O 65: Poster Wednesday: Surface Structure, Epitaxy and Growth

Time: Wednesday 17:45–20:00 Location: Poster B1

O 65.1 Wed 17:45 Poster B1

Polymorphic expressions of ultrathin oxidic layers of Mo on Au(111) — Taehun Lee[1], Yun-Jae Lee[1], Krisztián Palotás[2], Catherine Stampfl[3], and •Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary — [3]School of Physics, The University of Sydney, NSW, 2006, Australia

Ultrathin oxidic layers of Mo (O/Mo) on the Au(111) support have been investigated using first-principles density-functional theory calculations. Various polymorphic structural models of these O/Mo layers are proposed and compared with previous experimental results – covering both spectroscopic and microscopic approaches of characterization. We find that, through the control of metal-oxygen coordination in these ultrathin oxidic O/Mo films on Au(111), the oxidation state of Mo atoms in the O/Mo layers can be modulated and reduced without intentional creation of oxygen vacancies. This is also assisted by a charge transfer mechanism from the Au substrate to these oxidic films, providing a direct means to tune the surface electronic properties of ultrathin oxide films on metal substrates.

O 65.2 Wed 17:45 Poster B1

Structural investigation of strain induced effects in a Dy-Ag surface alloy — •Sina Mousavion[1], Johannes Seidel[1], Lu Lyu[1], Maniraj Mahalingam[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany

Studies of intermetallic compounds using lanthanide metals on noble metals have been subject of numerous studies due to their tunable structure as well as their electronic and magnetic properties [1]. In this study we focus on the structural properties of a Dysprosium-Ag surface alloy formed on the Ag(111) surface. Using LEED and STM, we observe the formation of a short range ordered Dy-Ag structure with an additional Moiré-like pattern. This is in contrast to most surface alloys which usually form a uniform Sqrt(3)xSqrt(3) structure on Ag(111). This intriguing surface structure can be explained by a non-uniform lattice strain in the adsorbate system due to the size mismatch of Dy and Ag. We propose that the formation of a Moiré pattern of the surface alloy can be used to control the structure formation of adsorbates on this surface alloy. [1] e.g., Nano Lett., 16, 4230-4235 (2016)

O 65.3 Wed 17:45 Poster B1

Two-dimensional CuI on Cu(111): A first-principles investigation — •Giyeok Lee, Taehun Lee, and Aloysius Soon — Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea

Of late, copper iodide (CuI), a *p*-type transparent semiconductor at room temperature, has been proposed as a choice material for various potential applications – from a hole conductor to a bipolar diode, forming a two-dimensional heterojunction with various *n*-type materials. However, the controlling the atomic structure of ultrathin (or interfacial) CuI layers for these targeted applications is challenging due to the existence of various polymorphic expressions (γ – zincblende structure as thermodynamic product, β – hexagonal phase, and α – rocksalt structure). The structures of ultrathin layers are determined by the orientation of metal substrates (e.g. Cu(100) and Cu(111)) and the surface coverage of precursors (e.g. $I_{2\,(g)}$ or $KI_{\,(aq)}$) used. In this work, we have performed van der Waals-corrected density-functional theory calculations to examine the initial/early stages of CuI ultrathin film formation on Cu(111) within the framework of *ab initio* atomistic thermodynamics, and report detailed surface atomic structures with their associated surface thermodynamics and electronic structure properties.

O 65.4 Wed 17:45 Poster B1

In-situ analysis of ultra-thin alkali metal films using optical transmission spectroscopy — •Hendrik Mathies Wrigge, Thomas Dziuba, Joerg Malindretos, Angela Rizzi, and Martin Wenderoth — IV. Physikalisches Institut, Georg August Universität Göttingen, Germany

Controlling the thickness of ultra-thin alkali metal films is a challenging task. Standard calibration techniques using e.g. ambient AFM, fail due to the high chemical reactivity of these metals. In this contribution, we present an alternative approach based on an in-situ optical transmission spectroscopy. Films are prepared by depositing pure alkalimetal from a dispenser on a glass substrate under UHV condition. While deposition, the optical transmission of the film is measured over a broad spectral range from 300 nm up to 1000 nm continuously (30 second per spectrum). We analyze distinct spectral features, which change according to the film thickness. Applying the scattering theory of non-spherical particle [1,2], the spectral features can be assigned to the film thickness and its nanoscopic structure. For comparison, we measured thin Ag films in the same setup. For Ag films, thickness as well as the structure is analyzed using AFM. In summary, our optical setup is able to measure deposition rate down to submonolayers per minute.

