

ABSTRACTS OF POSTER CONTRIBUTIONS

in alphabetical order of the presenting author's name

DEFECTS OF SiC NANOWIRES STUDIED BY STM AND STS

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Silicon carbide nanowires (SiCNWs) belong to the 1-D nanostructures family. These materials are very promising for nanotechnology applications [1]. The ideal SiCNWs are generally thin elongated SiC nanocrystals. However, like other 1-D nanostructures (e. g. carbon nanotubes) SiCNWs also possess various structural defects that can be divided into two classes: (i) ‘large-scale’ deformations (e.g. kinks, twists) and (ii) ‘atomic-scale’ defects (e.g. dislocations, vacancies). These two families of defects are in close relationship and furthermore, the local electronic structure of SiCNWs is expected to be perturbed in the vicinity of such defects.

In the present paper, the investigations of large-scale deformations of SiCNWs and their influence on the surface electronic structure were carried out. The scanning tunneling microscopy (STM) and spectroscopy (STS) were employed to determine the complex structures in SiCNWs produced via combustion synthesis route [2] and to detect the fluctuations of the local density of electronic states (LDOS) accompanying deformations. The local graphitization and the inhomogeneous concentration of doping impurities (e.g. nitrogen) were considered to explain LDOS fluctuations in the vicinity of SiCNWs deformations. Thus, new information for the understanding of surface electronic properties of 1-D nanostructures based on SiC compound have been achieved.

[1] W.M. Zhou, F. Fang, Z.Y. Hou, L.J. Yan, Y.F. Zhang, *IEEE El. Dev. Lett.* 27 (2006) 463.

[2] S. Cudziło, M. Bystrzejewski, H. Lange, A. Huczko, *Carbon* 43 (2005) 1778.

NANO- AND MICROTRIBOLOGICAL CHARACTERIZATION OF FLUOROSILANES DEPOSITED ON COBALT SUBSTRATE

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With advances in micro-/nanoelectromechanical systems (MEMS/NEMS), fluorosilanes on cobalt, silicon are of interest for a wide range of applications including medical implants, lubrication, corrosion, interfacial wetting, adhesion and friction. Fluorosilanes chemically bonded to the substrate are considered to be the best solution of lubrication.

Chemical vapor deposition (CVD) was used to grow fluorosilane film on cobalt surface. The films were characterized by means of a contact angle analyzer for hydrophobicity, ellipsometry for determining the thickness and X-ray photoelectron spectroscopy (XPS) for identification of fluoroorganic monolayers deposited on surfaces. Adhesion and friction measurements were performed using atomic force microscope (AFM) and compared with measurements made by microtribometer operating in milinewton (mN) normal load range.

Nano- and microtribological measurements indicated that cobalt modified by fluorosilanes has the lowest friction coefficient and indicated a decrease of friction coefficient with increasing fluoric alkylchain length.

MFM AND AFM STUDY OF THIN COBALT FILMS MODIFIED BY FLUOROSILANE

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Polycrystalline cobalt films 100 nm thick were thermally evaporated on oxidized Si(100) substrates. Then 1H, 1H, 2H, 2H perfluorodecyltrichlorosilane (FDTS) films of various thicknesses, in the range of about 1 nm to 30 nm, were grown on cobalt surfaces by chemical vapor deposition (CVD). The cobalt films modified by FDTS were investigated using magnetic force microscopy (MFM) and atomic force microscopy (AFM). MFM observation showed that the magnetic structure of the cobalt films modified by FDTS is composed of domains with a considerable component of magnetization perpendicular to the film surface. This in turn indicates that the cobalt films on Si(100) substrates crystallize in the hexagonal close-packed (HCP) phase and exhibit a texture with the hexagonal axis perpendicular to the film surface. The magnetic domains formed a maze structure. The domain width increased from typically 80–120 nm to 400–500 nm with increasing the thickness of FDTS films from about 1 nm to 30 nm. AFM imaging of the surfaces of FDTS films revealed the presence of an agglomerate morphology. The agglomerates varied in size from typically 30–70 nm to 150–300 nm as the film thickness was increased from about 1 nm to 30 nm.

INVESTIGATION OF InSb(110) AND InSb(111) SURFACES BY MEANS OF TARGET CURRENT (VLEED) SPECTROSCOPY AND LEED

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In this report we show InSb(110) and InSb(111) target current spectra (TCS) [1]. TCS spectra were recorded in 0-30 eV kinetic energy range in first derivative mode $\left(\frac{dI_T}{dE}\right)$. Spectra exhibit well pronounced structures, different for (110) and (111) orientations and are almost identical for InSb(111) and InSb($\bar{1}\bar{1}\bar{1}$) polar surfaces. Comparison with LEED intensities gives clear evidence that most of the fine structure in TCS originates from elastic scattering (diffraction) effects and reveals upper band critical points [2-4]. Our results are compared to previously published TCS data from CdTe(110) [5], CdTe(111) [6] and GaAs(110) [7]. Especially, in the electron energy range 4-8 eV above vacuum level, TCS spectra are very similar for (110) surfaces of all mentioned compounds and are sensitive to electron incidence angle. In addition we show preliminary results from thin Sn and In layers on InSb substrates.

[1] P.J. Møller, M.H. Mohamed, Vacuum 35 (1985) 29.

[2] R.C. Jaklevic, L.C. Davis, Phys. Rev. B 26 (1981) 5391.

[3] I. Bartoš, Prog. Surf. Sci. 59 (1998) 197.

[4] V.N. Strocov, Solid State. Comm. 106 (1998) 101.

[5] A. Dittmar-Wituski, P.J. Møller, Surf. Sci. 287-288 (1993) 577.

[6] A. Dittmar-Wituski, Zesz. Nauk. ATR Bydg. Fizyka (1)206 (1997) 167.

[7] J.-V. Peetz, W. Schattke, H. Carstensen, R. Manzke, M. Skibowski, Phys. Rev. B 46 (1992) 10127.

THEORETICAL INVESTIGATIONS OF THE DIFFUSION PROCESS OF TUNGSTEN ON TUNGSTEN

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We present theoretical investigations of the diffusion process of W atom on the W(112) surface. Our research has been focused on calculating the main features of activation barrier, such as its height and shape. We have considered only transitions between the nearest adsorption sites along the surface channel, examining also the influence of different substrate coverage. The obtained results agree very well with experiment [1] yielding an asymmetric shape of energetic barrier and values of activation energy close to the experimental value (0.84 eV). All calculations have been performed in the framework of ab-initio approach based on density functional theory. Electron-ion interactions are described by the projector-augmented wave method and the electronic wave functions are expanded in a plane wave basis. Additionally, two, namely LDA and PW91, types of exchange-correlation potentials have been tested. The diffusion process has been simulated, independently, by the use of constrained statistic method and nudged elastic band method. Both approaches have provided very consistent results.

[1] G. Antczak, Phys. Rev. B 73 (2006) 033406.

