is abruptly increased after 80,000hrs of measurement time which means the critical life time is exist in 30nm thick SiN/SiCN/SiN passivation layer. By C-CVD technology, defects and pin-hole free inorganic layer can be prepared that means diffusion path of water vapor can be effectively blocked in passivation layer. TEM analysis also revealed that inter-diffusion path, result in long life-time. Furthermore, XRD measurement exhibited each inorganic layer is amorphous that can hinder water vapor penetration into organic layer.

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13:30 **Investigation of SHG Properties of Some Azo-Molecules Doped in Sol-gel Thin Films**

Authors : I.C. Vasiliu1, I. Ionita2, A. Matei3, M.Elisa1, R. Iordanescu1, I. Feraru1, A. Emandi1
Affiliations : 1INOE 2000 - National Institute for Optoelectronics, 409 Atomistilor Str., Magurele RO-077125, Bucharest, Romania, icvasiliu@inoe.inoe.ro 2UB - University of Bucharest, 405 Atomistilor Str., Magurele RO-077125, Bucharest, Romania 3INFLPR - National Institute for Laser, Plasma and Radiation Physics, 409 Atomistilor Street, Magurele, RO-077125 Bucharest, Romania

Resume : We investigate the SHG behavior of SiO2-P2O5 thin films doped with some polyazo dye molecules comprising D – donor (NH2) ant A – acceptor (NO2) moieties, which change under illumination with visible light. Our data show that photoisomerisation, phototautomerization reactions and light-induced polar orientation are dependent on the molecular structure of the guest molecules. Polar structure and molecular size, as well as the chemical structure of SiO2-P2O5, are the dominant parameters that determine SHG. Two forms of azo-based dyes (trans ant cis forms) are responsible for the interaction with irradiating laser light and forming an anisotropic structure inside the SiO2-P2O5 /dye thin films

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add to my program (close full abstract)

13:30 **Growth and Characterization od ncNi-carbon nanolayered structure**

Authors : P.A.Karaseov1, A.I.Titov1, M.V.Mishin1, V.S.Protopopova2, A.Ya.Vinogradov3, O.A.Podsvirov1, P.G.Gabdullin1, E.N.Shubina1
Affiliations : State Polytechnic University, St. Petersburg, Russia; Aalto University, Helsinki, Finland; Ioffe Institute, St. Petersburg, Russia

Resume : It is well known that different varieties of carbon-based nanostructures demonstrate facilitated field-induced electron emission, even if they have no high-aspect-ratio surface morphology elements, such as sharp tips or ribs. Macroscopic properties of DLC films strongly depend on relative

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content of sp3- and sp2-hybridized carbon bonds and hydrogen content. The quality of DLC films and hence their properties can be tailored by tuning the ratio of sp2/sp3 carbon atoms and stress in the films, both of which can be changed by doping metals or non-metals in DLC matrix. In this contribution we report growth and study of properties of sandwich structures comprising layers of both Ni-C nanocomposite and α-C:H layers on (100) crystalline silicon substrates. α-C:H layers were grown using RF plasma of methane and methane -hydrogen mixtures. Process of deposition of α-C:H layers was carried out in the PECVD method. ncNi-carbon layers were grown by the MOCVD technique using bis-(ethylcyclopentadienyl) nickel (EtCp)2Ni as a precursor. The deposition process was carried out in low-pressure tube silica reactor in the temperature range 350-650°C. Nanocomposite layers contained 10-20 nm Ni particles presumably coated by nickel carbide shells were obtained. Results of investigation of DLC films and different sandwich structures by AFM, SEM, XPS and other techniques will be presented. This work was supported by RFBR grants № 12-08-01197 and 13-02-92709.

add to my program (close full abstract)

13:30 **DAMAGE FORMATION IN SILICON DURING SMALL CLUSTER ION IMPLANTATION**

Authors : P.A.Karaseev, A.I.Titov, K.K.Karabeshkin
Affiliations : State Polytechnic University, St.Petersburg, Russia

Resume : Structural damage formation in Si irradiated at room temperature by atomic (P+) and molecular (PF4+) ions is experimentally studied in a wide energy range (0.6-3.2 keV/amu). Strong molecular effect, caused by overlapping of collision cascades created by atoms comprising molecular ion, is revealed close to the sample surface in all cases considered. Theoretical assessments of depths where nonlinear processes are possible have shown good agreement with experimental data. Primary defect generation enhancement in the vicinity of Si surface is estimated about factor of 5. This work was supported by RFBR (grants 13-08-00666 and 14-08-01256).

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add to my program (close full abstract)

13:30 **Structure and optical properties of DLC:Cu thin films grown by using high density plasma**

Authors : Š. Meškinis, A. Čiegis, A. Vasiliauskas, K. Šlapikas, S. Tamulevičius, G. Niaura
Affiliations : Institute of Materials Science of Kaunas University of Technology, Savanorių 271, 50131 Kaunas, Lithuania

Resume : Diamond like carbon (DLC) is a metastable form of the amorphous carbon consisting from the sp2 bonded (graphite like) carbon clusters embedded into the sp3 bonded (diamond like) carbon matrix. DLC films remains under considerable interest of the researchers due to the high optical transmittance in visible light and IR ranges, high hardness and wear resistance, corrosion resistance, biocompatibility. Additional control of DLC properties can be achieved by doping with different metals. Particularly surface plasmon resonance effect was observed in group I metal containing DLC films. In addition good hemocompatibility and antibacterial properties were reported for group I metal containing DLC films. Taking into account interesting properties of DLC films mentioned above group I metal containing DLC films can become interesting material for fabrication of the advanced plasmonic biomedical sensors. In present study copper containing diamond like carbon films (DLC:Cu) films were deposited by using reactive high power pulsed magnetron sputtering. High power pulsed magnetron sputtering is novel high density plasma deposition method. High plasma density of the high power pulsed magnetron sputtering is advantageous for deposition of DLC films containing high amount of sp3 bonded carbon. Effects of the acetylene and argon gas flow ratio as well as pulse current density were studied. The dependence of the optical properties of DLC:Cu films on structure and composition was investigated.

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add to my program (close full abstract)

13:30 **Multiwavelength Raman analysis of SiOx and N containing amorphous diamond like carbon films**

Authors : Asta Tamulevičienė*, Vitoldas Kopustinskas*, Gediminas Niaura**, Šarūnas Meškinis*, Sigitas Tamulevičius*
Affiliations : *Institute of Materials Science of Kaunas University of Technology, Savanorių Ave. 271, LT-50131 Kaunas, Lithuania **Center for Physical Sciences and Technology, Institute of Chemistry, A. Goštauto 9, LT-01108 Vilnius, Lithuania

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Resume : Amorphous diamond like carbon films can be modified by introducing doping compounds during deposition process. As potential candidates for modification usually Si, O, N, Ag, Cu are used. In case of Si, O

and N incorporation, organosilicone compounds such as hexamethyldisiloxane (HMDSO) and hexamethyldisilazane (HMDSN) are used. Incorporation of SiOx gives better adhesion and optical properties (transparency, optical band gap) of the films. Using HMDSN one can form silicon carbonitride thin films with high hardness, low friction coefficient, etc. Even though these films show interesting properties, the structure of these films employing multiwavelength Raman scattering was not investigated. In the current research thin a-C:H:SiOx and a-C:H:SiN films were deposited on crystalline silicon and fused silica from HMDSO and HMDSN compounds respectively, using closed drift ion beam source and different ion beam energy. The structure of these films was studied employing multiwavelength (325 nm – 785 nm) Raman analysis. From the Raman spectra analysis, the characteristic parameters such as the positions of D and G peaks, D/G peak ratio as well as dispersion of G peak showing topological disorder of sp2 phase in doped a-C:H films were determined. Optical properties of the films were analysed versus composition and structure as well as doping conditions during deposition.

add to my program (close full abstract)

13:30 **FTIR STUDIES OF SILICON CARBIDE NANOSTRUCTURES**

Authors : I. Karbovnyk (1), P.Savchyn (1), A. Huczko (2), M. Cestelli Guidi (3), C Mirri (3), A. I. Popov (4,5)
Affiliations : (1) Dept of Electronics, Ivan Franko National University of Lviv, 79005, Lviv, Ukraine, (2) Department of Chemistry, Warsaw University, Poland (3) INFN-Laboratori Nazionali di Frascati, Italy (4) Institute of Solid State Physics, University of Latvia, LV-1063, Riga, Latvia; (5) Institute Laue-Langevin, F-38042 Grenoble, France;

Resume : The renewed interest in silicon carbide is connected with the synthesis of various one-dimensional nanostructures, which can be interesting in different applications. Stable 1D silicon carbide nanostructures have been obtained via combustion synthesis route. FTIR spectroscopy analysis has been done Daphne Light synchrotron facility of LNF INFN, Frascati. Infrared reflectivity spectra for unpurified and purified nano-SiC were compared with the spectra of commercially available SiC nanomaterials (experiments were carried out at 20 K and at room temperature). The performed measurements have proved that FTIR technique is very sensitive for silicon carbide nanomaterials. The manifestation of the fundamental Si and C sublattice was observed in the range of 770 to 1000 cm-1. In case of the synthesized 1D structures (nanowires) a different profile of the reflectivity peak was observed. This peak is strongly dependent on the purity of the investigated nanomaterial. For the raw synthesis product the main peak is strongly damped by background absorption. Generally, SiC nanowires show sharper reflectivity maximum than those of the nanoparticles. Small shift of the exact position of the main IR peak was also detected for 1D SiC, indicating the nanometric confinement effect.

