

ABSTRACTS OF ORAL CONTRIBUTIONS

in alphabetical order of the presenting author's name

FORMATION OF MONODISPERSE (WO₃)₃ CLUSTERS ON TiO₂(110)

A. Bondarchuk*, L-S. Wang, J.M. White

Centre for Materials Chemistry, Texas Materials Institute, University of Texas, Austin, TX 78712, USA

X. Huang, J. Kim, B.D. Kay, Z. Dohnalek

Fundamental Sciences Directorate and Institute for Interfacial Catalysis, Pacific Northwest National Laboratory, P.O. Box 999, M/S K8-88, Richland, WA 99352 USA

**Current address: SPECS GmbH, Voltastr. 5, 13355 Berlin, Germany*

In this study, we employed a qualitatively different deposition approach, which involved direct sublimation of tungsten trioxide, and prepared monodisperse WO₃ clusters on TiO₂(110). On the basis of atomically resolved imaging, X-ray photoelectron spectroscopy (XPS), mass balance of deposited WO₃, and supporting theoretical calculations, we conclude that the clusters are cyclic (WO₃)₃. To our knowledge, this is the first successful attempt to form monodisperse oxide clusters supported on another oxide. As such, this system shows great promise as an ideal platform for reactivity studies on well-defined supported model transition-metal oxide catalysts.

OXYGEN MEDIATED STRIPE-LIKE (1×5) Cu SUPERSTRUCTURE ON Ru (10 $\bar{1}$ 0)

J. Brona, A. Ciszewski

Institute of Experimental Physics, University of Wrocław, Plac Maksa Borna 9, 50-204 Wrocław, Poland

Currently, single-crystalline oxygen-rich ruthenium surfaces are intensively investigated. Several papers have recently been published yielding results of basic and applied research, in particular in catalysis [1]. These systems promise new applications in catalysis because the catalytic activity of oxygen-covered metal surfaces is often enhanced even by 2–3 orders of magnitude compared to the oxygen-deficient surface [2].

Formation and development of recently obtained on Ru(10 $\bar{1}$ 0) new (1×5) epitaxial superstructure of Cu has been studied [3]. Due to annealing, Cu deposited at room temperature on Ru(10 $\bar{1}$ 0) surface precovered with 1 monolayer oxygen evolves into a highly regular (1×5) superstructure. After heating at 850 K the superstructure is fully developed. The driving force behind the phenomenon is misfit strain between Cu adlayer and the substrate. The presence of oxygen adlayer is necessary to mediate the reconstruction. The experiment was performed using the scanning tunnelling microscopy (STM) and low-energy electron diffraction (LEED) techniques under ultrahigh vacuum (UHV) conditions. Physico-chemical features of the structure make the system to be of interest to catalysis and surface chemistry.

[1] see for example: D.W. Goodman et al., Surf. Sci. 601 (2007) L124; J. Assmann et al., J. Phys.: Condens. Matter 20 (2008) 184017; H. Over et al., Surf. Sci. 601 (2007) 5659; S. Zweidinger et al., J. Phys. Chem. C 112 (2008) 9966; N. Lopeza et al., J. Catal. 255 (2008) 29.

[2] M.S. Chen, Y. Cai, Z. Yan, K.K. Gath, S. Axnanda, D.W. Goodman, Surf. Sci. 601 (2007) 5326.

[3] J. Brona, A. Ciszewski, Surf. Sci. 603 (2009) 945.

FIM STUDIES OF OXYGEN CAUSED THERMAL FACETING OF IRIDIUM AND PALLADIUM MICROCRYSTALS

R. Bryl, T. Olewicz

Institute of Experimental Physics, University of Wrocław, Plac Maksa Borna 9, 50-204 Wrocław, Poland

N. Kruse

Universite Libre de Bruxelles, Chimie Physique des Materiaux, Campus de la Plaine CP 243, B-1050 Bruxelles, Belgium

It is known that the adsorption of oxygen on metal surfaces can lead to considerable morphological changes of the metal crystal. Even small amounts of oxygen (corresponding to exposure of at least 0.5 Langmuir) were previously found to induce faceting of W(111) after heating at temperatures in the range of 800 K – 1800 K. In the case of fcc metals, oxygen-caused faceting was observed on (210) planes (Ir, Pt, Cu, Ni). Faceting of platinum group noble metals has been studied recently for their role in numerous applications of heterogeneous catalysis.