NANOSCALE STUDIES OF (100) In₄Se₃ CRYSTAL FURROWED AND CHAINLIKE RELIEF SURFACES

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The layered crystal structures with the weak interaction of van der Waals type between the layers and the strong covalent-ionic interaction within the layer are recently studied giving new insights into understanding the properties of the natural low-dimensional, 2D structures and their potential applications in technology.

The crystallography, topography and local density of states of the (100) cleavage surfaces of a layered semiconductor In₄Se₃ crystal, obtained in ultrahigh vacuum, were analysed by low energy electron diffraction (LEED), scanning tunneling and atomic force microscopy (STM, AFM) *in situ*. The “structure” of surface LEED patterns, shape and dimensions of subsequent STM- and AFM-profiles [1] well correspond to the lattice parameters derived from the bulk-crystal structure obtained by X-ray diffraction (XRD). The local density of states and band gap for (100) In₄Se₃ have been obtained by scanning tunneling spectroscopy (STS), which gives the gap value the same as for bulk crystal.

The STM/STS results show a local energetic and phase inhomogeneity of (100) In₄Se₃ cleavage surfaces on atomic scale. The studies confirm that the (100) In₄Se₃ furrowed and chainlike surface structure is stable and unreconstructed under the cleavage and might be suitable as an anisotropy, low-conductive matrix/template for fabrication of surface-conductive nanowires or nano heterostructures.

[1] P.V. Galiy, T.M. Nenchuk, O.R. Dveriy, A. Ciszewski et al., *Physica E* 41 (2009) 465.

THE ANISOTROPY OF SURFACE BAND STRUCTURE OF THE LAYERED In_4Se_3 (100)

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The In_4Se_3 semiconductor crystal forms a layered structure characterized by weak interaction of van der Waals type between the layers and strong covalent-ionic interactions within the layer but the (100) surface is not “smooth”. The quasi two-dimensionality of layered crystals does not quite apply to this system as the layers are not perfectly flat but corrugated, resulting in quasi-one dimensional chain structures at the In_4Se_3 (100) surface as seen in both STM/AFM. In_4Se_3 is, in fact, is dominated by $(\text{In}_3)^{5+}$ multivalent clusters bonded with Se through ionic covalent bonds. The surface of In_4Se_3 provides, in fact, an opportunity to study the electronic structure of In chains in the presence of strong bonding with Se atoms.

It is possible to discern from ARUPS that the ordered surfaces of the In_4Se_3 (100) system exhibits band structure (i.e. discernable and significant band dispersion) both parallel and perpendicular to the cleavage plane. Along the principal high symmetry axis directions, parallel to the cleavage plane, the band structure is consistent with surface lattice constants of $b=12.3 \text{ \AA}$ and $c=4.08 \text{ \AA}$. Band widths (the extent of dispersion) of $\approx 1 \text{ eV}$ is observed along the surface chain rows, and about 0.5 eV perpendicular to the surface “furrows”. The downward dispersion (towards greater binding energy) of the band at the valence band maximum, away from the Γ point, can be understood as this band is dominated by In-s and Se-p_y bonds. The band widths (the extent of the dispersion) of 0.3 to 0.4 eV perpendicular to the chain direction or 1.25 eV along the chain direction, for bands within the valence region, is in line with the expectations from the calculated band structure.

STUDY OF Cr/6H-SiC(0001) CONTACTS FORMATION

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Early stages of Cr contact formation on 6H-SiC(0001) were investigated using the atomic force microscope (AFM) and current-sensing AFM with conducting tip. Cr layers were vapor deposited under ultra high vacuum onto samples cut out of a single crystal of n-type 6H-SiC(0001) that were ex situ hydrogen etched in a tubular flow reactor or in situ argon ion bombarded surface.

Hydrogen etching was carried out on the (0001)-oriented 6H-SiC wafer at various temperatures in the range from 1450 to $1650 \text{ }^\circ\text{C}$. Surface topography and morphology was characterized by the AFM. Optimal conditions have been found, under which all scratches due to the polishing process are efficiently removed and the atomically smooth, clean surface of SiC(0001) is achieved. The conditions of surface were examined by AFM and low electron diffraction (LEED).

Topography of the Cr/SiC interface, their local conductance patterns and local current-voltage characteristics of the Cr/SiC contact were examined simultaneously as a function of Cr-adlayer thickness and annealing temperature. Additionally the chemical analysis of the samples were carried out with x-ray photoelectron spectroscopy (XPS) using Mg K_α radiation ($h\nu = 1253.6 \text{ eV}$).

AES INVESTIGATION OF THE FRICTION NANO-LAYERS GENERATED ON STAINLESS STEEL SURFACE.

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Auger Electron Spectroscopy (AES) depth profiling of the Fe-oxide nano-layers prepared during friction process on stainless steel surface was performed. The structure was observed in the Auger spectra resulting from Fe $M_{2,3}$ VV transition. It has been established that native layer of oxide formed on stainless steel surface consists of Fe_2O_3 , Fe_3O_4 and FeO layers. The structure of Fe-oxide layers formed on stainless steel under different conditions of friction in oil has been determined.

ORDERED ZINC(II)-PHTHALOCYANINE LAYERS AT Cu(100)/ELECTROLYTE INTERFACES: AN IN-SITU STM STUDY

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The self-assembly of Zn(II)-Phthalocyanine on an iodide modified Cu(100) electrode has been studied by means of Cyclic Voltammetry (CV) and in-situ ElectroChemical Scanning Tunneling Microscopy (EC-STM). The iodide layer forms a $c(p \times 2)$ superstructure on the Cu(100) substrate on top of which the phthalocyanine molecules form an ordered monolayer. The flat-lying molecules form a square-shaped lattice with an intermolecular distance of 1.95 ± 0.02 nm. This molecular lattice is rotated by $62 \pm 2^\circ$ with respect to the [011] direction, i.e. the commensurate direction of the I-underlayer. This clearly excludes a template effect of the substrate surface, but rather hints to a molecular self-assembly.

DIRECTIONAL ELASTIC PEAK ELECTRON SPECTROSCOPY IN INVESTIGATION OF THE Ag/Au(111) SYSTEM

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The intensity of elastically backscattered electrons at different primary electron beam energies was measured to obtain a stereographic maps of the Ag/Au(111) adsorption system by means of the directional elastic peak electron spectroscopy (DEPES) [1,2]. The obtained data reveal the threefold symmetry of the clean substrate and adsorbed layers, which proves an epitaxial growth of the Ag adsorbate. Experimental DEPES results are compared with the theoretical data obtained by using multiple scattering calculations (MS) [3] taking into account both not- and reconstructed Au(111) clusters. A satisfactory agreement between experiment and theory is found when the third scattering order is taken into account in MS approximation. The lateral lattice misfit of the first layer leads to quantitative changes of theoretical intensities showing a sensitivity of DEPES on the short atomic chain axial order. This comparison proves that a main contribution of the experimental contrast originates from higher background level. Moreover, an anisotropy of the inelastic mean free path is suggested.

[1] S. Mróz, M. Nowicki, Surf. Sci. 297 (1993) 66.

[2] M. Nowicki, Phys. Rev. B 69 (2004) 245421.

[3] I. Morawski, M. Nowicki, Phys. Rev. B 75 (2007) 155412.