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13:30 **Investigation of the boundary reaction between InTe-C and InSb for the characterization carbon doping effect on In-Sb-Te ternary alloys**

Authors : Hyunsoo Kim13, Jinse Kim1, Jongmin Geum1, Hasub Hwang3, YongTae Kim*2, Man-Young Sung*1
Affiliations : 1 Electrical Engineering, Korea University; 2 Korea Institute Science and Technology (KIST); 3 Memory Division Samsung Electronics co. ltd

Resume : For the multi-bit storage phase change memory, new chalcogen alloys such as In-Sb-Te, Ga-Te-Sb and Si-Sb-Te have been suggested because GST has a limitation for the application of multibit storage. Therefore, it is very important to understand the phase change mechanism of a new chalcogenide material at the first because the feasibility of multibit storage strongly depends on the multi-level phase change mechanism. According to our previous results, In3Sb1Te2 (IST) shows multi-level phase transformation phenomena from amorphous to crystalline IST through several intermediate phases. However, this multi-level phase transformation leaded an abrupt volume change because of the movements of vacancy and the atomic migration. We proposed carbon doping In-Sb-Te materials, which is enhanced the reliability rather than InSbTe ternary alloy. In this work, we have prepared bi-layer of InTe-C and InSb and annealed them at over crystallization temperature. The crystallization mechanism of carbon doped IST can be explained by the observation of the boundary of InTe-C and InSb with a HR-TEM and AES. The boundary reaction between InTe-C and InSb bilayer shows that the carbon atoms in the InTe act interstitial impurity. Therefore, the bigger atoms such as Sb and Te atoms are not perfectly inter-diffused each layer by interruption of carbon atoms and the carbon atoms exist in the vacancy site of InSbTe, so the atomic migration is difficult to occur. It is increasing reliability.

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16:00 **PLENARY SESSION**

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PROGRAM VIEW : 2014 Spring
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Symposium : G

Carbon- or nitrogen-containing nanostructured thin films

26 May 2014 | 27 May 2014 | 28 May 2014 | **29 May 2014** | 30 May 2014

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start at	Subject	Num.
	Recent advances in transition metal nitrides-III : Jochen SCHNEIDER, Vladimir UGLOV	
08:30	**Erosion resistant, self-healing Cr2AlC nanolaminate MAX phase coatings** **Authors :** Christoph LEYENS **Affiliations :** Technische Universität Dresden, Institute of Materials Science, Chair of Materials Engineering, Helmholtzstraße 7, 01062 Dresden, Germany **Resume :** In aero engines, coatings are facing severe attack under multiple loading conditions. Sand erosion, e.g., can cause great damage to turbine hardware in the compressor, while hot corrosion and oxidation are of concern in the hotter parts of the engines. Today, coatings are widely applied to protect high pressure turbine airfoils, however, their use in the compressor and the low pressure turbine is scarce yet. The paper will review recent developments in the field of erosion protection of aerospace alloys such as titanium and nickel alloys indicating that Cr2AlC nanolaminate MAX phase coatings can substantially improve the component lifetimes under erosion attack. It has been shown that the Cr2AlC MAX phase exhibits good erosion protection due to its combination of metallic and ceramic properties. Furthermore, Cr2AlC has excellent oxidation resistance, particularly if doped with Y. Recently, for this MAX phase autonomous self-healing behaviour was demonstrated which fostered significant research efforts in this area. The current aim of ongoing research is to assess the potential of Cr2AlC MAX phase coatings as erosion resistant autonomous self-healing material by understanding the basic physical and chemical principles governing multiple crack closure to heal erosion damage. add to my program (close full abstract)	G.IX.1
09:00	**Design of superelastic interlayer for tribological coatings** **Authors :** T. Polcar, M. Callisti, B.G. Mellor **Affiliations :** University of Southampton, UK & Czech Technical University in Prague, Czech Republic; University of Southampton,UK **Resume :** In this study two different superelastic layers were fabricated by magnetron sputtering: Ni-rich Ni-Ti and a (Ni, Cu)-rich Ni-Ti-Cu film approx. 2 μm thick. In order to obtain superelastic properties, the films were isothermally annealed for 1 hour at 500°C in a high vacuum environment. Subsequently the superelastic layers were coated by magnetron sputtering with a tribological coating (DLC-W and self-lubricant WSC film). The chemical composition of every single layer was measured by Energy-dispersive X-ray spectroscopy (EDS), while the structure was evaluated by grazing-incidence X-ray diffraction (GIXRD) and transmission electron microscopy (TEM). The mechanical properties of the single layers as well as those of the bilayers were measured by nanoindentation. Finally, the tribological behaviour of the bilayers and of the single layers were characterised by pin-on-disc. add to my program (close full abstract)	G.IX.2
09:15	**Phase stability predictions of (Cr1-x,Mx)2(Al1-y,Ay)(C1-z,Xz) (M = Ti, Hf, Zr; A = Si, X = B)** **Authors :** L. Shang, D. Music, M. to Baben and J. M. Schneider **Affiliations :** Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany **Resume :** The phase stability of (Cr1-x,Mx)2(Al1-y,Ay)(C1-z,Xz) (M = Ti, Hf, Zr; A = Si, X = B, space group P63 / mmc, prototype Cr2AlC) was studied using ab initio calculations. Based on the energy of mixing data as well as the density of states (DOS) analysis, (Cr1-x,Zrx)2AlC and (Cr1-x,Hfx)2AlC are predicted to	G.IX.3

be unstable, whereas (Cr1-x,Tix)2AlC, Cr2(Al1-y,Siy)C and Cr2Al(C1-z,Bz) are predicted to be stable or metastable. The density of states analysis reveals that small differences in the position of the Fermi level alters the phase stability: (Cr1-x,Zrx)2AlC and (Cr1-x,Hfx)2AlC are predicted to be unstable or metastable as the Fermi level lies at a peak position. While the Cr dominated DOS for (Cr1-x,Tix)2AlC plateaus at the Fermi level indicating stability. Implications of these results for the vapour phase condensation of self-healing Cr2AlC based materials are discussed.

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09:30 **Development and characterization of bio- tribological Cr/CrN + a-C:H (dopped Cr) nano- multilayer coatings for medical tools application**

Authors : L. Major- 1, J.M. Lackner- 2, M. Kot- 3, M. Janusz- 1, J. Morgiel- 1
Affiliations : 1- Institute of Metallurgy and Materials Science, Polish Academy of Sciences, PL30-059 Cracow, 25 Reymonta Street, Cracow, Poland; 2- JOANNEUM RESEARCH- Materials- Institute for Surface Technologies and Photonics, Leobner Strasse 94, 8712 Niklasdorf, Austria; 3- AGH University of Science and Technology, Faculty of Mechanical Engineering and Robotics, Laboratory of Surface Engineering and Tribology, Al. Mickiewicza 30, PL-30059 Cracow, Poland