Field Ion Microscopy seems to be a suitable tool for studies of adsorbate-caused thermal faceting of metals. The specimen – metal tip of small radius of curvature – can be regarded as a good model of a morphologically diversified particle of a real catalyst grain.

In this presentation we want to demonstrate how oxygen-preadsorbed surfaces of palladium and iridium microcrystals develop during annealing. Faceting of an Ir [100] tip was observed after annealing at temperatures of at least 650 K when the tip was exposed to 2 or more Langmuirs of oxygen. We observed the existence of well developed {110}, {113}, {111} and {100} planes and sharp edges between them. The shape of the tip after oxygen-caused faceting will be compared to the shape obtained in the process of annealing without oxygen preadsorption. In case of a palladium tip exposed to oxygen (2–6 L) facets started to develop at temperatures as low as 500 K. It was found that the shapes obtained for palladium were considerably different from those obtained for iridium tips.

UPS AND PAX INVESTIGATIONS OF BIMETALLIC Au-Pt(111) SURFACES

T. Kobiela^{1,2}, M. Moors¹, W. Linhart³, I. Cebula³, A. Krupski³, C. Becker¹, K. Wandelt¹

¹*Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstraße 12, D-53115 Bonn, Germany*

²*Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland*

³*Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland*

Investigations of bimetallic systems concerning morphology and adsorption properties are of great interest for the development of new catalysts with higher efficiency and durability. The structure and the local electronic properties of ultrathin Au films deposited on Pt(111) and annealed at different temperatures have been studied by Ultraviolet Photoelectron Spectroscopy (UPS), Photoemission of Adsorbed Xenon (PAX) and Low Energy Electron Diffraction (LEED). The LEED measurements indicate an initial pseudomorphic growth of the Au films. The UPS and PAX experiments demonstrate a strong temperature dependence of the surface morphology. The surface covered with Au at 150 K is quite rough but smoothens significantly above room temperature. At a temperature of 750 K intermixing and the formation of an Au-Pt surface alloy starts at the interface. The electronic properties of the resulting Au-Pt surface alloy seem to be nearly independent from the originally deposited Au amount in the investigated range of 1–10 monolayers. The removal of Au from the surface regions has also been verified by Scanning Tunneling Microscopy. Adsorption experiments with CO as a titration agent show a significantly lower affinity of the Au-Pt surface alloy in comparison to the clean Pt surface.

STM/STS CHARACTERIZATION OF THE DEFECTS AND Ti CLUSTERS ON THE Si(100) SURFACE

W. Koczorowski, M. Bazarnik, M. Cegiel, R. Czajka

Institute of Physics, Faculty of Technical Physics, Poznan University of Technology, Nieszawska 13 A, 60-965 Poznan, Poland

Silicon and metal silicides are commonly used in nanoelectronic technology, in which the Si(100) surface is often used. Periodic buckled dimers structure characteristic for Si(100)-(2x1) surface reconstruction was studied earlier by theoretical and experimental methods. It is also known that titanium silicides grow in two, thermodynamically stable phases: C49 with high resistance and C54 with low resistance [1].

We have performed an STM/STS investigations of Si(100) and Ti clusters grown upon deposition of over 1 ML on the surface by the solid state epitaxy. Nanostructures of the titanium silicides in the C54 phase were observed after sample annealing at 970K temperature. The STM images show symmetrical, spherical nanostructures of the titanium silicides with lateral dimensions up to 20 nm and two nanometers in height. Additionally the I-V curves and CITS maps were recorded for both surface and nanostructures revealing different electronic properties for the substrate and nanostructures. We have also observed the lines of defects in the dimers structure on the Si(100) substrate. We believe that these line defects should allow formation of the titanium silicides nanowires (in the phase C49).