INTERACTION MECHANISMS AT THE PTCDA/Ag(111) INTERFACE: FIRST PRINCIPLES CALCULATIONS

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PTCDA is one of the most studied π -conjugated molecules that forms ordered structures on a wide range of metal surfaces. The interaction mechanism between PTCDA and metal surfaces has become a fundamental issue in understanding organic and molecular electronics. Adsorption process, nature of bonding, electronic structure and molecular distortion of PTCDA on Ag(111) surface is still controversial, although this interface has been intensively studied both experimentally and theoretically.

Therefore, we have performed large scale first principles simulations (using the VASP code [1]) to study the adsorption of the PTCDA on Ag(111) surface. Regarding the analysis of the molecular adsorption and the contact formation, we have analyzed the structural and electronic properties of the interface, fully relaxing a large unit cell containing two PTCDA molecules in non-equivalent adsorption configurations, which reproduces the characteristic herring-bone pattern observed in the experiments [2]. In particular, we have performed a detailed investigation of the interaction mechanism at a molecule-metal interface. We discuss the bond lengths inside the molecules, the distortion of the molecules due to adsorption, and their position and orientation relative to the substrate. Then, we analyze adsorption-induced chemical bond formation via differential charge density at the PTCDA/Ag(111) interface. We have found that the nature of this interface is characterized by multichannel molecular orbital interactions. The bonding mechanism has a chemisorptive character and occurs via two different channels: the perylene core of PTCDA and four terminal carboxylic oxygen atoms. The obtained projected density of states is in a very good agreement with recent STS [3] and photoemission experiments [4].

[1] G. Kresse, J. Hafner, Phys. Rev. B 47 (1993) R558; G. Kresse, J. Furthmüller, Comput. Mat. Sci. 6 (1996) 15; G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996) 11169.

[2] L. Kilian et al., Surf. Sci. 573 (2004) 359.

[3] A. Kraft et al., Phys. Rev. B 74 (2006) 041402(R).

[4] Y. Zou et al., Surf. Sci. 600 (2006) 1240.

MORPHOLOGY CHANGES OF W NANO-CRYSTAL DURING SEGREGATION OF CARBON

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Carbon is one of the major and toughest to remove contaminants of tungsten crystals. During annealing of W crystals carbon easily segregates to the crystal surface what changes not only surface structure, but also causes considerable changes of crystal morphology as it leads to adsorbate induced faceting of the W crystal.

Field Electron Microscopy is a good tool for studies of adsorbate-caused thermal faceting metal crystals. The specimen – metal tip of small radius of curvature – is terminated with a small nano-crystal. Faceting experiments carried out on curved surfaces of such specimen can show morphological changes of many different planes simultaneously, giving an insight into the adsorbate-caused evolution of the crystals.

In this work we want to show how the shape of a carbon contaminated W nano-crystal changes during annealing. Faceting of the surface cleaned bulk C contaminated W crystal was observed after annealing it at temperatures of at least 1100-1150 K and was ascribed to the segregation of carbon to the crystal surface. We found out that the pattern of crystal faceting depends strongly on the annealing time and temperature (and thus on the surface concentration of carbon) and can result in two different crystal shapes.

CO-ADSORPTION OF OXYGEN WITH SAMARIUM ON THE MOLYBDENUM (211) SURFACE

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Sm as a pure metal focuses oneself much scientific interest since electronic structure investigations shows that it could exist two different electronic configurations, namely $[Xe] 4f^6(5d6sp)^2 - Sm^{2+}$ and $[Xe] 4f^5(5d6sp)^3 - Sm^{3+}$ [1,2]. Up to now those two electronic configurations were connected with existence of Sm atoms in different valence state: di- (Sm^{2+}) and tri- (Sm^{3+}) valent. The Sm^{3+} atoms were assumed to be in the bulk, and Sm^{2+} on the surface. However recent theoretical calculations performed by Yakovkin shows that both electronic configurations ($[Xe] 4f^6(5d6sp)^2$ and $[Xe] 4f^5(5d6sp)^3$) has got similar LDOS around Fermi level and as a result should give similar photoelectron emission in valence band region [3] (identified earlier as Sm^{2+} emission). One of the author supposing about origin of Sm^{3+} signals in photoelectron emission (around 5 eV below Fermi level) was contamination of Sm by other elements (e.g. oxygen). During experiments concerning the adsorption of Sm on the Mo (211) face a presence of oxygen was not found [4], and electron photoemission spectrum has got both signals, from Sm^{3+} and Sm^{2+} . To check the influence of O on the electronic structure of Sm the XPS experiments of co-adsorption of O and Sm were performed. As a result of co-adsorption of O and Sm it was found that Sm^{2+} signal is attenuated and oxidized Sm layers shows only emission characteristic to Sm^{3+} . However, in spite of applying the smallest possible oxygen exposures (around 5×10^{-10} Torr) the O peak in XPS spectra was clearly visible which was absent during pure Sm deposition. Comparison of experimental results (adsorption of Sm vs. co-adsorption of Sm and O) shows that contamination of Sm layers with O atoms leads to electron emission from Sm^{3+} , but on this base it isn't possible to explain observed photoelectron emission spectra from metallic Sm.

[1] G.K. Wertheim, M. Campagna, Chem. Phys. Lett. 47 (1977) 182.

[2] G.K. Wertheim, G. Crecelius, Phys. Rev. Lett. 40 (1978) 813.

[3] I.N. Yakovkin, Surf. Sci. 601 (2007) 1001.

[4] M. Kuchowicz, J. Kołaczkiwicz, Surf. Sci. 603 (2008) 1018.

THEORETICAL STUDY OF ADSORPTION PROCESS OF Pb ON THE Ni(111) AND Ni₃Al(111) SURFACES

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The Ni₃Al(111) surface has been widely studied for over twenty years and it is applicable mainly as an ideal supporting surface of various nanosystems [1]. However, little is known about Pb adsorption on this surface. At the same time an adsorption of a Pb atoms on the Ni(111) face have been treated in number of works [2]. Recently, both supports are considered as a catalyzer for CO methanization [3]. From this point of view adsorption of CO on these surface has became to be of big interest. Adsorption in this case can be affected by Pb atoms [4], therefore it is interesting to look closer on the Pb adsorption process on both, Ni(111) and Ni₃Al(111) surface. I will present the results of the first-principles calculations based on density functional theory (DFT) used to study an adsorption process of lead on the Ni(111) and Ni₃Al(111) surfaces. The comparison of the substitutional adsorption (for Pb/Ni(111), resulting in a surface alloy) with simple deposition of adsorbate on surface will be presented for both systems.

- [1] M. Schmid, G. Kresse, A. Buchsbaum, E. Napetschnig, S. Gritschneider, M. Reichling, P. Varga, *Phys. Rev. Lett.* 99 (2007) 196104.
- [2] D.F. Li, H.Y. Xiao, X.T. Zu, H.N. Dong, *Physica B* 392 (2007) 217.
- [3] A.H. Zhang, J. Zhu, W.H. Duan, *Surf Sci.* 601 (2007) 475.
- [4] V. Matolin, I. Matolinova, N. Tsud, S. Fabik, J. Libra, V. Dudr, V. Chab, K.C. Prince, *Phys. Rev. B* 74 (2006) 075416.