Resume : Nanotechnology is the ability to manipulate atoms and molecules to produce nano- structured materials and functional nano- coatings on biomedical devices and surgical tools. The use of carbon fiber composites (CFC) for surgical applications is widespread due to the exceptional physical properties of this material. Carbon fiber structures provide strength, stiffness, and fatigue resistance. Carbon fiber components are also radiolucent and clinical-chemical resistant. Carbon-based materials show, however, significant oxidative degradation in air beginning at temperatures in the region of 400 degree C. The reinforcement of carbon with carbon fibers, complicates the anti- oxidative coating problem, due to the thermal and elastic anisotropy of the carbon fibers. Therefore, a coating concept for carbon–carbon composites should consist of an inner part, which serves as structural link with stress compensation ability to the carbon substrate, and an outer part, which acts as a diffusion barrier. In the presented paper, as the inner part chromium/ chromim nitride (Cr/CrN) multilayer structure has been selected. The literature data indicates the particular meaning of Cr and CrN multilayer coatings. They are characterized by an appropriate crystallographic adjustment of subsequent constituent layers of Cr and CrN and by the creation of a transition layer between them with a thickness of several dozen of nanometers. This ensures a good connection between particular constituent layers and as a result also good maintenance properties: high adhesion, wear and corrosive resistance. The CrN and Cr lattice parameters, 4.14Å and 2.88Å, respectively, allow a cube-on-cube, close to epitaxial growth with a low mismatch (1.6%). With this idea, Cr/CrN multilayers have been designed and deposited on CFC substrates. The outer part of the coating, in the presented paper, was hydrogenated amorphous carbon (a-C:H). It is well-known that a-C:H coatings have low- friction coefficients and low-specific wear rates. Thus, the amorphous carbon coatings are very promising tribo-materials. However, the poor adhesion strength to substrate, high residual stress and weak thermal stability would limit their application. Currently, many metallic elements (Ti, W, Ag, Cr etc.) have been utilized to modify their structure, and it has been proved that the metal doping is an effective method to reduce residual stress and enhance adhesion strength of the film. Among those doping metals, Cr as one of carbide formed elements possesses an attractive combination of properties (corrosion resistance, wear resistance, etc.). Thus, in the presented paper a-C:H part of the coating was implanted by Cr nanocrystals. Coatings were subjected to complex investigations. Influence of deposition conditions on bio- tribological properties were studied. Mechanisms of a mechanical wear of analyzed systems were presented focusing on the cracking propagation revealed in ball- on- disc and scratch tests. Cell-material interaction was analyzed in the direct cell deposition. Complex microstructure analysis of presented, nano- multilayer coatings, before and after mechanical and biological tests, were performed by means of transmission electron microscopy (TEM) and confocal laser scanning microscopy (CLSM). The bio- tribological investigation in connection with detailed microstructure interpretation were used as a screening tool before coatings could be deposited on medical tools.

G.IX. 4

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09:45 **Synthesis of Ti2AlN thin films by thermal annealing of Ti/AlN multilayers deposited on different substrates by magnetron sputtering**

Authors : M. Alkazaz, M.F. Beaufort, J.F. Barbot, and T. Cabioc'h.
Affiliations : Institut Pprime, CNRS - Université de Poitiers - ENSMA - UPR 3346

G.IX. 5

Département Physique et Mécanique des Matériaux Boulevard Marie et Pierre Curie - BP 30179 86962 FUTUROSCOPE CHASSENEUIL Cedex, France

Resume : Mn+1AXn phases (n=1, 2, 3) are a family of multifunctional, ternary carbides and nitrides, where M is a transition metal, A is an A -group element, and X is C and/or N. These phases are possessed of many unique properties with multiple applications and they combine the best properties of ceramics and metals. The synthesis of thin films of Ti2AlN (211 MAX phase) was achieved by using an indirect approach. Ti/AlN multilayers were first deposited onto single crystalline substrates (Al2O3(0001), MgO(111), GaN(0001) and 4H-SiC(0001)) by magnetron sputtering at the room temperature. Afterwards, the thermal annealing in vacuum at the temperatures, from 400° C to 750 °C, was carried out and the microstructure of the thin films so obtained was characterized by XRD and cross-sectional HRTEM observations. At 400°C, Al and N diffused into Ti allowing the formation of a solid solution with an hexagonal structure. A decomposition of this phase occurred at 600 °C leading to the formation of Ti2AlN, epitaxial layers being even obtained after further annealing at 750 °C on Al2O3(0001) and 4H-SiC(0001). Furthermore, some electrical properties of the thin films synthesized onto 4H-SiC were studied, a progressive evolution from a Schottky barrier behavior towards an ohmic behavior being obtained when annealing temperature was increased.

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10:00 **Coffee break**

New deposition methods - HIPIMS : Christoph LEYENS, Kostas SARAKINOS

10:30 **Trends in magnetron sputtering of Me-B-C coatings**

Authors : Ulf Jansson
Affiliations : Department of Chemistry - Angstrom, Uppsala University, Box 538, 751 21 Uppsala Sweden

Resume : Me-B-C coatings (Me = early transition metal) have interesting mechanical and tribological properties suggesting a potential use in many applications. Magnetron sputtering of these coatings usually leads to complex microstructures. Previous studies in the Ti-B-C have shown that nanocrystalline grains of TiB2 or TiC are formed, surrounded by an amorphous tissue-phase. However, the defect chemistry of the nanocrystalline grains and the nature of the tissue phase are unclear. In this paper, several Me-B-C systems (Me=Ti, Nb, Cr and Mo) will be compared. Phase composition, microstructure and properties of magnetron sputtered coatings will be discussed. In the Nb-B-C, Cr-B-C and Mo-B-C systems the boride grains can be substoichimetric which can be explained by trends in the stability of the MeB2 structure. With increasing carbon content, the coatings become less crystalline and completely amorphous nanocomposites are obtained in the Cr-B-C system. Superhard coatings (H>40 GPa) can be observed in the Nb-B-C system at low carbon contents, while much softer coatings (H< 20 GPa) are obtained in the Cr-B-C system. This trend can be attributed to variations in composition and thickness of the tissue phase as well the grain size of the carbon-containing boride grains. Furthermore, variations in tribological and electrical properties will be discussed based on trends in microstructure. In particular, the possible formation of lubricous tribofilms will be addressed.

G.X. 1

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11:00 **GROWTH OF CNX FILMS IN Ar-N2 AND Ne-N2 MIXTURES BY DC AND HIPIMS SPUTTERING**

Authors : C. Nouvellon1, N. Britun?, M. Michiels1, R. Snyders1,2
Affiliations : 1 Materia Nova Research Center - Parc Initialis, 1, Avenue Copernic, B-7000 Mons, Belgium 2Chimie des Interactions Plasma-Surface, CIRMAP, Universit? de MONS - 20, Place du Parc, B-7000 Mons, Belgium

Resume : CNx are extensively studied for tribological applications because of their high hardness and low friction coefficients. Considering the need to increase the nitrogen content in the today grown CNx films, increasing the dissociation of the nitrogen molecules in the plasma could be a promising strategy. Compared to other magnetron techniques, HiPIMS (High Power Impulse Magnetron Sputtering) enables a high ionization of the sputtered material and a strong dissociation of reactive molecules. Films have been synthesized using reactive HiPIMS of a graphite target in Ar-N2 and Ne-N2. Ne has been used because of its high ionization energy in order to increase the

G.X. 2

electronic temperature, and in turn the ionization rate. The results are compared to those obtained with a conventional DC reactive magnetron discharge at identical mean power (PD). We discuss the influence of the gas mixture on the peak current and therefore on the film chemistry, determined by XPS. Optical emission spectroscopy was performed in order to address the evolution of the plasma chemistry and temperature with respect to the gas mixture. In HiPIMS, the deposition rate increases with N2 content in Ne-N2 and is lower than in Ar-N2. In DC, the behaviour, with an opposite trend for the two gas mixtures, can be explained by the variation of the sputtering yield for the different gases. The chemical composition of the film reaches a saturation value in all cases.

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11:15 **Piezoresistive properties of metal containing diamond like carbon nanocomposite thin films deposited by HIPIMS**

Authors : R. Gudaitis, Š. Meškinis, A. Vasiliauskas, A. Čiegis, M. Andrulevičius, S. Tamulevičius, G. Niaura
Affiliations : Institute of Materials Science of Kaunas University of Technology, Savanorių 271, 50131 Kaunas, Lithuania

Resume : Diamond like carbon (DLC) films received significant attention due to their properties such as high hardness and Young modulus, low friction coefficient, high wear resistance, good corrosion resistance and biocompatibility. Doping with different metals provides additional control of DLC properties. Recently strong piezoresistive effect in DLC films was discovered. In combination with properties mentioned above it enables fabrication of the advanced DLC based embedded sensors able to work in different harsh environments. Deposition methods providing high ion to neutral ratios are necessary to grow sp3 rich diamond like carbon films. High power impulse magnetron sputtering (HIPIMS) is novel deposition method providing high ion to neutral ratio during film growth. In present study diamond like carbon nanocomposite films containing group I metal (copper, silver) nanoclusters were deposited by reactive high power impulse magnetron sputtering. Piezoresistive properties were studied by four point bending method. Structure of films was studied by multiwavelength Raman scattering spectroscopy and transmission electron microscopy. Chemical composition of films was investigated by the x-ray photoelectron spectroscopy. Effects of reactive HIPIMS deposition process technological conditions on piezoresistive properties of diamond like carbon nanocomposite films were investigated. The relationship between structure, composition and piezoresistive properties of the films was studied.

