

## O 59: Metal Substrates I

Time: Wednesday 16:00–19:15

Location: WIL A317

O 59.1 Wed 16:00 WIL A317

**Growth morphology of thin films on the metallic and oxide surfaces** — ●ALEKSANDER KRUPSKI — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

In this work we briefly review recent investigations concerning growth morphology of thin metallic films on the  $Mo(110)$  and the  $Ni_3Al(111)$  surfaces, and  $Fe$  and Copper Phthalocyanine ( $C_{32}H_{16}N_8Cu$ ) on the  $Al_2O_3/Ni_3Al(111)$  surface. Comparison of  $Ag$ ,  $Au$ ,  $Sn$ , and  $Pb$  growth on the  $Mo(110)$  surface has shown a number of similarities between these adsorption systems except surface alloy formation that has only observed in the case of  $Sn$  and  $Au$ . In the  $Pb/Mo(110)$  and  $Pb/Ni_3Al(111)$  adsorption systems selective formation of uniform  $Pb$  island heights during metal thin film growth has been observed and interpreted in terms of quantum size effects. Furthermore, our studies showed that  $Al_2O_3$  on  $Ni_3Al(111)$  exhibits a large superstructure in which the unit cell has a commensurate relation to the substrate lattice. In addition, Copper Phthalocyanine chemisorbed weakly onto an ultrathin  $Al_2O_3$  film on  $Ni_3Al(111)$  and showed a poor template effect of the  $Al_2O_3/Ni_3Al(111)$  system. In the case of iron cluster growth on  $Al_2O_3/Ni_3Al(111)$  the nucleation sites were independent of deposition temperature, yet cluster shape showed a dependence. In this system,  $Fe$  clusters formed a regular hexagonal lattice on the  $Al_2O_3/Ni_3Al(111)$ .

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**Annealing of oxidized aluminium alloy surfaces studied by PEEM combined with XPS** — ●LISA RULLIK<sup>1</sup>, FLORIAN BERTRAM<sup>1</sup>, JONAS EVERTSSON<sup>1</sup>, ANDERS MIKKELSEN<sup>1</sup>, YURAN NIU<sup>2</sup>, ALEXEI ZAKHAROV<sup>2</sup>, and EDVIN LUNDGREN<sup>1</sup> — <sup>1</sup>Div. of Synchrotron Radiation Research, Lund University, Lund, Sweden — <sup>2</sup>MAX-lab, Lund University, Lund, Sweden

Aluminium alloys are used in a wide range of applications due to their high tensile strength in concomitance with low density. Additionally, aluminium alloys form a native passivating oxide layer, which leads to high corrosion and weathering resistance. In industrial manufacturing, aluminium alloys acquire their desired properties upon heating and welding.

Here, we present how annealing affects the surface layer composition of different aluminium alloys. Using MEM, PEEM and XPS we were able to follow the diffusion process of aluminium and its alloying elements from and towards the surface. For temperatures up to 300°C only slight changes of the surface composition can be observed in PEEM images and XPS spectra. At 400°C a significant diffusion of magnesium to the surface occurs.

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**Growth of ultrathin Pb layers on the  $Ni_3Al(111)$  surface studied by AES/LEED/STM/DFT** — ●KATARZYNA MIŚKÓW and ALEKSANDER KRUPSKI — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

The morphology, atomic and electronic structure of ultrathin Pb layers deposited on the  $Ni_3Al(111)$  face in ultrahigh vacuum at the substrate temperature, ranging from 200 K to 950 K, were investigated with the use of Auger electron spectroscopy (AES), low-energy electron diffraction (LEED), directional elastic peak electron spectroscopy (DEPES), scanning tunnelling microscopy (STM). Density functional theory calculations (DFT) with the use of CASTEP code were used to describe atomic and electronic structure of the  $Pb/Ni_3Al(111)$  system. The analysis of AES and STM measurements indicate that two-dimensional growth of the first Pb monolayer wetting layer takes place. For  $T = 200$  K, lead on the  $Ni_3Al(111)$  grows layer-by-layer, while for  $T = 300$  K flat three atomic-layer-high islands seem to grow after the completion of the first lead monolayer. Above 350 K, the Stranski-Krastanov growth mode is observed. The ordered LEED patterns are observed. Above  $\theta > 1.0$  ML, a three-dimensional growth of the Pb islands was observed with a strongly preferred atomic-scale magic height (N), hexagonal shape and flat-tops. At coverage  $\theta = 3.5$  ML, only islands containing  $N = 3, 5, 7$  and 11 atomic layers of Pb are observed. At the higher coverage  $\theta = 5.5$  ML, three types of regular hexagonal islands with side lengths of 25, 30 and 45 nm are observed. Furthermore, three different island adsorption configurations were observed.