ELECTRON BEAM DEGRADATION OF POLYETHYLENES STUDIED BY ELECTRON SPECTROSCOPY METHODS AIDED WITH A LINESHAPE ANALYSIS

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The surfaces of polyethylenes of different density, branching, crystallographic order, and the length of the monomer, i.e. low density polyethylene (PELD), high density polyethylene (PEHD), polyethylene of ultra high molecular weight (PEUHMW), and electron beam surface degradation were investigated by XPS, XAES and EPES aided with the spectra lineshape analysis.

In the present work, the hydrogen content was evaluated from the electron recoil effect in EPES spectra [1], the Csp^2/sp^3 ratio - from the C 1s and C KLL spectra [2] and the lineshape analysis by the pattern recognition (PR) method called the fuzzy k-nearest neighbor (fkNN) rule [3]. The above approaches showed (i) the differences between various polyethylenes, (ii) their surface changes and degradation due to electron beam, (iii) the polyethylenes stability under electron beam. The results obtained from various approaches were found consistent [4,5].

- [1] B. Lesiak et al., *Polymer* 49 (2008) 4127.
- [2] Y. Mizokawa et al., *J. Vac. Sci. Technol. A* 5 (1987) 2809.
- [3] J.C. Bezdek et al., *Fuzzy Sets Syst.* 18 (1986) 237.
- [4] B. Lesiak et al., *Pol. Degrad. Stab.*, submitted (2009).
- [5] B. Lesiak et al., *Pol. Degrad. Stab.*, submitted (2009).

THE GROWTH OF THIN Hf FILMS ON 6H-SiC(0001) SURFACES

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The initial stages of Hf growth on SiC(0001) surface and annealing influence on the evolution of microstructure of formed Hf films have been investigated by X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). The shifts of the binding energies of Hf 4f, Si 2p C 1s, O 1s levels observed with increasing Hf depositions allow to state that even at room temperature hafnium oxide in the form of HfO_x is created. Further analysis of experimental data indicates that Hf grows irregularly with tendency to form nanocrystalite grains on terraces edges, and moreover, preferably on these parts of the surface which are not covered by additional graphite carbon layers which together with oxygen are present on the virgin SiC(0001) surface. The grain sizes are sensitive to the annealing and efficiently increase during sample heating at temperatures as low as 1000 °C. This surface morphology changes are going through merging smaller nanoparticles into clusters. For longer Hf depositions, with average thickness over 10 monolayers, excess of carbon segregates and migrates towards the surface, and simultaneously creates HfC and CO bonds. However, CO is not stable and during annealing at about 1000 °C desorbs from the surface.

LOW COVERAGE ALKALI METAL ADSORPTION ON Ge(100) SURFACE

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In our theoretical study we discuss the adsorption of individual atoms of alkali metals (Li, Na, K, Rb, Cs) at the Ge(100) surface. We present calculations for single atom adsorption (5×10 supercell) at the p(2×1) reconstructed Ge(100) surface. The structural properties of minimum energy configurations and adsorption energy are given. We also present geometrical and electronic properties of these structures and STM images. For comparison, we also calculated adsorption properties for surface with missing-dimer defect.

FLUORINE, CHLORINE AND IODINE ADSORPTION ON Ge(100) SURFACE: COMPARATIVE STUDY FOR COVERAGES OF 0.75 AND 1 MONOLAYER

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We present a theoretical investigation of the structural and electronic properties of fluorine, chlorine and iodine adsorbed on the Ge(100) surface, for 0.75 and 1 monolayer of adsorbate. Our calculations are performed using combination of two methods: plane-wave and local-orbital minimal basis techniques based on density functional theory. Results of molecular dynamics calculations are complemented by simulations of Scanning Microscopy Tunneling images.

PROPERTIES OF ULTRATHIN Pb LAYERS ON THE Ni(001) FACE

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The atomic structure and morphology of ultrathin Pb layers on the Ni(001) face deposited in ultrahigh vacuum at the substrate temperature ranging from 150 K to 900 K were investigated with the use of Auger electron spectroscopy (AES) and low-energy electron diffraction (LEED).

APPLICATION OF 1 MHz QUARTZ NEEDLE-SENSOR FOR COMBINED NON-CONTACT AFM AND STM

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A simultaneous measurement of atomic forces and tunneling current during imaging of surfaces is of great interest. We present combined ncAFM/STM images of a platinum surface obtained by means of a quartz needle-sensor with an attached platinum coated silicon tip. The needle-sensor is a 1MHz resonator where mechanical oscillations proceed along the quartz bar. High resonance frequencies and large values of the spring constant, on the order of 0.5MN/m, enable ultra low oscillation amplitudes and a fast scan rate at the reasonable low thermal frequency noise [1].

Tip-sample interaction forces were detected in the FM mode at a constant amplitude realized by means of a phase locked loop (PLL) control. The measurement circuit of the tunneling current was combined with a high frequency signal feeding quartz resonator. This setup enables electrical steering of the sensor as well as the detection of measured signals.

The frequency shift and tunneling current were detected simultaneously, while the feedback control loop for the topography signal was fed using one of them.

Size and shape of the tip apex influence the tip-sample force [3]. In case of a board tip apex, the total force is a sum of the long-range forces acting between particular pieces (atoms) of the tip and the sample surface. In general, a broad tip apex leads to smoothing of the topography signal providing a low lateral resolution. However, the tunneling current stays a local effect characterized by the single atom lateral resolution.

[1] T.R. Albrecht, P. Grütter, D. Horne, D. Rugar, J. Appl. Phys. 69 (1991) 668.

[3] F.J. Giessibl, Phys. Rev. B 56 (1997) 16010.

DEPENDENCE OF EXTENDED ENERGY LOSS FINE STRUCTURE ABOVE THE N AND O EDGES OF GOLD ON THE ENERGY OF PRIMARY ELECTRONS

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Electron Energy Loss Fine Structure (EELFS) has been established as an effective method in determination of the geometrical environment of atoms in the sample surface layer [1]. Interpretation of experimental data is based on theories elaborated for Extended X-ray Absorption Fine Structure (EXAFS). Position of particular maxima with respect to the edge position in the EELFS should be, according to these theories, independent of the energy of primary electrons. This independence was confirmed in numerous measurements performed for K, L, and M edges of light elements and transition metals (see, for example, [2]). Measurements for N edges are scarce and results are not so firm [3]. In the present work, EELFS spectra are presented for the gold N and O edges, with the use of crystalline Au₃Cu(001) sample. Our measurements were performed in the dN/dE mode, with the use of an RFA analyzer, for the primary electron energy E₀ ranging from 1000 to 1200 eV. The proper polynomials were fitted to and subtracted from particular spectra and results of this subtraction were integrated. Particular maxima of the fine structure were then clearly visible. It was found that the energy losses ΔE corresponding to particular maxima changed significantly and smoothly when the primary energy changes. For example, the maximum appearing at ΔE = 210 eV for E₀ = 1000 eV moves to 257 eV for E₀ = 1200 eV. Modification of theories based on these elaborated for EXAFS by introducing the curved-wave approximation (CWA) instead of plane-wave approximation (PWA) and used in [3] for the palladium N_{2,3} edge does not explain this dependence. Further effort in the theory seems to be necessary here.