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Ag CHAINS ON HIGHLY ORDERED Si(557) SURFACE

M. Krawiec, M. Jałochowski

Institute of Physics, M. Curie-Skłodowska University, pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

An attractive route to create nanostructures with reduced dimensionality is a process of self-organization of atoms into very regular arrays of parallel metallic chains on stepped (vicinal) Si surfaces. Those surfaces are often decorated with gold, which stabilizes them and allow to grow one dimensional structures on them [1]. The Si(557) surface stabilized by deposition of 0.2 ML of Au is one of these systems [1-4]. The terraces of this surface are formed from (111) facets and have a width of 1.92 nm. Each terrace contains a row of gold atoms running parallel to the step edge. However, scanning tunneling microscopy (STM) shows two non-equivalent chains, one associated with step edge Si atoms, and the other one with Si adatoms in the middle of terrace [2-4]. The surface may serve as a template for growing other monoatomic chain structures.

Here we report on Ag chains fabricated on Si(557)-Au surface. We have applied STM and STS to study structural and electronic properties of monoatomic Ag chain structures. The STM and STS data show that presence of silver atoms significantly modifies structural and electronic properties of the Si(557)-Au surface. The experimental results are supplemented by density functional theory (DFT) calculations, which allowed to find a structural model of Ag chains on Si(557)-Au surface, as well as to explain STS characteristics. The DFT calculations remain in good agreement with all the available experimental data.

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[2] J. N. Crain *et al.*, Phys. Rev. B 69 (2004) 125401.

[3] M. Krawiec *et al.*, Phys. Rev. B 73 (2006) 075415.

[4] S. Riikonen, D. Sanchez-Portal, Phys. Rev. B 76 (2007) 035410.

STRUCTURAL AND ELECTRONIC PROPERTIES OF GOLD OVERLAYERS ON THE MOLYBDENUM (112) SURFACE

N. Lozova, Ya.B. Losovyj, J. Scott

Center for Advanced Microstructures and Devices of Louisiana State University, 6980 Jefferson Highway, Baton Rouge, LA 70806, USA

S.M. Zuber

Institute of Experimental Physics, University of Wroclaw, pl. M. Borna 9, Wroclaw, Poland

K. Fukutani, P.A. Dowben

Department of Physics and Astronomy and the Nebraska Center for Materials and Nanoscience, 116 Brace Laboratory, University of Nebraska, P.O. Box 880111, Lincoln, NE 68588, USA

Atomic-scale structure of the growth of a gold film on (112) plane of Mo single crystal were investigated by means of low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) over up to 3 monolayers (ML) of gold coverage. Both LEED and STM results establish that the gold grows on Mo(112) in a layer-by-layer mode, for at least the first two monolayers of gold. Both the first and second layers adopt the Mo(112) 1x1 surface structure upon completion. With growth of the third gold monolayer a three-dimensional growth mode becomes manifests.

During first monolayer growth gold film consists of atomic wires running along the Mo(112) corrugation and repeating substrate lattice constant. The wires are randomly separated across substrate rows up to coverage 0.66 ML where a 3x1 missing row structure surface structure is adopted followed by 1x1 structure for complete first monolayer. The second gold layer exhibits island growth of a 4x1 structure, which “fills in” as the coverage increases to 1.5 ML. This latter structure is consistent with paired atomic wires separated by two empty rows. The 3x1 missing row structure at 1.66 ML coverage is seen but coexists with the LEED signature of 4x1 structure. The 4x1 structure is followed by 5x1 structure and form at 1.75 and 1.8 monolayers of gold respectively.

The band mapping of the electronic structure along the gold atomic wires, constructed from angle-resolved photoelectron spectroscopy, reveals the changes in the band structure details in spite of an intra-wire lattice that remains constant independent of coverage and critical points consistent with the $[1\ 1\ \bar{1}]$ Mo(112) lattice constant. The changes in band structure are due to changes in spacing between the atomic gold chains, which decrease as coverage increases. Perturbation of the surface charge density of the Mo(112) surface in the submonolayer regime is certainly implicated.