Work supported by DFG through SPP 1666

Reference: [1] K. Lance Kelly *et al.*, J.Phys. Chem. B, 107, 668-677 (2003) [2] Luis J. Mendoza Herrera *et al.*, Journal of Applied Physics 116, 233105 (2014)

O 65.5 Wed 17:45 Poster B1

Verkleinerung der mechanischen Spannungen im System <Aluminium-Anodenoxid des Aluminiums> — Basov Georgi und •Vladimir Schulgov — Belorussische Staatliche Universität für Informatik und Radioelektronik(BSUIR) Brovka Str. 6 BY 220013 Minsk Belarus

Das Aluminium und seinen Anodenoxid stellen die mehrschichige Struktur mit verschiedenen Eigenschaften von den Materialien vor. Im Laufe der Herstellung und der Betrieb können in ihr die thermischen Spannungen entstehen, die zur Übertretung der Ganzheit von Isolationsdeckung führen.

Im Laufe des Wachstums an der Trennungsgrenze Al - Al2O3 entsteht die Zone der plastischen Deformation des Aluminiums, in der die Relaxation des Teiles von der elastischen Spannungen geschieht. Sie ist ungefähr drei Radien des Zellegrunds vom porösen Oxids gleich. Der Zelledurchmesser des porösen Oxids nimmt proportional zur Anodisierungsspannung zu. Deshalb muss man die poröse Anodisierung bei den grossen Grössen der Anodisierungspannung durchführen.

Die vergleichende Einschätzung des Niveaus der thermischen Spannungen in den Filmen führten nach der Messung der Probedurchbiegung durch, der in die inneren Spannungen im Temperaturbereich 298 - 623K nachgerechnet wurde.

Schlussfolgerungen: Die Zusätze der Oberflächenaktivstoffen lassen mehr als in 2 Male die Größe der Durchbiegung und in 10 Male das Niveau der Spannungen zu verringern, die bei den Hochtemperaturbehandlungen an der Trennungsgrenze Al - Al2O3 entstehen sind.

O 65.6 Wed 17:45 Poster B1

Growth studies of Fe_3O_4 on $SrTiO_3$(001) by SPA-LEED — •Andreas Alexander, Jascha Bahlmann, and Joachim Wollschläger — Universität Osnabrück Fachbereich Physik, Barbarastr. 7, 49076 Osnabrück

Because of its electric and magnetic properties, Fe_3O_4 (Magnetite) is a promising candidate for spintronic applications, such as magnetic tunneling junctions (MTJs) or magnetic data storage (Magnetoresistive Random Access Memory = MRAM). Previously, magnetite films were grown on lattice matched MgO substrates. Here, we study Fe_3O_4 epitaxy on $SrTiO_3$(001) (lattice mismatch -7.5%) by means of high resolution low energy electron diffraction with spot profile analysis (SPA-LEED) to shed light on strain effects. The magnetite films were grown by stepwise deposition and linescans were performed after each deposition step for different energies.

Due to the lattice mismatch an (111) oriented epitaxial interface layer is observed first. The thickness depends on growth conditions. Thereafter, the magnetite film reorientates and grows with (001) direction. Additionally, the profile analysis of the diffraction spots reveals information about the surface morphology, such as atomic steps, roughness or surface defects.

O 65.7 Wed 17:45 Poster B1

Strain induced enhanced magnetization of ultrathin epitaxial $NiFe_2O_4$ films on $SrTiO_3(001)$ — •Jari Rodewald, Tabea Nordmann, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin epitaxial ferrite films as $NiFe_2O_4$ are in the focus of spintronics owing to their semiconducting and ferrimagnetic properties. Thus, they are well-suited to be used as spin filters due to spin dependent tunneling barrier. Here, the homogeneity of the films is essential to form tunneling barriers. Furthermore, the cation ordering on the different sublattices of the inverse spinel structure determines the magnetic properties of the ferrite films which is crucial for the performance as a spin filter. Therefore, the formation of ferrite films has to be carefully controlled if high quality devices are aimed for.