G.X. 3

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11:30 **Impact of the nanostructure and phase transition of TaNx x=[0,1.8]buffers films elaborated by HiPPiMS on the CNT morphology**

Authors : Brigitte Bouchet-Fabre1, Marie-Christine Hugon 2, Mathieu Pinault 1, Eddy Foy 3, Martine Mayne-L'Hermite 1; Cécile Reynaud 1; Tibériu Minéa 2
Affiliations : 1 IRAMIS/NIMBE/LEDNA, CEA-Saclay, F- 91191 Gif / Yvette Cedex 2 LPGP, U-Psud-CNRS, Université Paris-Sud, F-91401 Orsay Cedex 3 IRAMIS/SIS2M/LAPA CEA-Saclay, F- 91191 Gif / Yvette Cedex

Resume : The comprehensive study focuses on the interplay interfaces Ta-Nx, x= [0,1.8] coating/ CNT during the growth by assisted catalyst CVD at 850°C, while using ferrocene as catalyst source. We show that the use of Ta-Nx buffer films grown by High Power Pulsed Magnetron Sputtering HIPPIMS is of special interest because it allows a larger incorporation of nitrogen inside the films and generates specific nanostructures. The CCVD process promotes reactions among C, N, O on one side, Ta, Fe on the other side. The abundant evidences collected in our experiments confirm the strong influence of these chemical reactions occurring during the CVD process, thus justifying a close scrutiny of the chemical and structural changes due to the temperature and the CCVD process. Therefore, we present here the interfaces modifications studied by grazing incidence X-ray scattering GIWAXS, high resolved electron scanning microscopy SEM-Feg and XPS. The together techniques are very helpful for exanimating the temperature effect on the morphology of the interface, giving a good picture of the nanocrystalline evolution of the buffers involved in the CNTs growth process. The CNT morphology and nanostructure is followed by TEM and Raman spectroscopy. We conclude on the huge impact of the nanostructure an surface morphology of tantalum nitride on the CNT morphology and growth, and then its influence on potential applications.

G.X. 4

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11:45 **Influence of HIPIMS Pulse Duration on the Properties of TiAlN Films Deposited at Low Substrate Temperature**

Authors : Tetsuhide SHIMIZU 1), Tomotaro WATANABE 2), Yoshikazu TERANISHI 2),

G.X. 5

Hiroshi NAGASAKA 2), Hidetoshi KOMIYA 2), Kazuo MORIKAWA 2), Ming YANG1)
Affiliations : 1) Division of Human Mechatronics Systems, Tokyo Metropolitan University, 2) Tokyo Metropolitan Industrial Technology Research Institute
Resume : Transition metal nitrides like TiN, ZrN, TiAlN, and VN were successfully used as protective coatings against wear and corrosion in medical devices. In particular, because of the cost-efficiency and biocompatibility of polymers, thin film deposition on polymeric substrate is strongly required. One of the high potential methods for low temperature deposition, which can expect the excellent film properties, is high power impulse magnetron sputtering (HIPIMS). In the present paper, to achieve the low temperature deposition less than 150 °C, TiAlN films were deposited on Si substrates using HIPIMS. The pulse duration was varied from 60 to 300 μs with a low frequency of 333Hz to investigate the effects on substrate temperature, deposition rate and film structure. Chemical composition, surface morphology and phase composition of the films were analyzed by means of EDS (Energy Dispersive Spectroscopy), SEM (Scanning Electron Microscopy) and XRD (X-ray Diffraction), respectively. Mechanical properties were additionally measured by nanoindentation tester. As results, decreasing of pulse duration at constant mean power of 5kW leads to a decrease of substrate temperature of around 20 °C in 10 min film deposition. Nevertheless, due to the high peak currents under the shorter pulse duration, the hardness is rather higher in lower substrate deposition. Thin film growth under low substrate temperature in HIPIMS deposition was discussed.

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12:00 **Lunch break**

Analysis methods for nanostructured thin films : Valentin CRACIUN, Ulf JANSSON

14:00 **In situ study of the texture development during sputter deposition of V-C thin films**

Authors : Sunil Kotapati1, Bärbel Krause1, Marthe Kaufholz1, , Richard Thelen3, Michael Stüber4, Sven Ulrich4 and Tilo Baumbach1, 2
Affiliations : 1)IPS, Karlsruhe Institute of Technology (KIT), Germany; 2) ANKA, Karlsruhe Institute of Technology (KIT), Germany; 3) IMT, Karlsruhe Institute of Technology (KIT), Germany; 4) IAM-AWP, Karlsruhe Institute of Technology (KIT), Germany.
Resume : Magnetron sputtered coatings based on transition metal carbides are used in industry as protective hard coatings and for tribological applications. Depending on the growth conditions and the carbon content, composite or single phase coatings can form. Coexisting phases, texture and grain size have a strong influence on the mechanical properties of these coatings. In order to understand the influence of microstructure formation processes on the mechanical properties, a combined approach using several complementary in situ and ex situ analysis methods is required. Here we present a systematic study of V-C1-x/a-C nanocomposites. The development of the texture during the deposition was studied by In situ x-ray diffraction (XRD) experiments at the synchrotron radiation source ANKA (Karlsruhe). The coatings were deposited from a composite target using DC magnetron sputtering. The structural and mechanical properties of the films were studied as a function of different process parameters including substrate temperature, bias and gas pressure. Complementary ex situ atomic force microscopy, nanoindentation, X-ray photoemission spectroscopy and plasma diagnostic measurements were performed. The experimental results are summarised in a structural growth model.

G.XI. 1

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14:15 **Cross-Sectional X-ray Nanodiffraction as a Powerful Tool to Reveal Structure-Property Relationships in Nanocrystalline Coatings**

Authors : A. Riedl (a)*, R. Daniel (b), M. Stefenelli (a), J. Todt (c), C. Krywka (d), C. Mitterer (b), and J. Keckes (c)
Affiliations : (a) Materials Center Leoben Forschung GmbH, Roseggerstraße 12, 8700 Leoben, Austria (b) Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, 8700 Leoben, Austria (c) Erich Schmid Institute for Materials Science, Austrian Academy of Sciences, 8700 Leoben, Austria (d) Helmholtz Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht, Germany
Resume : Hard nanocrystalline coatings commonly exhibit complex microstructures and stresses across their thickness due to inherently varying

G.XI. 2

growth conditions, self-organization phenomena and/or post-deposition mechanical and thermal loads caused, e.g. by friction between coating and counterpart. The determination of these depth-gradients, as well as how they influence the mechanical properties of the coating at the macroscale, is not trivial. Cross-sectional X-ray nanodiffraction using monochromatic beams with diameters down to 100 nm can provide representative position-resolved data on the depth-evolution of phases, crystallographic texture, crystallite size and residual stresses in thin coatings. This contribution shows our recent activities in the field of advanced coating characterization at the nanofocus endstation of the P03 beamline of Petra III in Hamburg, Germany. For the examples of CrN, TiN and TiAlN coatings, we demonstrate that scanning nanodiffraction studies can serve not only as an effective tool to characterize the inhomogeneous properties of coatings at the sub-micron scale but, coupled with indentation, allow for the characterization of microstructural and stress changes during deformation. Finally, in-situ nanodiffraction is a very powerful tool to understand the relationship between macroscopic mechanical response and local properties of inhomogeneous coatings. Corresponding author: angelika.riedl@mcl.at

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14:30 **In situ X-ray study during off-normal sputter deposition of VN**

Authors : B. Krause, M. Kaufholz, S. Kotapati, T. Baumbach
Affiliations : (1) IPS, Karlsruhe Institute of Technology (KIT) (2) ANKA Synchrotron Radiation Facility, Karlsruhe Institute of Technology (KIT)

Resume : Off-normal deposition offers very interesting possibilities to tailor the nanostructure of sputter deposited thin films. Under certain deposition conditions, transition metal carbides and nitrides exhibit columnar growth. The orientation, size, and porosity of these columnar structures depend on the deposition angle. The direction of the incoming flux influences also the texture formation and can lead to tilted or biaxial textures. Both the texture and the shape of the columns allow for the control of the mechanical properties of the coating. However, for the prediction of these properties a detailed understanding of the growth process is required. Here we present an in situ X-ray study during reactive magnetron sputtering of VN under various deposition angles. The structure formation of thin films with thicknesses up to 200 nm was followed with sub-nm resolution using in situ X-ray reflectivity (XRR) and X-ray diffraction (XRD) measurements performed at the synchrotron radiation source ANKA (Karlsruhe). The XRR measurements give access to the time-dependent thickness and roughness increase of the coating, while the XRD measurements show the development of the (111) texture. The results were compared with SIMTRA simulations. The in situ study was complemented by ex situ measurements including nanoindentation, atomic force microscopy and pole figure measurements.