STM STUDY OF SUPRAMOLECULAR ORGANIZATION IN POLY(DIALKYLTER-THIOPHENES)

R. Nowakowski, T. Jaroch, A. Maranda-Niedbała

Polish Academy of Sciences, Institute of Physical Chemistry, Kasprzaka 44/52, 01-224 Warszawa, Poland

M. Zagórska

Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, 00-664 Warszawa, Poland

A. Proń

CEA-Grenoble, INAC, 17 rue des Martyrs, Grenoble 38054, France

The possibility of precise tuning of the electronic and optoelectronic properties of organic semiconductors by their chemical modification is an important advantage of organic electronics. However, another factor which seriously influences the final properties of organic electronic devices is the active material supramolecular organization. Significant progress in this field is expected to be reached by the use of well-defined ordered thin organic layers. Elucidation of the interchain interactions which have a strong effect on the resulting supramolecular structures is therefore essential for the optimization of such systems.

Here we present the results of STM studies of poly(dialkylterthiophenes), a family of polymers of potential use in the fabrication of organic field-effects transistors. The microscopic observations of monomolecular layers on HOPG processed from monodispersed fractions of different molecular mass have been compared for polyterthiophene derivatives with different positions of the alkyl side groups in the repeat unit. Two problems of crucial importance have been addressed: i) the evolution of their 2D structure caused by increasing length of the macromolecule and ii) the effect of the position of the alkyl substituent on this supramolecular organization. The position of the alkyl substituent in the molecule turns out to be the key parameter which determines the resulting structure *via* different patterns of the side groups interdigitation. Expected consequences of this effect on the electronic properties of the layer are also discussed.

GOLD NANOSTRUCTURES ON DEFECTED RUTILE TiO₂(110)

T. Pabisiak, A. Kiejna

Institute of Experimental Physics, University of Wrocław, Plac M. Borna 9, 50-204 Wrocław, Poland

The discovery of enhanced catalytic properties of dispersed gold nanoparticles on oxide supports have attracted a lot of interests on adsorption of gold atoms on rutile TiO₂ surfaces. Experimentally, it has been proposed that one-dimensional Au structures can be formed in a controlled manner, using ordered oxygen vacancies created on a TiO₂(110) surface during irradiation [1]. We examine from first principles the adsorption of small Au aggregates (atomic rows and clusters), of a size ranging from a monomer to a dozen of Au atoms per cell, on a partially reduced rutile TiO₂(110). The calculations apply density-functional theory, plane wave basis, and the projector augmented wave method. Our previous results for the infinite monomer, dimer, and triple Au rows [2] are extended to thicker infinite-rows, as well as finite rows, and the three-dimensional clusters [3]. The discussion is focused on the structure and bonding of one-dimensional Au rows on the missing row defected TiO₂(110) surface and their comparison with the respective properties of Au clusters and finite rows adsorbed on the partially defected bridging O row. The calculations show a strong bonding to the substrate and the metallic nature of the Au rows. The adhesive bonding of gold clusters to the vacancy defected bridging oxygen row at the TiO₂(110) is of covalent nature. We examine electron charge transfer and discuss the charging of rows and clusters and their dependence on the gold-structure size. Our results provide an insight into the nature of Au-Ti bond, the role of oxygen vacancies, and the amount of deposited metal on the observed electronic properties, and the growth behavior of the Au nanostructures on TiO₂(110).

[1] A. Locatelli et al., J. Phys.: Condens. Matter 19 (2007) 082202.

[2] T. O. Montes et al., Phys. Rev. B 76 (2007) 155413.

[3] T. Pabisiak, A. Kiejna, Phys. Rev. B 79 (2009) 085411.