O 59.4 Wed 16:45 WIL A317

**Three-dimensional atomic imaging by means of electron diffraction** — ●TOBIAS LÜHR<sup>1</sup>, AIMO WINKELMANN<sup>2</sup>, GERT NOLZE<sup>3</sup>, and CARSTEN WESTPHAL<sup>1</sup> — <sup>1</sup>TU Dortmund - Experimentelle Physik I, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D 06120 Halle, Germany — <sup>3</sup>Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, D 12205 Berlin, Germany

Diffraction patterns obtained with angle-resolved x-ray photoelectron diffraction (XPED) provide the information of the sample structure on an atomic length scale. Over the last three decades there were many attempts in order to obtain the sample structure applying a holographic reconstruction, due to common properties of XPED-patterns and holograms. However, anisotropic electron scattering, multiple scattering effects, as well as twin image formation generally prevented identifiable reconstructed images of the structure. Here, we demonstrate that all these problems can be circumvented by using electron diffraction patterns at kinetic energies of  $E_{kin} \geq 10$  keV. Without adding any structure information, the reconstruction reveals a three-dimensional image displaying up to thousands of atoms located at their correct position. Demonstrating the reconstruction scheme on a bcc-structure we are presenting results on more complex systems as graphite with different emitter types, and polyatomic crystals. In all cases studied up to now, the spatial image reflected the respective crystal structure with all atoms at their correct location.

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**Thickness-dependent growth study of Pt-Ce alloys on Pt(111)** — ●JEANNETTE KEMMER, ANDREAS KRÖNLEIN, PIN-JUI HSU, and MATTHIAS BODE — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently angle-resolved photoemission spectroscopy has revealed the formation of the coherent low-energy heavy-fermion band near the Fermi level on the CePt<sub>5</sub> surface alloy on Pt(111) [1]. We have investigated the coverage-dependent morphology of the various Pt-Ce surface alloys which form upon Ce deposition onto Pt(111) with a home-built low-temperature scanning tunneling microscope. Within the coverage range from  $9.6 \times 10^{18}$  atoms/m<sup>2</sup> to  $34 \times 10^{18}$  atoms/m<sup>2</sup> topographic constant-current images show several superstructures similar to those previously reported by Baddeley *et al.* [2]. While the coexistence of different superstructures is observed for low Ce coverages, much higher amounts of Ce lead to the formation of clusters, possibly due to segregation of excess Ce. An optimal surface quality is found for a Ce coverage of  $19 \times 10^{18}$  atoms/m<sup>2</sup>. We will also discuss the electronic properties of the Ce superstructures as observed by scanning tunneling spectroscopy.

[1] M. Klein *et al.*, Phys. Rev. Lett. **106**, 186407 (2011).[2] C. J. Baddeley *et al.*, Phys. Rev. B **56**, 12 589 (1997).

O 59.6 Wed 17:15 WIL A317

**Comparison of lithium- and magnesium battery anode materials on a microscopic level using DFT** — ●MARKUS JÄCKLE<sup>1,2</sup> and AXEL GROSS<sup>1,2</sup> — <sup>1</sup>Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — <sup>2</sup>Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany

Lithium and magnesium exhibit rather different properties as anode materials with respect to the phenomenon of dendrite formation which can lead to short-cuts in batteries. Diffusion processes are the key to understanding structure forming processes on surfaces. Therefore we have determined adsorption energies and barriers for the self-diffusion on Li and Mg using periodic density functional theory calculations. In addition, the adsorption of sulfur on these electrodes was studied as it represents a common pollutant in catalytical- and electrochemical systems.

According to our calculations, there are characteristic differences between Li and Mg, as far as the self-diffusion is concerned. On Mg, diffusion is much faster than on Li. The structural origins of this difference will be addressed. Furthermore, we will discuss the relevance of our findings for the understanding of the dendrite growth on Li anodes.

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**Temperature Dependent Electronic Structure of the CuN**

**c(2x2) on Cu(100) Overlayer** — ●IVAN BAEV, HENRIKE HÜMPEL, MICHAEL MARTINS, and WILFRIED WURTH — Institut für Experimentalphysik, Universität Hamburg

CuN c(2x2) on Cu(100) is a promising surface insulator to study nanoparticles. If the size of deposited particles is small, then the coupling of the particles to the surface is often stronger than the size dependent effects within the particles itself. In such a case CuN can be used to decouple the particles from the metallic substrate without the disadvantages of a bulk insulator. Former characterizations of the CuN layer were focused on LEED and STM techniques. Only a few studies involving core level photoemission exist.