[1] M. De Crescenzi, Surf. Sci. Rep. 21 (1995) 89.

[2] A.P. Hitchcock, C.H. Teng, Surf. Sci. 149 (1985) 558.

[3] B. Luo, J. Urban, J. Electr. Spectr. Rel. Phen. 57 (1991) 399.

METAL-SEMICONDUCTOR TRANSITION ON THE SURFACE AND IN THE BULK OF SOME RARE EARTH METALS: COMPARISON BETWEEN TERBIUM AND GADOLINIUM

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H₂ interaction with hexagonal rare earth metals (RE) leads to spontaneous three-hydride formation when appropriate thermodynamic conditions are fulfilled. In the course of this process the (RE) metals are transformed into semiconductors. The question arises whether the metal-semiconductor (MS) transition starts already on the surface when hydrogen coverage reaches an appropriate value, or whether the adsorbate penetrates below the surface first, to find defined interstitial sites in the metal lattice, and then hydride formation occurs. To answer this question, surface phenomena accompanying H₂ interaction with (RE) have to be correlated with the change of bulk properties known for the process of hydride formation. This can be done by studying hydrogen interaction with thin (RE) films deposited on glass under UHV conditions, thus having a clean surface. During (MS) transition, light-reflecting thin metal film is transformed into a transparent semiconductor. Measurements of work function changes ΔΦ were chosen to illustrate the surface phenomena, while changes of the relative electrical resistance R(H)/R₀, relative transparency for light T(H)/T₀ and the light absorption spectrum correspond to known bulk properties. The correlation of surface and bulk phenomena has been compared for thin Gd and Tb films. Samples of known weight were completely evaporated from a tungsten heater and deposited on glass. Successive calibrated H₂ doses were introduced into the reactor of known volume, disconnected from pumps, with simultaneous monitoring of the pressure and surface or bulk phenomena. In this way the atomic concentration of hydrogen in the thin film could be determined and correlated with the surface and bulk properties. (MS) transition on the surface has been postulated on the basis of the ΔΦ course dependent on hydrogen uptake.

A PORTABLE EVAPORATOR FOR LOW TEMPERATURE SINGLE ATOM STUDIES WITH SCANNING TUNNELING AND ATOMIC FORCE MICROSCOPY

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Here we present a concept for deposition of single adatoms in studies with low temperature scanning tunneling and dynamic force microscopy [1]. A portable evaporator is presented which enables the deposition of material at very low coverage, i.e. single atoms, onto a sample while it is placed on a microscope stage at low temperature. The material for deposition will be loaded, e.g. from a SAES-Li-getter [2], onto the filament of the portable evaporator. This can then be placed in the vicinity of the cold sample. By heating the filament, atoms of the load material are evaporated and then adsorbed onto the cold substrate. A significantly lower vapor pressure of the evaporator's carrier filament as compared to that of the material for deposition prevents contamination of the deposit. The construction of the evaporator is based on a modified halogen lamp with a tungsten filament. Filament temperature and therefore the evaporation flux can be controlled by the heating current and very stable evaporation conditions were obtained. The installation of this evaporator on the manipulator enabled its transportation directly to the sample at the microscope. In this way the controlled deposition of Li on Ag(001) as well as on MgO/Ag(001) samples placed in the microscope at low temperature was possible. The images recorded after the deposition show the presence of single Li atoms on investigated surfaces, which in the case of silver would move into the surface to form an alloy if deposited with the substrate at higher temperature. This directly proves the usefulness of the proposed low temperature evaporation procedure.

[1] H.-P. Rust, T. König, G.H. Simon, M. Nowicki, V. Simic-Milosevic, G. Thielsch, M. Heyde, H.-J. Freund, in preparation.

[2] SAES Getters, Via Gallarate, 215, 20151 Milano, Italy.

ANALYSIS OF INDIUM SURFACE DIFFUSION ON THE TUNGSTEN SUBSTRATE

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Indium layers, having coverage ranging from 1.6 to 3.2 ML were deposited in room temperature on one half area of the tungsten substrate of 12 mm diameter. Thermodesorption and Auger electron spectroscopy studies have been used to determine mechanism of growth of indium on tungsten. Annealing performed at the temperature range of 400-680 K caused surface diffusion of In atoms. Surface diffusion of In on the W polycrystalline surface was studied by using X-ray Photoelectron Spectroscopy. Measuring the photoelectron intensity as a function of distance and energy, we observed movement of In atoms on the tungsten surface. On the basis of the change of surface coverage with distance surface diffusion coefficient was evaluated at the temperature range of 400-680 K. Results have been compared with previously obtained data for In/W(110).

[1] M. Trzeciński, A. Bukaluk, A. Goldmann, M. Bürgener, *Vacuum* 74 (2004) 157.

[2] M. Gabl, M. Trzeciński, N. Memmel, A. Bukaluk, E. Bertel, *Surface Science* 600 (2006) 4390.

[3] M. Trzeciński, M. Gabl, N. Memmel, K. Okulewicz, E. Bertel, A. Goldmann, A. Bukaluk, *Surface Science* 601 (2007) 4470.

PROPERTIES OF THE CLEAN AND Fe IMPURED GRAIN BOUNDARIES IN CHROMIUM

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The structural, cohesive and magnetic properties of (111) and (210) tilt grain boundaries (GB) in pure antiferromagnetic Cr and in Cr with different concentration of Fe additions are studied from first principles. Our calculations show that Fe atoms in the interstitial positions adjacent to the GB enhance cohesion. Fe atoms substituted for one of the Cr layers atoms has very small or negligible effect on the cohesion. We found that Fe additions in Cr should segregate to the boundaries. The changes in the magnetic moments on GB host atoms are not meaningful. The magnetic moments on Fe atoms are much reduced compared to that on atoms in ideal iron bulk, but in most cases they are much higher than the local moments on the Cr host atoms.

ADSORPTION OF 2-CHLOROPHENOL ON $\text{Cu}_2\text{O}(111)\text{-Cu}_{\text{CUS}}$: A FIRST-PRINCIPLES DENSITY FUNCTIONAL STUDY

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It is widely accepted that copper surfaces enhance the formation of polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs), or dioxins for short. In particular, copper oxide compounds are believed to be the most efficient catalysts for such processes. Copper oxides operate through two pathways. The first is the so-called de novo route which is characterized by the burnoff of the carbon matrix (highly ordered carbon composites present in the ash) together with chlorination and oxidation reactions followed by the release of dioxins from the carbon matrix. The second route is through catalyzing the self-coupling of direct precursors such as chlorophenols, chlorophenoxy radicals and chlorobenzenes. The 2-chlorophenol molecule $\text{C}_6\text{H}_5\text{ClO}$ is composed of a benzene ring with a hydroxyl group and a chlorine atom bonding to adjacent positions on the benzene ring.