G.XI.3

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14:45 **Identification of the coating defects responsible for pitting corrosion on PVD deposited steel samples by a novel method: Large Area High Resolution (LAHR) mapping**

Authors : Martin Balzer
Affiliations : fem - Forschungsinstitut für Edelmetalle und Metallchemie, Katharinenstrasse 17, 73525 Schwäbisch Gmünd, Germany

Resume : Coatings deposited by PVD techniques have been characterised for decades for their corrosion protection capabilities. The film density was often stated to be the key factor and improvements were published, based on different electrochemical corrosion measurements. However, these improvements mostly did not prove true when being verified by exposing the coated samples to neutral salt spray test. The pitting corrosion then observed has usually been explained by the presence of coatings defects. With the Large Area High Resolution (LAHR) mapping a method has recently been developed at the fem which allows localizing and characterising all coating defects responsible for pitting corrosion attacks. It is based on scanning the topography of the entire surface (several cm2) of lab sized coated samples with a lateral resolution in sub-µm range by confocal microscopy. The defect data are generated by complex custom-built templates based on Mountains Map™ and Visual Basic™. Using this method on the same sample before and after a corrosion test enables to trace back all corrosion sites to their responsible coating defects. Furthermore reliable defect statistics, defect maps as well as coordinates for each specific defect are available. The method will be introduced in detail including problems that had to be solved like dust particles being present on the sample surfaces during the scan, or different measurement artefacts. Finally results for TiN coated steel samples will be presented.

G.XI.4

add to my program (close full abstract)

15:00 **Optical and EPR study of a-SiCxNy films obtained by magnetron sputtering**

Authors : D. Savchenko(1), V. Kulikovsky(1),(2), V. Vorlíček(1), J. Lančok(1), E. Kalabukhova(3)
Affiliations : (1) Institute of Physics, AS CR, Praha, Czech Republic (2) Institute for Problems of Materials Science, NASU, Kiev, Ukraine (3) V.E. Lashkaryov Institute of Semiconductor Physics, NASU, Kiev, Ukraine

Resume : Amorphous silicon carbonitride (a-SiCxNy) thin films deposited on the SiO2 substrates by reactive magnetron sputtering from SiC target without and with different nitrogen (N) incorporation have been studied by Raman and electron paramagnetic resonance (EPR) spectroscopy. Raman analysis indicates the presence of C-N, Si-N, C-C bonds in a-SiCxNy films. Three EPR signals were revealed in a-SiCxNy/SiO2. One of them with isotropic g factor at g=2.0033 and Lorentzian lineshape was attributed to the carbon-dangling bonds (CDB) located within a-SiCxNy film. Based on the lineshape and linewidth (~ 1.2 mT) the EPR signal was attributed to the unpaired electron delocalized over the sp2 carbon cluster. With increase of the N content the spin density of the CDB significantly increases. From the temperature dependence of the linewidth and integral intensity of the CDB EPR signal which obey Curie-Weiss law it was concluded that antiferromagnetic ordering occurs in the spin system. The value of the antiferromagnetic exchange constant between dangling bonds was found to be J=−32 K. The second EPR signal having g=2.009 was attributed to the interface defect representing threefold-coordinated Si dangling bond which may appear due to the formation of the oxidized silicon on the top surface of the film. The third EPR signal with g=2.05 was tentatively attributed to the trapped holes at Si atom. The work was supported by GA ČR 13-06697P and SAFMAT project CZ.2.16/3.1.00/22132.

G.XI. 5

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15:15 **Thermal stability and long term hydrogen release from soft to hard hydrogenated amorphous carbons analyzed using in-situ Raman spectroscopy. Application to tokamak deposits**

Authors : C. Pardanaud1, C. Martin1, G. Giacometti1, P. Roubin1, B. Pégourié2, C. Hopf3, T. Schwarz-Selinger3, W. Jacob3
Affiliations : 1 Aix-Marseille Université-CNRS, PIIM, 13397 Marseille cedex 20, France; 2 CEA, IRFM, 13108 Saint-Paul-lez-Durance, France; 3 Max-Planck-Institute für Plasmaphysik, EURATOM Association, Boltzmannstr. 2, 85748 Garching, Germany

Resume : Hydrogen isotopes plasma/walls interactions in carbon tokamaks lead to a severe safety issue avoiding carbon use in the future ITER project. A complete analysis of the D retention in the Tore Supra tokamak, including both in-situ gas balance measurements and ex-situ post-mortem characterizations, has revealed that deuterium was depleted in the deep layers of the deposits, indicating that an unexpected long term D-release occurs. To mimic the variety of hydrogenated deposits found in Tore Supra, we used several reference samples and heated them to relevant temperatures (120-1000°C). These samples had various C(sp2)/C(sp3)/H content and were PECVD layers with properties ranging from soft to hard films (DC bias from -100 to -300 V corresponding respectively to H/(H+C) equal to 37 and 29 at.%). We have studied the thermal stability of these samples using in-situ Raman microspectroscopy under argon atmosphere, recording their evolution during hours or days. Ultra High Vacuum thermal desorption spectroscopy and ion beam analysis were done separately for comparison. We have identified selected Raman parameters as C(sp3)-H and/or C(sp2)-H sensitive. For example, for the -300 V DC bias sample, carbon reorganization with aromatization and loss of C (sp3) occurs in the first 100 minutes at 500 °C. A similar reorganization is detected in the temperature range of 450 - 600°C. H release occurs on a longer timescale of about 10 hours at 500 °C and H release from C(sp2) is only partial, even after several days. These processes occur more rapidly with higher initial H content. Similar analyses have been done for deposits produced in the Tore Supra tokamak to get insights into their structure and on the long term D release processes.

G.XI. 6

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15:30 **PECVD synthesis and characterization of BCxNy films from N-triethylborazine and hydrogen**

Authors : V.S. Sulyaeva, M.L. Kosinova, Yu.M. Rumyantsev, F.A. Kuznetsov
Affiliations : Nikolaev Institute of Inorganic Chemistry SB RAS 3, Acad. Lavrentiev Ave., Novosibirsk, 630090, Russia

Resume : Boron carbonitride thin films attract more attention since demonstrate excellent properties and can be used as promising materials:

G.XI. 7

optical, dielectric and protective layers. In this paper BCxNy films were obtained by plasma enhanced chemical vapor deposition method using a single-source precursor N-triethylborazine B3N3H3(C2H5)3 and hydrogen as plasma activating gas. The effect of temperature synthesis on the chemical composition and properties of the BCxNy films was investigated. Substrate temperature was varied in the range of 100-700ºC. Total pressure in the system was 2.1•10-2 Torr, plasma power was 30 W. The BCxNy films were investigated by SEM, FTIR and Raman spectroscopy, EDX, XPS, ellipsometry and spectrophotometry techniques. Results indicated that BCxNy films produced at low temperatures (< 400 C) are the polymer-like hydrogenated films with high transparency. BCxNy films produced at high temperatures (> 400 C) contain additional phase of disordered carbon which is dramatically reduce transparency. The band gap of the films varied from 0.6 to 4.5 eV, with variation in deposition temperature. Surface morphology examination yield presence 20-30 nm nanoparticles. The refractive index of the BCxNy films increased from 1.5 to 2.5 with increasing temperature of the synthesis. The XPS study suggested that synthesized films contain B-N, B-C, C-C, and C-N bonds.

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15:45 **Coffee break**

Energy related applications : Gregory ABADIAS, Thien-Phap NGUYEN

16:30 **Use of transition metal nitride films as electrode in energy storage microdevices**

Authors : J.F. Pierson1, S. Bouhtiyya1, R. Lucio Porto2, F. Capon1, T. Brousse2
Affiliations : 1 Institut Jean Lamour, Université de Lorraine, Nancy, France 2 Institut des Matériaux Jean Rouxel, Université de Nantes, Nantes, France

Resume : The high hardness and the low friction coefficient of transition metal nitride (TMN) films allow their use as protective coatings. These materials exhibit also functional properties that make TMN films suitable for applications in energy storage devices. This talk aims to screen the potential use of nitride thin films in supercapacitors. TMN films were deposited on glass substrates by reactive magnetron sputtering of TM targets (TM = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Nb and Ru). Only Cu- and Ni-based films crystallized in a TM3N-like structure while most of the deposited films exhibit a metal to nitrogen atomic ratio of 1. Only limited information about the structure of MnN and RuN is available in the literature. Subsequently, the structure of these two nitrides is described for the first time. X-ray diffraction analyses and the Rietveld's method evidence that both RuN and MnN thin films crystallize in a ZnS-like structure with lattice constant of 0.451 and 0.428 nm, respectively. The electrochemical properties of the deposited films were determined by cyclic voltammetry in electrolytes KOH. ScN, Ni3N, FeN, CrN have shown a poor capacitance suggesting that only double layer is involved in the charge storage mechanism. The large capacitance of MnN, RuN and VN and the nearly rectangular shape of the voltammograms suggest a pseudofaradaic process. These electrochemical results are discussed in connection with the film structure and composition.