RESISTIVE SWITCHING IN $\text{Sr}_{1-0.05}\text{La}_{0.05}\text{TiO}_3$

M. Pilch

Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland

K. Szot, W. Speier

Forschungszentrum Juelich, IFF-6, 52425 Juelich, Germany

The analysis of the electronic structure of La-doped SrTiO_3 single crystals, $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ with $x=5$ at % (LSTO), shows that additional electrons in the host matrix are accommodated by a change of the valence of Ti ions from Ti^{+4} to Ti^{+3} . We found, however, no evidence of a metallic peak near the Fermi level by electron spectroscopy. Similarly, electrical characterisation of the material revealed only semiconducting behaviour. This stands in contrast to the general idea of a macroscopic insulator-to-metal transition (I/M-transition) in LSTO at a doping level of a few percent of La. By means of conducting AFM we found evidence of an inhomogeneity of the in-plane conductivity at the nano-scale and the possibility of locally manipulating the electric resistivity by means of an electrical stimuli, i.e. resistive switching. The observed inhomogeneity is attributed to a non-uniform distribution of La doping and a high density of extended defects in LSTO crystal.

Of particular interest is the reversible I/M-transition as it holds great promise in the context of resistive switching and its potential application for Terabit memories. LSTO is widely recognized as model system for substitutional doping in perovskites: its electrical properties ranges from a band insulator, SrTiO_3 , a metallic conductor for $0 < x < 1$ to a Mott insulator, LaTiO_3 . However, the material shows a lack of reproducibility in the conductivity data (see [1], and references therein). In fact, the critical concentration of La for the I/M-transition is not well determined and can vary between 0.001at% and 20at%, depending critically on the preparation conditions. At the same time, the ease with which this material can be driven from one electronic state to another [2] immediately raises the question concerning the stability of the different electronic phases, but also opens the pathway of easily manipulating the electronic properties of the material. This requires a detailed analysis of the different physical and chemical properties at the macro- and nano-scale induced in the perovskite matrix by doping or generated by, e.g., an electrical field.

Further studies demonstrated that the origin of the complicated pattern of electrical conductivity at the nano-scale is accompanied by a very high density of extended defects and a local variation of the concentration of La. TEM investigations of LSTO give evidence that the dominating types of extended defects are stacking faults and elemental analysis (combining EDX, EELS and TOF-SIMS) revealing that the distribution of La is modulated at the nano- as well as at the macro-scale.

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[2] S. Hirose et al., *Journal of Applied Physics* 104 (2008) 053712.

SELFNEUTRALISATION PHENOMENON IN SrTiO₃ SINGLE CRYSTAL

J. Szade

A. Chełkowski Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland

B. Psiuk

Institute of Glass, Ceramics, Refractory and Constructions Materials, Department of Refractory Materials, Toszecka 99, 44-101 Gliwice, Poland; A. Chełkowski Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland

M. Pilch

A. Chełkowski Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland

K. Szot

Institute of Solid State and CNI – Center of Nanoelectronic Systems for Information Technology, Research Center Jülich GmbH, 52425 Jülich, Germany; A. Chełkowski Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland

It is known that for XPS (X-ray Photoelectron Spectroscopy) measurements on insulating materials neutralization with use of electron gun is necessary. Otherwise photoemission from insulating materials leads to charging effect what can be visible as gradual shifts of XPS spectra towards higher values on binding energy scale (after appropriately long time the process reach equilibrium). The presence of the band gap of 3.2 eV in undoped SrTiO₃ causes that it can be included to insulators. However our photoemission studies show that for insulating samples of SrTiO₃ after a long enough time of exposure to soft x-rays the position of photoemission lines tends aback to the standard position established in experiments with proper neutralization. This new and surprising effect we called selfneutralisation. Series of experiments allowed us to relate the observed phenomenon to the gradual increase of conductivity through the bulk sample. In our opinion this increase should be connected to conducting filaments found earlier in SrTiO₃ single crystals [1].

[1] K. Szot, W. Speier, G. Bihlmayer, R. Waser, *Nature Materials* 5 (2006) 312.