Hence, in this work ultrathin $NiFe_2O_4$ films of different thicknesses are prepared via reactive molecular beam epitaxy (RMBE) on $SrTiO_3(001)$. Chemical composition and structural ordering at the surface are examined by x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively. In order to investigate structural strain and ordering effects in the films, synchrotron radiation based grazing incidence x-ray diffraction (SR-GIXRD) experiments are performed. Magnetic properties are characterized via superconducting quantum interference device (SQUID) magnetometry, revealing unexpectedly high magnetic moments exceeding bulk values of up to four times for ultrathin films below 13 nm film thickness.

O 65.8 Wed 17:45 Poster B1

Formation of cobalt ferrite by interdiffusion of CoO/Fe_3O_4 bilayers — •Jannis Thien, Jascha Bahlmann, Andreas Alexander, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

With their magnetic and electronic properties thin $CoFe_2O_4$ (CFO) films are among the most promising candidates for the development of spin filters at room temperature, where spin-polarized electron currents are generated due to the spin-dependent tunnelling barrier. Since the efficiency of spin-filtering greatly depends on the band structure of the material and the presence of defects, the fabrication of these films has to be carefully controlled if efficient spin filters are aimed for. To prepare thin CFO films pulsed laser deposition or sputter deposition is commonly used. Another approach of preparing CFO films might be the interdiffusion of CoO/Fe_3O_4 bilayers mediated by post-deposition annealing as recently shown for $NiFe_2O_4$ using Fe_3O_4/NiO bilayers.

Therefore, CoO/Fe_3O_4 bilayers were consecutively grown by reactive molecular beam epitaxy on $SrTiO_3(001)$ and post-annealed at different temperatures afterwards. The film structure and chemical properties of the annealed bilayer system have been studied after each annealing step using synchrotron radiation by means of (grazing incidence) X-ray diffraction and soft/hard X-ray photoelectron spectroscopy, respectively.

The measurements revealed interdiffusion of CoO and Fe_3O_4 films after an annealing temperature of 673K and probable formation of $Co_xFe_{3-x}O_4$.

O 65.9 Wed 17:45 Poster B1

N_2 physisorption on the KCl(100) surface — •Jochen Vogt — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

Molecular nitrogen is known to only weakly interact with ionic materials like NaCl and KCl [1,2]. Experimental information on the adsorbate structures is sparse so far [1]. This contribution compares results from quantitative low-energy electron diffraction (LEED) experiments for these systems. While in the case of N_2/NaCl(100) a p(1×1) symmetry is observed even at the lowest accessible temperature of 20 K, lattice mismatch induced strain causes a different behavior in the N_2/KCl(100) system. Here, the p(1×1) phase transforms into an oblique 2D phase of higher density at elevated N_2 partial pressure and temperatures below 40 K. For the p(1×1) phase, LEED I(V) analysis supports an adsorption site of N_2 on top of Na^+ on the NaCl substrate [1], while on the KCl(100) surface the N_2 molecules appear laterally displaced on the line connecting neighboring cations. This is interpreted in terms of strain-induced structural disorder that causes local coalescence of neighboring molecules. [1] J. Vogt, J. Chem. Phys. **137** (2012), 174705 [2] J. Vogt, H. Weiss, Z. Phys. Chem. **218** (2004), 973

O 65.10 Wed 17:45 Poster B1

From Fe_3O_4/NiO bilayers to $NiFe_2O_4$-like thin films through Ni interdiffusion — •Olga Kuschel[1], Ralph Buss[1], Timo Kuschel[2], Karsten Kuepper[1], and Joachim Wollschläger[1] — [1]Osnabrück University, Germany — [2]Bielefeld University, Germany