In order to better understand these processes, we have used density-functional theory and a periodic-slab model to investigate the adsorption of a 2-chlorophenol molecule on the $\text{Cu}_2\text{O}(111)\text{-Cu}_{\text{CUS}}$ surface, which is a CuO(111) surface with a vacant Cu surface site. Several vertical and flat configurations have been studied. All of these molecular configurations interact very weakly with the $\text{Cu}_2\text{O}(111)\text{-Cu}_{\text{CUS}}$ surface, an observation which also holds for clean copper surfaces and the $\text{Cu}_2\text{O}(110)\text{:CuO}$ surface. Hydroxyl-bond dissociation assisted by the surface was found to be endoergic by 0.42-1.42 eV (9.7-39.7 kcal/mol), depending predominantly on the position of the isolated H on the surface. In addition, the corresponding adsorbed 2-chlorophenoxy moiety was found to be more stable than a vacuum 2-chlorophenoxy radical by about 0.76 eV (17.5 kcal/mol). Despite these predicted endoergicities, however, we would predict the formation of 2-chlorophenoxy radicals from gaseous 2-chlorophenol over the copper (I) oxide $\text{Cu}_2\text{O}(111)\text{-Cu}_{\text{CUS}}$ surface to be a feasible and important process in the formation of PCDD/Fs in the post flame region where gas-phase routes are negligible.

NANOSTRUCTURE IN A DIMER PHASE: MONTE CARLO STUDY OF Co/Cu(111)

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The epitaxial growth of Co on Cu(111) at coverage 0.03 monolayer (ML), is studied by kinetic Monte Carlo (kMC) simulations performed beyond temperature of dimer formation in order to find nanostructure made of dimers as an analogue of nanostructure made of monomers [1]. The surface-state mediated interaction between the Co adatoms has a long range and oscillates between attraction and repulsion as a function of the adatom-adatom distance [2]. First repulsion barrier and first minimum of attraction are at 4.43 Å and 11.14 Å, respectively [3]. The repulsion barrier of the interaction potential prevents dimer formation up to 20 K, so the distance between monomers equals to the position of the minimum. As the temperature increases, adatoms aggregate to form dimers, linear trimers and other small clusters. In order to obtain the largest possible fraction of dimers the simulation procedure consist of deposition of adatoms ($T = 9$ K, flux 0.01 ML/s) and simulated annealing. After 60-120 s of annealing at 21-22 K the fraction of dimers comprise about 90% of the small clusters in the submonolayer. The dimers form big two-dimensional percolating island with weak hexagonal order. Average separation between two dimers (11.9(2) Å) is nearly the same as between two monomers (11.7(1) Å). We call the island as a nanostructure in a dimer phase. Mobility of dimers is very low and the energy required for dissociation of dimers is of the order of 1.4 eV. It makes the nanostructure in a dimer phase stable up to 200 K. The stability of the nanostructure together with magnetic moment of Co may make this nanostructure interesting from technological point of view.

[1] J.M. Rogowska, M. Maciejewski, Phys. Rev. B 73 (2006) 235402.

[2] P. Hyldgaard, M. Persson, J. Phys.: Condens. Matter 12 (2000) L13.

[3] V.S. Stepanyuk et al., Comput. Mater. Sci. 35 (2006) 272.

SURFACE STRUCTURE OF Pd₈Ni₉₂(111) BY DYNAMICAL LEED STUDY

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The structure of (111) surface of a single crystal Pd₈Ni₉₂ alloy was studied using low energy electron diffraction (LEED). The *IV*-spectra were acquired at two polar incidence angles, $\theta = 0^\circ$, $\theta = 20^\circ$. The range of incident beam energies was from ~50 to ~430 eV, the exact range depending upon angle of incidence. In all, 29 non-equivalent beams were used representing a total energy range of 5000 eV. The structure and segregation profile of Pd₈Ni₉₂(111) surface was determined by comparison of the experimental *IV*-spectra to spectra computed by TensEr LEED code [1]. The compositions of the first four atomic layers and the first four interlayer spacings were determined. The composition and spacings of deeper layers were fixed at their bulk values – layer spacing was 2.0306 Å and concentration of Pd was 8%.

Quantitative comparison of experimental and calculated *IV*-spectra was performed by evaluating Pendry R-factor [2]. The minimum Pendry R-factor was $R_p=0.26$ and $R_p=0.38$ for the incidence angles of $\theta = 0^\circ$ and $\theta = 20^\circ$, respectively. The best-fit structure for the incidence angles of $\theta = 0^\circ$ exhibits the Ni enhancement in surface region and contraction of all interlayer spacings, while for the incidence angles of $\theta = 20^\circ$ we find the same behavior of interlayer spacings but the concentration profile is different. The enrichment in Pd is then observed and this requires further investigation by using for example GIXRD.

The results for Pd₈Ni₉₂(111) are compared to the results for the nickel–platinum alloy Pt₁₀Ni₉₀(111) [3] and it is found that they are quite in line.

[1] V. Blum, K. Heinz, *Comput. Phys. Commun.* 134 (2001) 392.

[2] J.B. Pendry *J. Phys. C* 13 (1980) 937.

[3] R. Baudoing, Y. Gauthier, M. Lundberg, J. Rundgren, *J. Phys C* 19 (1986) 2825.

THE INFLUENCE OF ATOM INTERMIXING IN Zr/W(100) SYSTEM ON THE INTERACTION WITH OXYGEN

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Low-work-function materials find wide applications in modern electronics. They are used for high-efficient cathode production of electron microscopes or other devices with bright electron sources required. Usually they are complex-materials whose utility crucially depends on the surface stability under working conditions. From this point of view, the O/Zr/W(100) system is one of most promising. The early studies of the Zr/W system, carried out using the field emission techniques, revealed that annealing the Zr adlayer deposited on the W tip surface caused an intensified emission from the W(100) plane. Explanation of this effect was not unequivocal. It was admitted that the effect was due to either oxygen contamination [1] or the formation of surface alloy [3].

It was established that the presence of oxygen highly decreases the work function (WF) of the Zr/W(100) system [2]. Satoh et al. [4] have shown that annealing the Zr adlayer in oxygen produces ZrO_2 which after short flashing at 2100 K evolves into Zr-O complex. Such complex causes reduction of the WF down to 2 eV [4]. The role which tungsten atoms play in the complex is unknown.

The aim of our project is to investigate to what extent Zr and W atoms intermix in the Zr/W(100) system and how the intermixing influences the interaction of the system with oxygen, as well as to answer the question if there is any impact of the intermixing on the WF reduction. In this report preliminary results concerning the influence of oxygen on the WF changes of the Zr/W(100) adlayers of various thickness annealed at different temperatures prior to oxygen exposure will be given.

[1] L.W. Swanson, L.C. Crouser, J. Appl. Phys. 40 (1969) 4741.

[2] L.R. Danielson, L.W. Swanson, Surface Science 88 (1979) 14.