G.XII. 1

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17:00 **Investigation of oxynitride thin films for photocatalytic water splitting**

Authors : Markus Pichler, Daniele Pergolesi, Christof Schneider, Thomas Lippert, Alexander Wokaun
Affiliations : Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Resume : Hydrogen is an eco-friendly energy carrier and a promising alternative to fossil and nuclear fuels. The sustainable hydrogen production by photocatalytic water splitting is a topic of intense research activity. The efficiency of current photocatalysts is limited by the large energy band gap which reduces the usable part of the solar spectrum to the UV range. Oxynitrides are oxide materials in which oxygen is substituted by nitrogen. As a result, additional energy levels are created above the valence band making these materials able to use a larger part of the solar spectrum. Many questions are still open concerning the fabrication and the ultimate limits of these materials. The aim of this work is the fabrication of highly ordered oxynitride thin films used to investigate the correlation between crystallographic properties and photocatalytic activity. Oxynitride thin films are fabricated by Pulsed Reactive Crossed-Beam Laser Ablation. X-ray diffraction is used to characterize the crystalline properties, while the photocatalytic activity is tested by photoelectrochemical measurements. The latter require a conducting substrate

G.XII. 2

or seed layer. Besides providing a suitable lattice matching with the oxynitride films, the selected conducting material has to be stable under the experimental environment required for the oxynitride deposition (high temperature and reducing atmosphere). The investigation of different materials used as conducting buffer layers will be presented.

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17:15 **"On-Chip" Nanoporous Titanium Nitride Electrodes** G.XII.3

Authors : Micheal Burke, Brendan Kennedy,Mary Manning, Alan Blake, Aidan Quinn.
Affiliations : Tyndall National Institute

Resume : We describe a wafer-scale, clean-room fabrication process for nanoporous titanium nitride electrodes using anodized aluminum oxide (AAO) nanopore arrays on silicon (with aspect ratios > 10) combined with ~20 nm coatings of titanium nitride from a tetrakis(dimethylamino)titanium (TDMAT) precursor using plasma enhanced atomic layer deposition. The electrochemical performance of these nanoporous titanium nitride electrodes are characterised using electrochemical techniques such as cyclic voltammetry and electrochemical impedance spectroscopy (EIS). Subsequently their suitability for applications in "on-chip" energy storage is discussed.

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17:30 **Functionally graded PDMS/Ag nanocomposites for broadband solar thermal harvesting applications** G.XII.4

Authors : P. Nikolaou1, C.Mina1, L.E. Koutsokeras1, G. Constantinides1, S. Kalogirou1, E. Lidorikis2, A. Avgeropoulos2, P.C. Kelires1, P. Patsalas3
Affiliations : 1Cyprus University of Technology, Department of Mechanical and Materials Science and Engineering, Research Unit for Nanostructured Materials Systems, Limassol, Cyprus; 2University of Ioannina, Department of Materials Science and Engineering, 45110 Ioannina, Greece; 3Aristotle University of Thessaloniki, Department of Physics, 54124 Thessaloniki, Greece;

Resume : Thin films that combine broadband absorbance, limited infrared emittance, high thermal conductivity, ease of use and processing, and environmental friendliness are essential for solar photothermal harvesting. Plasmonic nanoparticles (PNPs) have been proven to absorb parts of the visible and infrared spectra depending on their sizes and shapes; therefore, if they were supported in a matrix that would provide all the aforementioned essential properties, they should become effective solar harvesters. In this work, we produce functionally graded nanocomposites consisting of Ag PNPs supported in a Poly-Di-Methyl-Siloxane (PDMS) matrix. The PDMS was selected due to its high optical transparency, non toxicity and ease of use. The Ag PNPs were formed by annealing sputtered Ag ultra-thin films and were subsequently capped by a spin-coated PDMS layer. We investigate the factors that affect their plasmonic behavior, such as the PNPs' size, the annealing conditions and the surrounding environment. In order to achieve broadband solar absorption we developed PDMS/Ag(PNPs) multilayers with graded PNPs' size. The morphology of the Ag PNPs was investigated by Electron and Atomic Force Microscopy. The optical measurements were performed using a UV/VIS spectrometer. Finally, the solar photothermal performance of the produced films was evaluated in realistic conditions, using a large-scale solar simulator and monitored in real-time their thermal behavior using an ultrafast thermal camera.

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17:45 **Porous Carbon Nanoparticle Networks with Tunable Absorbability** G.XII.5

Authors : Wei Dai1, Seong Jin Kim1, 2, Won-Kyung Seong1, Sang Hoon Kim1, Kwang-Ryeol Lee1, Ho-Young Kim2, and Myoung-Woon Moon1,*
Affiliations : 1Institute for Multi-disciplinary Convergence of Matter, Korea Institute of Science and Technology, Seoul 130-650, Republic of Korea 2 School of Mechanical and Aerospace Engineering, Seoul National University, Seoul 151-744, Republic of Korea

Resume : Porous carbon materials with high specific surface areas and superhydrophobicity have attracted much research interest due to their potential application in the areas of water filtration, water/oil separation, and oil -spill cleanup. Most reported superhydrophobic porous carbon materials are fabricated by complex processes involving the use of catalysts and high temperatures but with low throughput. Here, we present a facile single-step method for fabricating porous carbon nanoparticle (CNP) networks with selective absorbability for water and oils via the glow discharge of hydrocarbon plasma without a catalyst at room temperature.[1] Porous CNP networks were grown by the continuous deposition of CNPs at a relatively high deposition pressure. By varying the fluorine content, the porous CNP networks exhibited tunable repellence against liquids with various degrees of surface tension. These porous CNP networks could be applied for the separation of not only water/oil mixtures

but also mixtures of liquids with different surface tension levels. Reference [1] W Dai, S J Kim, W-K Seong, S H Kim, K-R Lee, H-Y Kim, and M.-W. Moon, Porous carbon nanoparticle networks with tunable absorbability, Scientific Reports, 3(2013),2524.

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18:00 **Photoluminescence spectrum transformation in Si rich silicon nitride versus silicon nitride stoichiometry**

Authors : T.V. Torchynska1, J.L. Casas Espinola1, E. Vergara Hernandez1, A. Slaoui2 and L. Khomenkova3,
Affiliations : 1ESFM-Instituto Politecnico Nacional, Mexico DF, 97738, MEXICO 2ICube, 23 rue du Loess, BP 20 CR, 67037 Strasbourg Cedex 2, FRANCE 3 V. Lashkaryov Institute of Semiconductor Physics, 45 Pr. Nauky, 03028 Kyiv, UKRAINE

Resume : Si-rich Silicon nitride films were grown by PECVD technique on silicon substrates. The film stoichiometry was controlled via variation of NH3/SiH4 ratio from 0.45 up to 1.0. Thermal annealing at 1100°C and 30 min in nitrogen flow was applied to form Si nanocrystals (NCs) in the films that have been investigated by means of photoluminescence and Raman scattering spectra. Temperature dependence of photoluminescence spectra have been studied also. Several emission bands composed PL spectra were detected with the peak positions at: a)2.9-3.0eV, b)2.5-2.7eV, c) 1.90-2.25eV, d) 1.8-1.90eV, e) 1.5eV. The former three PL bands were assigned to the defects in silicon nitride. The position of these PL bands depends on silicon nitride stoichiometry. The PL band at 1.8-1.90 eV is, apparently, due to the exciton emission inside Si NCs. The fifth PL band 1.5 eV was attributed to the second order diffraction peak of the first PL band (3.0eV). The temperature dependences of PL spectra were studied with the aim to confirm the types of optical transitions and the nature of light emitting defects in silicon nitride. The mechanism of photoluminescence is discussed.

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Carbon- or nitrogen-containing nanostructured thin films