We have performed annealing temperature dependent X-Ray photoemission spectroscopy with an energy resolution sufficient to separate various contributions to the resulting core level photoemission lines. Complimentary, we also performed LEED and STM investigations in a so far not investigated temperature and nitrogen-dose range.

The results show that an interpretation of the CuN system involving LEED and STM experiments only, is dangerous. Our stoichiometric evaluation together with core level binding energy shifts shows, that a full monolayer coverage of CuN is formed under rather different conditions than it is generally perceived in the literature. Also, we can show that the usual preparation technique involving low energy sputtering of nitrogen onto Cu(100) is probably not suitable to achieve a large homogeneous CuN coverage density.

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**Stability of surface adsorption patterns of Se on Mo(110): a first principles study** — ●GUIDO ROMA<sup>1</sup>, ELAHEH GHORBANI<sup>1</sup>, HOSSEIN MIRHOSSEINI<sup>1</sup>, JANOS KISS<sup>2</sup>, and CLAUDIA FELSER<sup>2</sup> — <sup>1</sup>Joh. Gutenberg University, Mainz, Germany — <sup>2</sup>MPI for Chemical Physics of Solids, Dresden, Germany

The selenization of molybdenum is technologically relevant for the production of thin film chalcopyrite solar cells. But it could become very important also for the production of nanostructures based on the layered compound MoSe<sub>2</sub>. However, the control of the process is still very poor, due to the lack of basic knowledge of the surface thermodynamics of the system. We present a theoretical study of the stability of surface adlayers of Se on the Mo(110) surface, predicting surface patterns and their stability range in terms of temperature and selenium partial pressure. Our results, based on density functional theory, show that the attainable Se coverages range from 1/4 to 3/4 of a monolayer for systems in equilibrium with a gas formed of Se molecules. We provide simulated scanning tunneling microscopy images to help the experimental characterization of adsorbed surface patterns.

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**STM and LEED studies on alloying and oxidation effects at the Mn/Cu(001) interface** — ●JIAMING SONG<sup>1</sup>, CHII-BIN WU<sup>2</sup>, and WOLFGANG KUCH<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>Chung Yuan Christian University, Department of Physics, 200 Chung Pei Rd., Chung Li, Taiwan 32023, R.O.C.

Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) are applied for characterizing the interface properties of Mn/Cu(001) at room temperature. STM reveals a three-dimensional growth mode of Mn on clean Cu(001). When a submonolayer Co is introduced in between, the Mn growth mode is stabilized in a two-dimensional mode. This two-dimensional growth mode can be attributed to the formation of an intermixed alloy of MnCo or even Mn-CoCu. Growth of Mn on the “missing row” phase of oxidized Cu(001) occurs without the surfactant effect known from the growth of Co, Ni and Fe on that surface. The absence of the surfactant effect of oxygen could be due to a larger binding energy between Mn and oxygen atoms compared to the surface energy. Nevertheless, the Mn growth mode on this oxidized Cu(001) surface is still two-dimensional. This might be due to a reduction of the surface energy of the substrate by the oxygen during the Mn growth, leading to a smoother morphology.

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**Thermodynamical assessment of stress evolution and jumps during the deposition of polycrystalline films** — ●AMIRMEHDI SAEDI and MARCEL J. ROST — Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

During Volmer-Weber thin film growth at conditions with sufficiently high atom mobility, the intrinsic film stress becomes compressive in the later stages. Moreover, upon deposition interruptions, the film reacts

with a huge tensile jump, that surprisingly, is fully restored back to the original stress values before the interruption, if the deposition is switched on again.

Several mechanisms have been proposed to explain these phenomena, but none of them were able to explain all the details of the experimental results and they remain as mere hypotheses waiting for their proof to come. One suggestion is that the diffusion of adatoms into/out of the grain boundaries (GB) during the deposition/interruption would be responsible for the observed effects. There are some models, based on kinetic arguments, attempting to show that this mechanism is capable of reproducing the experimental observations. However all of these models suffer from a critical shortcoming as they do not take into account the thermodynamical aspects. These include e.g. relationships between the flux, adatom densities, chemical potentials of the surface and grain boundaries, and the elastic energy of the bulk. Here our aim is to check for the first time whether the adatom-GB theory can really survive the test of a rigorous thermodynamical analysis.