[3] P.R. Davis, Surface Science 91 (1980) 385.

[4] H. Satoh, H. Nakane, H. Adachi, Applied Surface Science 100/101 (1996) 216.

THE ADSORPTION OF Fe ON THE Mo(111) CRYSTAL FACE

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The adsorption of Fe on the Mo(111) crystal face has been investigated by means of TDS technique. The desorption energy E and desorption frequency ν were determined by using the Arrhenius plot slope. These parameters, as well as desorption order x have been also obtained by comparison (fitting) with numerically calculated spectra. On the basis of them a growth mechanism of Fe on the (111) bcc crystal face has been suggested. The fitting method was also used to revised previous results for Ni on the Mo(111) surface.

STRESS RELAXATION IN THE Hf ADLAYERS ON THE W(100) SURFACE

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Hafnium adsorption on the W(100) surface was investigated by the STM, LEED and AES techniques. The adsorbate was vapor deposited under ultrahigh vacuum conditions (background pressure below 2×10^{-10} Torr). Room temperature deposition results in the Volmer-Weber growth type. Then revealed is formation of grainy layers with islands of up to 7 Å in height and 3 nm size. The layers are atomically ordered with quite a short-range order; if are too big in thickness, do not give LEED patterns typical of an ordered structure. Local ordering that fulfils the LEED imaging is attained after heating the adlayers at ~1100 K.

The crystal field of the substrate affects the adlayer structure strongly so that Hf adlayers on W(100) are pseudomorphic, i.e. have the substrate's structure bcc rather than that of hcp typical of bulk Hf. In this state the Hf layers are strongly stressed. Stress relaxation of such layers can be attained by annealing. Depending on the heating temperature and the adlayer thickness, the stress relaxation leads to a variety of changes in morphology and topography of both the adlayer and the substrate.

SLOW ION IRRADIATION OF SUGAR: MORPHOLOGICAL TRANSFORMATION

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As a result of ion irradiation of saccharose, humic films insoluble in water were obtained. The films having fractal nature were produced by slow hydrogen and argon ions. The argon ions form thicker and more condensed structure than hydrogen ones as a consequence of larger energy transfer to the nuclear system of the target.

The use of hydrogen ions simulated roughly the interaction of solar wind protons with interplanetary dust grains. The film generated by this process could play a similar role to a cell wall isolating, at least partially, a grain interior from a harmful influence of an external environment, which could condition a chemical evolution of the grain.

RECOMPOSITION OF THE FLOAT GLASS SURFACE INDUCED BY PLASMA TREATMENT

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Float glass is a flat, multicomponent oxide glass produced in the float process, in which a ribbon of glass is formed by floating the glass melt on a bath of molten tin in a hot reducing atmosphere. Consequently, the bottom and top surfaces differ in the chemical composition and structure from those of the bulk.

Both surfaces of a commercial float glass were treated simultaneously by a low-temperature argon plasma generated by an inductively coupled rf power supply. The effect of plasma processing on the outer surface composition of both sides of the glass was analysed by means of the ion scattering spectroscopy (ISS) technique.

The observed recomposition of the outer surface atoms was interpreted as a result of the action of the thermal and electric fields created by the plasma on particular glass constituents.

CRYSTALLINE STRUCTURE OF Co LAYERS ON Cu(111)

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The Auger signal and the height of the elastic peak were measured as a function of the incident angle of the primary electron beam with the use of an retarding field analyzer (RFA) to find the crystalline structure of Co layers on the Cu(111) surface. Auger peak kinetics were recorded during the continuous Co deposition at RT. Experimental DEPES (directional elastic peak electron spectroscopy) profiles [1,2] measured for clean Cu(111) and Co/Cu(111) present very well distinguished intensity maxima for incident angles corresponding to the closely packed rows of atoms. DEPES scans were obtained for the $[\bar{2}11]$ - $[2\bar{1}\bar{1}]$ azimuth of the clean Cu(111) face and for different primary electron beam energies in the range 0,5 - 2 keV. Although no long range order within the adsorbed Co layers was found with the use of low energy electron diffraction (LEED), the intensity maxima on DEPES profiles for the Co/Cu(111) system at different coverages prove the presence of the short atomic chain axial order within the adsorbate. Experimental profiles were compared with the theoretical data obtained with the use of a multiple scattering approximation [3]. The characteristic energy losses were recorded for clean Cu and Co on Cu(111) as a function of the incident angle of the primary beam and different primary electron energies. Very well visible intensity maxima on the profiles recorded for energy losses and ultrathin Co layer reflect the crystalline order of Co atoms within the first atomic layers. The above result shows the usefulness of this method in investigating the structure of the substrat/adsorbate interface at early stages of growth.

[1] S. Mróz, M. Nowicki, Surf. Sci. 297 (1993) 66.

[2] M. Nowicki, Phys. Rev. B 69 (2004) 245421.

[3] I. Morawski, M. Nowicki, Phys. Rev. B 75 (2007) 155412.

TITANIUM DIOXIDE-BASED NEW MATERIALS

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Titanium oxides are widely used and still extensively investigated. In this report we present new nanostructured materials obtained on the basis of titanium dioxide. Thin films doped with metals were prepared successfully using electron beam evaporator. This simply method allows for obtaining stoichiometric TiO₂ on SiO₂ substrates. Oxides were obtained in a vacuum chamber of base pressure 10⁻⁷ Pa in a reactive atmosphere.

The influence of dopant and annealing treatment on morphology has been discussed. Thin films were investigated by X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). We also carried out AFM measurements. Additionally we checked the films' activity under UV and visible light to see their usefulness for hydrophilic capping layer.

ADSORPTION OF Nd ON THE Mo (110) FACE.

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The adsorption of Nd on the Mo (110) have been investigated by low energy electron diffraction (LEED) , Auger electron spectroscopy (AES) and work function change measurements ($\Delta\Phi$). LEED patterns shows that linear chain structures of adatoms commensurate to the surface were formed. At temperature 300 K variety of adsorbed structures were observed: (18x2); (14x2); (11x2); (10x2); (8x2); (6x2) and (4x2), which were appearing one after other with increasing coverage. At higher temperatures additionally structures were observed: (17x2), (13x2), (12x2) and (7x2). In every studied case after (4x2) structure (5x3) was observed and then appeared non-commensurate hexagonal structure of Nd. An numerical calculations indicates that Nd atoms were forming zigzag chains which correspond to lower total energy of occupied adsorption sites. Diffraction patterns produced by zigzag chains were numerically simulated using kinematic approximation.

SPECTROSCOPIC ELLIPSOMETRY STUDY OF THE DIELECTRIC RESPONSE OF Au-In AND Ag-Sn THIN-FILM COUPLES

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Ultrathin metallic multilayers and intermetallic compounds are recently of great interest due to their application in modern branches of technology. The most promising candidates for modern joints in the microelectronic and optoelectronic devices are diffusion solders formed of noble metals and indium and noble metals and tin.