26 May 2014 | 27 May 2014 | 28 May 2014 | 29 May 2014 | **30 May 2014**

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start at	Subject	Num.
	Graphenes - I : Bodgana MITU, Pierre-Yves TESSIER	
08:30	**Carbon Foams made of Nanotubes and Graphene Nanoflakes: a Monte Carlo and Tight-Binding Molecular Dynamics Study** **Authors :** C. Mathioudakis, P. C. Kelires **Affiliations :** Research Unit for Nanostructured Materials Systems, Department of Mechanical and Materials Science Engineering, Cyprus University of Technology, P.O. Box 50329, 3603 Lemesos, Cyprus **Resume :** In the low-density regime of carbon materials, nanoporous formation along with nanostructuring and coexistence of various hybridizations give rise to three-dimensional (3D) structures with outstanding properties. Carbon nanofoams (CNFs) belong to this class of materials. They are open, random and light structures resembling a foam. We have recently studied [1] CNFs made up of schwarzites, nanostructures with negative Gaussian curvature. Here, we investigate two other forms of this exciting material. One is made of carbon nanotubes (CNT) and the other of graphene nanoflakes (GNF). These 3D randomly interconnected structures offer an alternative route for promising applications. Our studies are based on Monte Carlo simulations for the network formation, followed by tight-binding molecular dynamics simulations for full relaxation and calculation of the mechanical and optoelectronic properties. We find that both foam types are rigid, despite their porous nature, so they can be utilized in applications (catalysis, tribology, energy storage) as thin films. The GNF foams exhibit high conductivity, approaching that of single-layer graphene, and high optical absorptivity. Similar properties are exhibited by the CNT foams. This makes these 3D manifestations invaluable for applications in electronics and optics. [1] C. Mathioudakis and P. C. Kelires, Phys. Rev. B 87, 195408 (2013). add to my program (close full abstract)	G.XIII.1
08:45	**Electron microscopy and spectroscopy studies of plasma functionalised graphene** **Authors :** Ehsan Rezvani1, Niall McEvoy2, Hugo Nolan1,2, Clive Downing, Toby Hallam and Georg Duesberg1 **Affiliations :** 1) School of Chemistry, Trinity College Dublin, Dublin 2, Ireland, 2) CRANN, Trinity College Dublin, Dublin 2, Ireland. **Resume :** Graphene, an atomically thin sheet of sp2-hybridised carbon atoms arranged in a honeycomb lattice, has attracted a great deal of interest among the scientific community primarily because of its extraordinary electronic properties. The introduction of dopants has been proposed for applications in nanoelectronics and sensing. In particular, nitrogen dopants can act as electron donors in nitrogen-doped (N-doped) graphitic systems. N-doping of graphene is advantageous for high frequency semiconductor device applications and this material is considered an excellent candidate for energy storage and solar cell applications. Most recently, N-doped graphene has been reported to act as a catalyst in oxygen reduction reactions (ORR) which are crucial in energy conversion. For chemical functionalisation there are several sub-categories, namely surface doping and substitutional doping which can both give rise to either p-type or n-type electronic behaviour. Substitutional nitrogen doping of graphene has been reported by means of different techniques such as chemical vapour deposition, annealing under ammonia atmosphere, arc-discharge of graphite under pyridine/ammonia ambient, wet chemical routes and nitrogen	G.XIII.2

plasma treatment. In spite of its crucial importance, details on the mechanism of incorporation of heteroatoms into graphene remain unclear. We have developed a downstream plasma doping technique using a custom-built apparatus in which the samples are placed at a location remote from the plasma source, thereby minimising the destructive effect of plasma species. Using this approach, an initial oxygen plasma treatment is performed on the pristine sample creating active sites for accommodating further functional groups. A subsequent plasma treatment is then carried out with a mixture of hydrogen and ammonia which simultaneously reduces and N-dopes the graphene. Elsewhere, a similar approach has been shown to simultaneously reduce and N-dope graphene oxide powder. Here we report on the TEM and energy-filtered TEM characterisation of plasma functionalised CVD graphene. Comparative TEM/EELS studies were performed on three different CVD-grown graphene sample types. Namely pristine graphene, O2 plasma treated graphene and O2 followed by H2+NH3 plasma treated graphene. The results show the evolution of pristine untreated graphene to a disordered oxygenated graphene upon O2 plasma treatment and subsequent partial restoration of crystallinity of the graphene lattice following H2+NH3 plasma. This study further probes our N-doped graphene using several spectroscopic techniques, thus offering further information on the nature of doping in graphene. In conclusion, we report on the application of EELS in conjunction with two other spectroscopic techniques for full characterisation of remote plasma-treated CVD -grown graphene. This allowed for a highly detailed analysis of nitrogen-doped graphene; elucidating the structural evolution, along with the nature and bonding states of dopants present. TEM and EELS studies show distortion of the graphene lattice upon oxygen-plasma treatment which is further confirmed by Raman spectroscopy via the emergence of defect related peaks; as well as XPS, with an increased contribution from sp3 carbon bonds and oxygen functional groups. A subsequent H2+NH3 plasma treatment results in partial lattice restoration which is evident from the electron diffraction pattern; this is further corroborated by the better defined peaks and additional features and shoulders in the EEL spectrum. Again, these results are supported via Raman spectroscopy with the re-emergence of long range order and suppression of defect-related peaks. XPS indicates the restoration of the lattice to a graphitic structure with the removal of oxygen groups and the introduction of nitrogen as a dopant. The nature of the nitrogen functional groups was also established. These results show that EELS can be applied to chemically and crystallographically monitor the chemical changes in graphene and its derivatives and, hence, shed light on an established technique as a new avenue for better understanding of the structural variations of graphene upon chemical treatments. Furthermore, the restoration of the graphene crystalline lattice in conjunction with the introduction of nitrogen dopants following the two-step plasma treatment suggests that this plasma treatment technique is a viable method of producing nitrogen-doped CVD graphene for incorporation into further device applications.

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09:00 **ELECTRON SPECTROSCOPY OF COMPOSITE MATERIALS CONTAINING 2D CARBON**

Authors : S. Kaciulis, A . Mezzi, S.K. Balijepalli, M. Lavorgna, H. Xia
Affiliations : Institute for the Study of Nanostructured Materials, ISMN – CNR, Roma, Italy; Institute of Composite and Biomedical Materials, IMCB – CNR, Napoli, Italy; State Key Laboratory of Polymer Materials Engineering, Sichuan University, China

Resume : Composite materials with 2D carbon (graphene and/or single wall carbon nanotubes) are very promising due to their extraordinary electrical and mechanical properties. Graphene and natural rubber composites, which may be used for gaskets or sealants, were prepared by ultrasonically assisted latex mixing exfoliation and in-situ reduction process, varying the distribution of the filler in the samples. They present a low electrical conductivity and barrier properties, in spite of excellent spatial distribution. On the other hand, natural rubber composites, prepared by latex mixing and co-coagulation, exhibit a segregated 3D graphene network where the graphene sheets are stacked within the interstices of the coagulated latex particles. These vulcanized composites exhibit good electrical conductivity and high mechanical strength together with excellent barrier properties. The standards for the compositional characterization of these materials still are not established. In addition to the mostly used techniques, such as Raman spectroscopy and electron microscopy, also Auger electron spectroscopy (AES) can be employed for the identification of graphene. In this study, the shape of C KVV peak, excited by electron beam (AES) and X-ray photons (XAES), has been investigated in different composite

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materials containing graphene and SWCNTs. A new method for 2D carbon recognition, based on the D parameter, determined from C KVV spectra excited by X-ray photons, was proposed and verified.

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09:15 **Synthesis and doping of graphene with plasmas assistance and its application in lithium ion batteries**

Authors : Chundong Wang,1 Wenjun Zhang,2 Chris Van Haesendonck1
Affiliations : 1. Laboratory of Solid-State Physics and Magnetism, K.U. Leuven, BE-3001 Leuven, Belgium 2. Center of Super-Diamond and Advanced Films (COSDAF), and Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China

Resume : Graphene, being a two-dimensional material with carbon atoms arranged in a honeycomb lattice structure, has drawn enormous attention recently because of its superior mechanical strength, extraordinary high carrier mobilities and thermal conductivities, ease for surface functionalization, supreme optical properties, etc. There have been a variety of methods developed to synthesize graphene, e.g. mechanical exfoliation from highly ordered pyrolytic graphite (HOPG), chemical reduction of graphite oxide, high temperature annealing of single crystal silicon carbide, chemical vapor deposition (CVD), etc. In this work, we developed two different methods to synthesize graphene from solid carbon sources (PMMA and PDMS) with plasma enhanced CVD. The utilization of reactive hydrogen plasmas enable the graphene growth at reduced temperature as compared to conventional thermal chemical vapor deposition processes, which favors to in-situ fabricate graphene pattern on low temperature substrates. Meanwhile, two facile N-doping approaches (ex-situ and in-situ) were demonstrated to efficiently incorporate nitrogen atoms into graphene lattices. First principle calculations revealed that the incorporated nitrogen atoms with the Pyridinic-N and Pyrrolic-N formats in the graphene sheets would tune the band gap of graphene effectively which may provide a new step toward controlled graphene electronics, and this technique may lead to precise determination of graphene-based device characteristics in the future. Moreover, a unique three-dimensional graphene scaffold has been fabricated to support Si, Sn and Ge nanostructures, which shows outstanding integrative electrochemical properties, excellent cyclability and rate performance. In addition, silicon nanowires/nanotubes grown by VLS, of which were incorporated with rGo or decorated with conductive carbon nanoparticles were realized stable cycling performance in LIBs. References: 1. C.D. Wang, Y.S. Chui, Y. Li, X.F. Chen, W.J. Zhang, Binder-free Ge-3D graphene electrodes for high-rate capacity Li-ion batteries. Appl. Phys. Lett. 2013, 103, 253903. 2. C.D. Wang, Y.Li, Y.S. Chui, Q.H. Wu, X.F. Chen, W.J. Zhang, Three-dimensional Sn-graphene anode for high-performance lithium-ion battery, Nanoscale, 2013, 5, 10599-10604. 3. C.D. Wang, Y.S. Chui, R.G. Ma, J.G. Ren, T.L. Wong, Q.H. Wu, X.F. Chen, W.J. Zhang, Three-dimensional graphene scaffold supported thin film silicon anode for lithium-ion battery, J Mater Chem. A., 2013, 1, 10092- 10098. (Back cover page). 4. C.D. Wang, Y.G. Zhou, L.F. He, T.W. Ng, G. Hong, Q.H. Wu, F. Gao, C.S. Lee, W.J. Zhang, In situ nitrogen-doped graphene grown from polydimethylsiloxane by plasma enhanced chemical vapor deposition, Nanoscale, 2013, 5, 600-605. 5. C.D. Wang, M.F. Yuen, T.W. Ng, S.K. Jha, Z.Z. Lu, S.Y. Kwok, T.L. Wong, X. Yang, C.S. Lee, S.T. Lee, W.J. Zhang, Plasma-assisted growth and nitrogen doping of graphene from solid carbon source, Appl. Phys. Lett, 2012, 100, 253107. 6. J.G. Ren, C.D. Wang, Q.H. Wu, X. Liu, L.F. He, W.J. Zhang, Silicon Nanowires-Reduced Graphene Oxide Composite as A High-Performance Lithium-Ion Battery Anode Material. Nanoscale, 2014. In press (DOI: 10.1039/C3NR05093A). 7. Z.Z. Lu, T.L. Wong, T.W. Ng, C.D. Wang, Facile synthesis of carbon decorated silicon nanotube arrays as anode material for high-performance lithium-ion batteries. RSC Advance, 2014, 4, 2440-2446. (Corresponding author)