O 59.11 Wed 18:30 WIL A317

**Role of stacking, bonding and interaction with substrate in formation of bilayer silicene** — ●PAUL PFLUGRADT, LARS MATTHES, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität and European Theoretical Spectroscopy Facility (ETSF), Max-Wien-Platz 1, 07743 Jena, Germany

The properties of the two-dimensional systems of group-IV materials are of increasing interest. Unlike graphene, the corresponding silicon-based honeycomb crystal, silicene, is claimed to be experimentally realized as monolayer on silver substrate. However, such conclusions are controversially debated in literature, because of the strong adsorbate-substrate interaction. Very recently promising bilayer silicene has been prepared, whose geometry and properties are widely unknown.

We predict an atomic geometry for this bilayer system, in contrast to the suggestions of experimentalists. Based on ab-initio density functional theory including van der Waals interaction, we make a comprehensive analysis of this new structure. We find a surprising silicene configuration, not stable as monolayer. The translational symmetry, the resulting lattice spacing, and the height of the topmost monolayer are in agreement with the STM findings. The band structure of the complete adsorbate system but also of the peeled-off silicene do not show conical linear bands near the Fermi level, as expected for free-standing 2D crystal.

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**Lateral Segregation in Pt<sub>50</sub>Rh<sub>50</sub>(111) induced by a h-BN nanomesh** — ●ROLAND STANIA<sup>1</sup>, IRAKLI KALICHAVA<sup>1</sup>, BERND SCHÖNFELD<sup>2</sup>, JÜRIG OSTERWALDER<sup>1</sup>, WOLFGANG HECKEL<sup>3</sup>, TOBIAS C. KERSCHER<sup>3</sup>, STEFAN MÜLLER<sup>3</sup>, PHILIP R. WILLMOTT<sup>1</sup>, and THOMAS GREBER<sup>1</sup> — <sup>1</sup>Universität Zürich, Physik-Institut — <sup>2</sup>ETH Zürich, LMPT — <sup>3</sup>Hamburg University of Technology, Institute of Advanced Ceramics

Epitaxially grown hexagonal boron nitride (*h*-BN) on Rh(111) forms a corrugated monolayer with a 13 on 12 super-honeycomb-structure known as the *h*-BN nanomesh [1]. In contrast *h*-BN on Pt(111) forms a flat layer with an approximate 10 on 9 superstructure being weaker bonded than the nanomesh [2]. The investigation of *h*-BN/Pt<sub>50</sub>Rh<sub>50</sub>(111) reveals a corrugated nanomesh-like 11 on 10 superstructure with a periodicity of 2.8 nm. Lateral segregation occurs in the topmost layer of the substrate during growth of *h*-BN, where Rh atoms form islands under the pores of the nanomesh which are surrounded by Pt atoms under the wires. The unit cell size is obtained by surface X-ray diffraction, while angular resolved photoemission indicates the nanomesh structure and the lateral segregation. The picture of lateral segregation at the nanometer scale is perfectly confirmed by density functional theory within a cluster expansion approach.

[1] Corso et al. Science **303** (2004) 217.

[2] Čavar et al. Surface Science **602** (2008) 1722.

O 59.13 Wed 19:00 WIL A317

**Physisorbed molecular networks as surfactants for the growth of Ag on Ag(100)** — ●CLAUDIUS MORCHUTT<sup>2,3</sup>, GUSTAVO RUANO<sup>2,3</sup>, KLAUS KERN<sup>1,2,3</sup>, and MAGALI LINGENFELDER<sup>1,2,3</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, D-70569 Stuttgart — <sup>2</sup>Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne — <sup>3</sup>Max Planck-EPFL Center for Molecular Nanoscience, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

Homoeptaxial growth of Ag on Ag(100) proceeds by a quasi layer-by-layer fashion at room temperature (RT). This means that higher-layer islands nucleate before the completion of lower layers and it leads to kinetic roughening of the multilayer film. Previous studies have shown that deposition of metal atoms such as Sb can act as surfactants improving the smoothness of the films. However, these surfactants are difficult to remove from the surface after growth. Here we show by Scanning Tunneling Microscopy (STM) in ultra-high vacuum (UHV)

that the growth mode of Ag on Ag(100) at RT is significantly modified by the presence of physisorbed molecular networks. The islands consisting of terephthalic acid (TPA, benzene-1,4-dicarboxylic acid) are stabilized via hydrogen bonds. Upon Ag deposition the Ag atoms penetrate the molecular islands without disrupting their supramolecular network that in turn enhances the coarsening of the Ag islands underneath. Furthermore, the organic molecules can easily be removed by post-annealing at moderate temperature.