FUNCTIONALIZATION OF ZnO NANOWIRES FROM FIRST-PRINCIPLES CALCULATIONS

A.L. Rosa, Th. Frauenheim

University of Bremen, Am Fallturm 1, 28359 Bremen, Germany

Nanostructures offer novel and unique properties to fabricate bio-sensors, because the dimension of such structures are similar to those of the target molecules. ZnO is a well known bio-friendly semiconductor with potential applications in electronics and biosensing, In this work we employ density functional theory to investigate ZnO nanowires and nanotubes. We find that the band gap of bare wires decreases as the size of the nanowire increases, revealing strong quantum confinement effects [1]. We have further investigated ZnO nanowires functionalized with H and OH groups [1]. We find that the conductivity of these wires can be tuned from semiconductor to metallic, depending on how hydrogen and functional groups adsorb on the nanowire surfaces. Furthermore, we show that thick-walled ZnO nanotubes are energetically more favorable than single-walled ones. The formation energies of thich-walled ZnO hexagonal ZnO nanotubes are mainly dependent on the thickness of the wall but not on the tube diameter [2].

[1] W. Fan, H. Xu, A.L. Rosa, Th. Frauenheim, R.Q. Zhang, *Phys. Rev. B* 76 (2007) 073302; *Phys. Rev. B* 79 (2009) 073402.

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THORNY WAY TOWARDS EQUILIBRIUM: KINETIC BARRIERS IN THE THERMAL EVOLUTION OF OXYGEN-COVERED TUNGSTEN CRYSTAL

A. Szczepkiewicz

Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland

In this presentation I report on the recent experimental findings about time effects in the thermal evolution of oxygen-covered tungsten crystals. I discuss obstacles to the microscopic observation of the equilibrium surface topography:

- it is not enough to wait “long enough” at a given temperature,
- it is not enough to freeze the surface configuration “very fast” (6000 K/s).

I estimate the time of the formation of W{211} pyramids, and calculate the exponent describing the growth in time of the W{211} steps.

Cr-INDUCED COHESION CHANGES IN Fe GRAIN BOUNDARIES

E. Wachowicz, A. Kiejna

Institute of Experimental Physics, University of Wrocław, Pl. Maxa Borna 9, 50-204 Wrocław, Poland

The mechanical properties of macroscopic polycrystalline iron are to much extent governed by cohesion at grain boundaries (GBs) which, in turn, is highly dependent both on the local atomic structure and impurities segregated to the GBs. Iron and chromium form a perfect solid solution which is ferromagnetic to quite low concentrations of iron.

We present results of extensive first principles calculations of structural, cohesive, and magnetic properties of two symmetric tilt grain boundaries in pure bcc Fe and in dilute FeCr alloys. Different concentration and position of Cr solute atoms are considered. Our calculations show that Cr atoms placed in the GB interstice enhance the cohesion by 0.5-1.2 eV, depending on concentration. Substitutional Cr in the layers adjacent to the GBs shows anisotropic effect on the GB cohesion: it is neutral when placed in (111) oriented Fe grains, and enhances cohesion (by 0.5 eV) when substituted in the boundary layers of the (210) grains. The strengthening effect of the Cr solute is dominated by the chemical component of the GB energy. We found that unlike the free iron surfaces, Cr impurities in Fe grains segregate to the boundaries. The magnetic moments on GB atoms change meaningfully. The variation of the magnetic moment at the atoms in the vicinity of the boundary correlates with the corresponding lattice relaxation pattern.

VALENCE OF "DIVALENT" RARE EARTH METALS

I.N. Yakovkin

Institute of Physics, National Academy of Sciences of Ukraine, Prospect Nauki 46, Kiev 03028, Ukraine

It is generally recognized that light rare earths change their valence from 2 to 3 when forming a bulk metal. In particular, the Sm is believed to be trivalent in the bulk and divalent at the surface and even can have an intermediate valence. However, the avowed concept of the different bulk and surface valence of rare earth metals is inherently controversial. Any surface cannot be separated from the bulk, and therefore the surface electronic structure cannot be considered independently. Because of the *s-d-f* band hybridization in the "divalent" rare earth metals, the *f* band must be considered as a part of the valence band. As such, the *4f-5d* transition cannot change the valence, which should be defined as the number of all electrons in the *s-d-f* valence bands. The possibility of alternative interpretation of UPS spectra of the "divalent" rare earths (Pr, Nd, Sm, and Eu) is illustrated by DFT/GGA calculations of local densities of states for excited atoms in the crystal lattice. In particular, the appearance of the -5.3 eV peak in photoemission spectra for Sm, obtained with higher photon energies, is attributed to excitations induced by impinging radiation.