In this work, the optical properties in terms of the complex dielectric function ($\mathcal{E}(E) = \varepsilon_1(E) + i\varepsilon_2(E)$) of In/Au and Sn/Ag composite layers created during interdiffusion of elements were determined from ellipsometric quantities Ψ and Δ measured in the photon energy range 0.6-6.5 eV at different angles of incidence. Pure metal layers were deposited sequentially in a vacuum for the proper film composition In(Sn):Au(Ag)=1:2. The XRD patterns indicated formation of intermetallic phases in the samples at room temperature, mainly the AuIn₂ and Ag₃Sn intermetallic compounds were found. The free-carrier parameters and optical resistivity were evaluated using a semiclassical Drude-Lorentz model of the dielectric function. There was noticed a significant dependence of the optical resistivity on sample composition and its microstructure.

ABSENCE OF CO DISSOCIATION ON Mo: TPD AND DFT STUDY

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The problem of the CO dissociation on Mo surfaces has been addressed by means of temperature-programmed desorption (TPD) and density-functional (DFT) calculations. The TPD spectra show a first-order CO desorption, which indicates the desorption from a "virgin" state, not a recombinative form of desorption. The height of the potential barrier for the dissociation (~ 2.8 eV), estimated from DFT calculations, substantially exceeds the energy of CO chemisorption (~ 2.1 eV), which makes the thermally induced CO dissociation on Mo improbable. Monte Carlo simulations of TPD spectra, performed using estimated chemisorption energies, are in good agreement with experiment and demonstrate that the two-peak shape of the spectra can be explained without involving the CO dissociation. Thus, the results of the present study finally refute the concept of a dissociative form of CO adsorption on Mo surfaces.

MAGNETIC ANISOTROPIES AND NATURE OF THE SPIN-REORIENTATION TRANSITION IN THIN HEISENBERG FILMS

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It was shown experimentally for a variety of systems that the anisotropy characterizing the thin films is extremely sensitive to lattice geometry and film thickness as well as type of substrate. We consider the spin reorientation transition (SRT) in a ferromagnetic Heisenberg system Ni/Cu(100) with different kind of magnetic anisotropies as a function of temperature and Ni film thickness. The Heisenberg type Hamiltonian describing the Ni/Cu(100) system assumes the magnetization vector to precess around the surface normal and its direction is completely determined by two angles of rotation: polar and azimuth. We use the thermodynamic approach to the problem, which is, in general, based on the free-energy functional construction determined by means of internal energy and entropy calculations. The equilibrium values of all parameters characterizing the magnetic properties of the system are obtained by minimizing free energy with respect to these parameters. The sensitivity of the SRT on exchange anisotropy, shape anisotropy and uniaxial anisotropy parameters is then analyzed in details. It is shown that the direction of magnetization is determined by the competition between uniaxial and shape anisotropy. The use of the Valenta model for the thin film description allows us to present the SRT phenomenon in the layer resolved mode. It is shown that interplay between anisotropies can induce non-collinear spin structure in thin magnetic films.

[1] M. Farel, B. Mirwald-Schulz, A.N. Anisimov, W. Platow, K. Baberschke, Phys. Rev. B 55 (1997) 3708.

PECULIARITIES OF Pb WETTING LAYER ON Si(111)-7×7

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The thickness of the wetting layer on Si(111)-7×7 substrate strongly depends on the substrate temperature. It spans from 1.3 ML at room temperature up to 6 ML at 18K. This wetting layer plays an essential role in formation of crystalline nanostructures of Pb. It includes phenomena known as islands “magic height” [1], formation of crystalline Pb nanowires arrays on vicinal surfaces [2], and unusual type of surface diffusion [3].

Here we present Angle Resolved Photoemission Spectroscopy (ARPES) studies of the Pb wetting layer supplemented by Scanning Tunneling Microscopy (STM), “*in situ*” electrical conductivity, and Reflection High Energy Electron Diffraction (RHEED) measurements.

Photoemission data reveal almost dispersion less band with high density of states at the Fermi level. Between the Fermi level and binding energy of 5eV there are bands with weak dispersion introduced by the presence of wetting layer and strongly dispersive band of bulk silicon. The high density of states at the Fermi level suggests metallic character of the layer, that is confirmed by low electrical resistivity equal to $1.6 \times 10^{-4} \Omega \text{cm}$ at 180 K. STM images of the thinnest films reveal grainy structure commensurate with Si(111)-7×7 substrate reconstruction. The RHEED measurements of thicker film show diffraction pattern characteristic of amorphous-like material.

This work has been supported by the Grant No N N202 1468 33 of Polish Ministry of Education and Science.

[1] K. Budde, E. Abram, V. Yeh, M.C. Tringides, Phys. Rev. B 61 (2000) R10602.

[2] M. Jałochowski, E. Bauer, Surf. Sci. 480 (2001) 109.

[3] M. Hupalo, M.C. Tringides, Phys. Rev. B 75 (2007) 235443.

LOCALIZED VS CHARGE-TRANSFER EXCITED STATES OF CATECHOL AND POLYACENE DERIVATIVES ADSORBED ON TiO₂ AS PHOTSENSITIZERS

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The extensive investigations of the molecule-solid interaction with the participation of molecular electronic excited states stems from the prospects of the possible applications of dyes to produce new type photocells and the useful solid state photocatalysts. The adsorption capacity and energetics of electronic states make the nanoparticles of TiO₂ dioxide very promising in this respect [1].

The interpretation of valuable spectroscopic observations for these systems requires the knowledge of the involvement of the oxide's metal atoms into the excited state orbital. This paper presents the experimental data which enable an assessment of the excited state delocalization. This is obtained with electroabsorption, an adequate spectroscopic technique which provides the differences between the dipole moments ($\Delta\mu$) and polarizabilities ($\Delta\alpha$) between the ground and excited states of the adsorbed dye. The electronic structure of the excited state of adsorbed dyes has not been directly addressed by experiment as yet. We examined several dyes [2] which are tentatively considered to form charge-transfer excited state on TiO₂ surface.

The main results of our work are the quantitative characterization of excited state delocalization in organic molecules adsorbed to TiO₂ and its dependence on the surface electric field. These data provide new detailed insights into the electronic excited state.

[1] M. Grätzel, Chem. Rev. 95, (1995) 49.

[2] A. Nawrocka, A. Zdyb, S. Krawczyk, Chem. Phys. Lett. (2009) in press.

ADSORPTION OF ISOPROPANOL ON Si(100) AND Si(110) SURFACES

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Alcohol additives to KOH-based systems for etching silicon wafers have been widely employed in microelectronics for a long time. It has been reported that the additive of IPA modifies the anisotropy of the etching process, which results in reduction of etch rates of (hkl) type planes, but does not reduce etch rates of (hll) planes [1]. In order to better understand the formation process of the IPA/silicon interface, we concentrated on the adsorption of isopropanol on Si(100) and Si(110) surfaces under ultra-high vacuum conditions. Low energy electron diffraction and scanning tunneling microscopy were employed to examine the IPA adsorption on these silicon surfaces at room temperature. It was found that the adsorption rate of IPA on the Si(100) plane is lower than that of the Si(110).

[1] I. Zuber, M. Kramkowska, Surf. Sci. 602 (2008) 1712.