G.XIII.4

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09:30 **Exfoliated graphene doped mesoporous titania films: functional nanocomposites from integrated processing**

Authors : Luca Malfatti, Paolo Falcaro, Alessandra Pinna, Barbara Lasio, Maria F. Casula, Danilo Loche, Andrea Falqui, Benedetta Marmiroli, Heinz Amenitsch, Roberta Sanna, Alberto Mariani, Plinio Innocenzi
Affiliations : LMNT, University of Sassari, Italy; CMSE-CSIRO, Clayton South, Australia; Department of Chemical and Geological Sciences, University of Cagliari, Italy; IIT Italian Institute of Technology, Genova, Italy; Institute of Inorganic Chemistry, Graz University

G.XIII.5

of Technology, Austria; Department of Chemistry and Pharmacology, University of Sassari, Italy.
Resume : An integrated approach has been designed to obtain mesoporous graphene nanocomposite films by exploiting the potential of self-assembly in a single step. The synthesis allows incorporating graphene sheets with a small number of defects into highly ordered and transparent mesoporous titania films. The graphene is well-dispersed, and the films do not lose their cubic ordered mesoporous structure after thermal treatment. The films retain a high optical transparency and can be integrated in a bottom-up and top-down process; well-defined and sharp patterns with a thickness up to 1 μm have been obtained by deep X-ray lithography. The films show an enhanced photocatalytic activity which is due to three specific contributions: the insertion of exfoliated graphene with a minimized amount of defects, the formation of anatase nanocrystals with photocatalytic properties, and the highly organized mesoporosity which enhances the diffusivity inside the matrix. A scalable and straightforward synthesis is now available for the preparation of photocatalytic nanocomposite devices based on thin transparent films. Such a protocol can be successfully exploited for the microfabrication of new integrated devices, such as dye-sensitized solar cells and optical limiting devices, which will take advantage of the functional properties of graphene mesoporous nanocomposites.

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09:45 **Coffee break**

Graphenes - II : Saulius KACIULIS, Rony Snyders

10:00 **Sigmoidal kinetics of graphene growth under continuous carbon supply**

Authors : Kemal Celebi, Matthew T. Cole, Ning Yang, Nalin Rupesinghe, John Robertson, Kenneth B. K. Teo, Hyung Gyu Park
Affiliations : Department of Mechanical and Process Engineering, ETH Zurich; Department of Engineering, University of Cambridge; Aixtron Ltd.
Resume : It has been claimed that graphene growth on copper by chemical vapor deposition is dominated by crystallization from the surface initially supersaturated with carbon adatoms, which implies that the growth is independent of hydrocarbon addition after the nucleation phase. Here, we present an alternative growth model based on our observations that oppose this claim. Our Gompertzian sigmoidal growth kinetics support the postulate that the growth can be controlled by adsorption−desorption dynamics and the dispersive kinetic processes of catalytic dissociation and dehydrogenation of carbon precursors on copper. Growth and nucleation behavior of the secondary layer could be explained by dissociative dehydrogenation cascade with limited active reactants.

G.XIV.1

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10:15 **Transport and Vibrational properties of CVD-grown graphene on PMN-PT substrate**

Authors : Wenjing Jie, Jianhua Hao
Affiliations : Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Hong Kong
Resume : Graphene has attracted much attention because of its fascinating optical, electrical and mechanical properties. Chemical vapor deposition (CVD) synthesized monolayer graphene was transferred onto single-crystal [Pb (Mg1/3Nb2/3)O3]0.7-[PbTiO3]0.3 (PMN-PT) substrates by standard transfer method. PMN-PT is an excellent substrate which is capable of providing large strain due to its giant electromechanical or converse piezoelectric response. Herein, the effects of piezoelectric potential and tunable strain on the transport properties and Raman spectra of the graphene were investigated. Graphene-based FET gated by PMN-PT was fabricated and exhibited p-type characteristics in air ambient at room temperature. The curve of drain current as a function of gate voltage revealed a large memory window, which should be very useful for graphene/ferroelectric memory application. On the other hand, detailed analysis by X-ray diffraction (XRD) technique and Raman spectroscopy indicated that the blue shifts of graphene 2D band mainly resulted from biaxial strain induced by the PMN-PT substrate. The calculations based on the shift of 2D band showed that small percentage of biaxial strain could be delivered from the PMN-PT to the graphene layer, and subsequently, a continuous Raman 2D

G.XIV.2

band shift could be detected. Such time-dependent Raman shift may be caused by different strain distribution between domain and domain boundaries in CVD-grown graphene.

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10:30 **Graphene Oxide Scrolls Fabricated by Molecular Combing**

Authors : Jumiati Wu, Hai Li, Hua Zhang
Affiliations : School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

Resume : Carbon nanoscroll (CNS), a wrapped graphene sheet with tubular structure, has been receiving increasing interest in recent years. Several methods have been reported to fabricate CNS, such as scrolling of the mechanically exfoliated graphene sheets with the aid of isopropyl alcohol in water, sonication of graphite intercalation compounds and microwave-assisted scrolling in liquid nitrogen. In this work, well-aligned graphene oxide (GO) scrolls are fabricated by folding/scrolling of GO on various hydrophobic substrates, such as the aged gold substrate, polydimethylsiloxane (PDMS) film, poly(L-lactic acid) (PLLA) film, and octadecyltrimethoxysilane (OTS)-modified silicon dioxide, using molecular combing. We then extend this concept to hydrophilic-hydrophobic patterned substrate. Alternative bead-string like GO architectures are fabricated over large area by molecular combing GO solution on hydrophilic-hydrophobic alkanethiols self-assembled monolayers (SAMs), which are patterned by microcontact printing. GO has been found to be spread over hydrophilic SAMs (16-mercaptohexadecanoic acid, MHA) but folded within hydrophobic SAMs (1-octadecanethiol, ODT). The shape, orientation and position of GO sheets can be easily controlled by using the hydrophilic-hydrophobic micropatterned SAMs as templates. Followed by hydrazine reduction, the reduced GO scroll and architecture based devices have been demonstrated to detect NO2 gas at low concentration.

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10:45 **CVD synthesis and wetting properties of various BN nanostructure films**

Authors : Amir Pakdel, Yoshio Bando, Dmitri Golberg
Affiliations : National Institute for Materials Science (NIMS), Tsukuba, Japan

Resume : Boron nitride (BN) nanostructures are among the most promising inorganic nanosystems explored so far due to their unique properties, such as wide optical bandgap, deep UV emission, good thermal conductivity, excellent stiffness, and outstanding thermal and chemical stability. In this study various BN-based nanostructure films consisting of nanosheets, nanotubes, nanobamboos, nanofunnels, etc were grown on silicon/silicon dioxide (Si/SiO2) substrates via a thermal CVD method. They were then employed as a platform to investigate the influence of surface nanomorphology on the static and dynamic interaction of the BN films with liquids. Moreover, post-treatment techniques such as UV-ozone and air plasma treatments were applied to BN nanostructure films to study the effect of surface functionalization on their wetting properties. As a result, a wide range of wetting properties from superhydrophilicity with contact angle (CA) of ~5° to superhydrophobicity with CA of ~160° was obtained by changing the surface nanomorphology or chemical composition. Highly-rough vertically-standing nanotube and nanosheet films demonstrated great water-repellency whereas conical nanostructure films were less hydrophobic. On the other hand, chemically-modified BN nanostructure films were totally wetted by water.

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11:00 **DISCUSSION**

12:00 **Lunch**

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