Ferrites with (inverse) spinel structure display a large variety of electronic and magnetic properties, making some of them interesting for potential applications in spintronics. Especially, $NiFe_2O_4$ thin films are of huge interest since they are magnetic insulators or semiconductors with spin dependent band gap. Therefore, they can be used as spin filters or for thermal induction of spin currents via the spin Seebeck effect. Furthermore, electrical charge transport and spin currents can be manipulated by the spin Hall magnetoresistance using $NiFe_2O_4$ thin films adjacent to nonmagnetic spin-Hall material.
For this purpose, thermally induced formation of nickel ferrite starting with a distinct Fe_3O_4/NiO bilayer grown on Nb-doped $SrTiO_3(001)$ was investigated. After synthesis a systematic three-step annealing cycle was performed. After each annealing step surface crystallographic and 'bulk' electronic structure changes were investigated by means of low energy electron diffraction (LEED), soft and hard x-ray photoelectron spectroscopy (HAXPES). Furthermore, structural analysis before and after the overall annealing cycle were carried out employing x-ray reflectivity (XRR) and synchrotron-radiation-based x-ray diffraction (SRXRD), as well as element- and site-specific x-ray magnetic circular dichroism (XMCD) to analyze the resulting magnetic properties.
[1] O. Kuschel et al., Phys. Rev. B 94, 094423, (2016)

O 65.11 Wed 17:45 Poster B1

Structures and energetics of surface steps of SiC — •Kaori Seino[1,2] and Atsushi Oshiyama[1] — [1]Institute of Materials and Systems for Sustainability, Nagoya University, Nagoya, Japan — [2]X-Ability Co., Ltd., Tokyo, Japan

Silicon carbide (SiC) is a material of considerable interest due to applications in power semiconductors. Stepped surfaces of SiC are important from the viewpoint not only of a crucial role in epitaxial growth but also of substrates for epitaxial graphene. There exist, however, only a small number of theoretical *ab initio* studies of surface steps of SiC [1].

Here we present density functional theory (DFT) calculations of structural properties and energetics for surface steps of 3C-SiC(111) surfaces. The calculations are performed using the real-space DFT (RSDFT) program code [2]. In the present work, we reveal atom-scale structures of single-bilayer steps inclined toward different directions. Further, we discuss the energetics of the step structures by calculating step formation energies. Based on the results, the morphology of the surface steps during epitaxial growth could be discussed.
[1] K. Sawada, J.-I. Iwata, and A. Oshiyama, Appl. Phys. Lett. **104**, 051605 (2014).
[2] J.-I. Iwata, https://github.com/j-iwata/RSDFT.

O 65.12 Wed 17:45 Poster B1

SPA-LEED studies on the Sn/Ge(111) $(3\times3) \leftrightarrow (\sqrt{3}\times\sqrt{3})$ Mott-insulator to metal phase transition — •Fabian Thiemann, Semih Özdemir, Christian Brand, Bernd Hafke, Tobias Witte, and Michael Horn-von Hoegen — Universität Duisburg-Essen

An ordered adsorbate layer of 1/3 monolayer of Sn on a Ge(111) surface exhibits a reversible Mott-insulator to metal transition at 173 K [1, 2] which is accompanied by a structural transition from a (3×3) to $(\sqrt{3}\times\sqrt{3})$ superstructure. Employing spot-profile-analysis low-energy-electron-diffraction allowed the acquisition of high-resolution line profiles and thus an accurate determination of the temperature dependent intensity of the characteristic superstructure spots. Through temperature cycling of the sample starting from the (3×3) ground state at 110 K to the metallic $(\sqrt{3}\times\sqrt{3})$ phase at temperatures above the transition temperature of 173 K we followed the reversible phase transition through $k_\parallel$-dependent line profiles taken for each temperature step. The contribution to the spot intensity through the Debye-Waller factor and the structure factor were individually determined.
[1] J. Avila et. al., Phys. Rev. Lett. **82**, 442 (1999).
[2] A. V. Melechko et. al., Phys. Rev. B **61**, 2235 (2000).