SCATTERING POTENTIALS AT IMPURITY DIMERS AND ATOMIC SWITCH DESIGN ON Ge(001) AND Si(001): FIRST-PRINCIPLES STUDY

B. Yan

BCCMS, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany; Center for Advanced Study, Tsinghua University, 100084 Beijing, China

K. Tomatsu, F. Komori

Institute for Solid State Physics, The University of Tokyo, 5-1-5, Kashiwanoha, Kashiwa-shi, Chiba 277-8581, Japan

G. Zhou, W. Duna

Department of physics, Tsinghua University, 100084 Beijing, China

A.L. da Rosa, T. Frauenheim

BCCMS, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany; Center for Advanced study, Tsinghua University, 100084 Beijing, China

On the Si/Ge (001) surface, Si/Ge atoms form buckled dimers with π and σ bonds. The dimers line up and make a dimer row. The π^* band lies in the bulk gap and localizes at the lower atom of the dimer. It behaves as a 1D conduction channel along the dimer row. By controlling the conduction of π^* electrons using the buckled Sn-Ge dimer on Ge(001), Tomatsu *et al.* have fabricated an atomic switch using STM (Science 315 (2007) 1696). Collaborated with Tomatsu *et al.*, we investigated the *ON/OFF* mechanism of the atomic switches. Using first-principles method we calculated the scattering potentials induced by different impurity dimers and obtained good agreement with STM phase shift measurements. We further studied the switch mechanism related with dimer flip motion by electron injection from STM tip. We propose that the flip motion is caused by a resonant scattering of the π^* electrons with localized electronic states. On the other hand, we studied theoretically the scattering by impurity dimers on Si(001) and proposed that it is possible to fabricate good atomic switches using X-Si (X=Ge, Sn and Pb) impurity dimers.

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[2] K. Tomatsu, B. Yan *et al.* Phys. Rev. B 78 (2008) 081401(R).

[3] B. Yan, K. Tomatsu *et al.*, submitted.

MAGNETIZATION AND STRUCTURE OF ULTRATHIN Fe FILMS

R. Zdyb

Institute of Physics, Maria Curie-Skłodowska University, Pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

E. Bauer

Department of Physics, Arizona State University, Tempe, Arizona, AZ 85287-1504, USA

T.O. Mentes

Sincrotrone Trieste, S.S. 14 km 163.5, 34012 Basovizza (TS), Italy

The structure, morphology and magnetic properties of iron films grown on Au layers with different thickness on a W(110) surface are investigated with spin polarized low energy electron microscopy and low energy electron diffraction. The iron thickness of the onset of ferromagnetic order depends approximately linearly on the thickness of underlying gold film. The easy axis direction also depends upon Au thickness. It is parallel to the tungsten $[1\bar{1}0]$ direction at the onset of magnetization for one and two monolayers (ML) of gold. In the latter case, right after the onset of magnetic order which occurs at about 1.6 ML Fe, spin reorientation transition starts and the easy axis rotates towards $[001]$, being most close to it between 2 and 4 ML Fe. Above 4 ML it rotates back towards the $[1\bar{1}0]$ direction reaching 25° off the $[001]$ axis at about 7 ML. Then it rotates again to the $[001]$ direction where it remains for larger thicknesses. For thicker gold films the easy axis is parallel to the $[001]$ direction from the onset of ferromagnetic order.

The observed changes of the direction of the easy axis and the onset of ferromagnetic order are discussed in terms of magnetic anisotropies, interaction between iron overlayer, gold and tungsten substrate, Fe film crystallographic structure and morphology.