O 65.13 Wed 17:45 Poster B1

2D Supramolecular Self-assembly of C8-BTBT on Cu(111) — •Sebastian Becker[1,3], Lu Lyu[1], Benjamin Stadtmüller[1,2], Sina Mousavion[1], Maniraj Mahalinam[1] und Martin Aeschliemann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [3]Department of Chemistry, University of Kaiserslautern, Erwin-

Schrödinger-Straße 52, 67663 Kaiserslautern, Germany

Benzothieno[3,2-b]-benzothiophene (BTBT) is one of the most attractive core structures because of its chemical stability as well as its electronic properties and its derivatives with different end groups have been synthesized which demonstrate a very promising mobility up to 100 cm2V-1s-1. Here we use the VT-STM and LEED to systematically investigate the self-assemble behavior of monolayer 2,7 Dioctyl[1]-BTBT (C8-BTBT) on Cu(111). STM shows three different phases of C8-BTBT at 106 K. When increasing the sample temperature, phase transitions exist in different phases, which coincides with a temperature-dependent LEED measuring. Our findings will open insight into understanding of the mechanism of single-crystal organic semiconductor to further improve the performance.

O 65.14 Wed 17:45 Poster B1

Influence of the sample preparation on hydrogen-induced surface reconstruction on Pd(110) — •Robert Schindhelm[1], Markus Leisegang[1], Jens Kügel[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

The three main impurities to be considered when cleaning Pd(110) surfaces are hydrogen (H), carbon (C), and oxygen (O). Especially, H-induced vacancy rows reconstructions were investigated by STM [1,2]. We have systematically investigated the influence of some preparation parameters, i.e., the annealing temperature and the hydrogen pressure, on the temporal evolution of H-induced surface reconstructions by means of room-temperature STM. Whereas most results are in agreement with literature, our quantitative analysis regarding the relation between vacancy rows and adatom rows reveals some significant differences. We will discuss the suitability of these Pd(110) surfaces for studies of the direct [3] and remote [4] charge carrier-induced vibrationally excited motion of *cis*-2-Butene, a prominent example for molecular switches [3].

[1] E. Kampshoff *et al.* Surf. Sci. **360**, 55 (1996).
[2] M. Kralj *et al.* Surf. Sci. **600**, 4113 (2006).
[3] Kawai *et al.* Phys. Rev. Lett. **95**, 246102 (2005).
[4] Leisegang *et al.* Nano Lett. **18**, 2165 (2018).

O 65.15 Wed 17:45 Poster B1

Photoelectron holography – an experimentalist's approach to computer calculated reconstructions — •Matthias Gianfelice[1], Christopher Kohlmann[1,2], and Carsten Westphal[1,2] — [1]Experimental Pysics I - TU Dortmund University, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - TU Dortmund University, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund

The determination of atom locations within surface structures is of great importance for basic science and for applications. Atomic force microscopy allows the analysis of the uppermost atomic layer, however this technique does not provide any information about the three-dimensional subsurface structure.

D. Gabor proposed a holographic approach suggesting electron waves for three-dimensional atom imaging. The electron wave length is in the order of the atom distances and thus should be well suited for the determination of atom structures. Unfortunately it is very hard to reconstruct atom images from a detection hologram because of non-isotropic electron scattering.

In this contribution we present recent progress on reconstructing three-dimensional atom images from electron holograms.

O 65.16 Wed 17:45 Poster B1

Thermal motion slows down the In/Si(111)(8x2)-(4x1) phase transition — •Marvin Krenz, Uwe Gerstmann, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn

The optically induced In/Si(111)(8x2)-(4x1) insulator-metal transition serves as a prototypical model for the interplay of electronic and structural degrees of freedom during photoreactions [1,2]. Interestingly, at 20 K, the photo-induced (8x2)-(4x1)phase transition occurs extremely fast, in the quantum limit, and requires only a few hundred femtoseconds [1]. Here we present ab initio molecular dynamics calculations on excited-state potential energy surfaces based on constrained DFT. The calculations that account for temperature effects at 100 K indicate that thermal motion has a small effect on the transition time with a tendency to a slightly slow down the transition.

[1] T Frigge et al., Nature 544, 207 (2017). [2] CW Nicholson et al., Science 362, 821 (2018).