

O 31: Poster Session - Metal substrates: Structure, Epitaxy and Growth

Time: Monday 18:15–20:00

Location: P1C

O 31.1 Mon 18:15 P1C

Influence of strain on dendrite growth in battery materials — ●DANIEL STOTTMEISTER and AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The growth of dendrites to this date represents a significant safety problem in the operation of high-performance batteries. Unraveling the underlying mechanics of dendritic growth has been the focus of many studies, and recent results strongly suggest that strain effects might influence the growth mechanism. Density functional theory (DFT) is a well-established method for the description of metal systems on an atomic level and can help to understand the underlying processes behind dendrite growth. In this contribution, ab initio calculations were performed in order to investigate the effects of strain on diffusion processes for a selection of promising battery materials such as lithium, sodium, and potassium. In order to address the possible influence of the electrochemical environment on the dendrite growth, first attempts to include the presence of electrolytes in the calculations will be presented.

O 31.2 Mon 18:15 P1C

Production and transfer of h-BN monolayers: Exploratory study — ●MARCO THALER, TOBIAS BONCZYK, and ERMINALD BERTEL — Physikalische Chemie, Universität Innsbruck, Österreich

Hexagonal Boron Nitride (h-BN) monolayers belong to the rapidly growing family of two-dimensional materials. h-BN is intensely studied, on the one hand as a template for graphene growth, on the other hand as a dielectric barrier in graphene-based electronic and spintronic devices. In electro-catalysis, h-BN can serve as support for active clusters, but is active also by itself^{1,2}. Recently, h-BN monolayers were found to host defects acting as single-photon sources with excellent spectral properties³. In view of these diverse applications, an easy, clean, and reproducible procedure for h-BN synthesis and transfer is highly desirable. We present a simple, load-lock equipped UHV chamber allowing the preparation of Pt foils as recyclable templates and the deposition of h-BN monolayers. The morphology and cleanliness of Pt templates after various pretreatments is studied by AFM and XPS. h-BN deposition is monitored by XPS and different transfer protocols for the monolayers to metallic or dielectric substrates are evaluated.

¹ Elumalai, G. et al., Phys. Chem. Chem. Phys. **16**, 13755(2014).

² Lyalin, A. et al., The Chemical Record **16**, 2324(2016).

³ Li, C. et al., Nanophotonics **8**, 2049 (2019).

O 31.3 Mon 18:15 P1C

Inverse melting of Ni on Re(0001) — JOHANNES REGEL, ●TORGE MASHOFF, and HANS-JOACHIM ELMERS — Institut für Physik, Johannes Gutenberg-Universität, Mainz

Usually, cooling a metal sample down to cryogenic temperatures leads to an immobility of the surface atoms. In rare cases an opposite behavior has been observed under extreme conditions, where cooling leads to an increase in entropy and thus to a higher mobility of the surface atoms. This process is known as inverse melting. In our case a combination of a small force induced by the STM-tip and the weakened bonding between the Ni atoms results in mobile Ni atoms at island edges.

We prepare coverages between 0.1 ML and 10 ML of Ni on a Re(0001)-surface and investigate the mobility of the Ni atoms using scanning tunneling microscopy at temperatures between 4.8 K and room temperature. Sequences of STM-images show an increased mobility of Ni atoms at low temperatures.

O 31.4 Mon 18:15 P1C

Al₂Cu(001) studied by photo electron spectroscopy — ●HOLGER SCHWARZ¹, NIELS RÖSCH¹, STEFAN PÜSCHEL², PETER GILLE², MARC ARMBRÜSTER³, and THOMAS SEYLLER¹ — ¹Institute of Physics, TU Chemnitz, Chemnitz, Germany — ²Department of Earth and Environmental Sciences, LMU München, München, Germany — ³Institute of Chemistry, TU Chemnitz, Chemnitz, Germany

Intermetallic compounds have received interest because of their performance as catalysts in, e.g., hydrogenation reactions. However, compared to the enormous number of surface studies on pure metals and on alloys, there are considerably fewer studies on the surface prop-

erties of intermetallic compounds. Recently, Al₂Cu(001) showing a $(2\sqrt{2} \times \sqrt{2})R45^\circ$ reconstruction was studied using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) in combination with ab initio calculations [1]. A structure model was derived which consists of a bulk termination with incomplete Al planes. The aim of our work is to further characterize the Al₂Cu(001) surface by additional techniques, in particular X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). The poster will present and discuss first results of our work, focusing on surface composition and structure as well as electronic structure.

[1] L. N. Serkovic Loli, et al., Phys. Rev. Lett. **108** (2019) 146101.

O 31.5 Mon 18:15 P1C

Structure analysis of ultrathin NaCl-layers on metallic substrates — ●KIRA KOLPATZECK, EBRU EKICI, VIJAYA BEGUM, MARKUS GRÜNER, ROSSITZA PENTCHEVA, and ROLF MÖLLER — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

To observe radiative transitions in molecules, single atoms or clusters it is necessary to decouple those from any metallic substrate. On the other hand, for surface science methods, such as scanning tunneling microscopy, a non-vanishing surface conductivity has to be ensured. Ultrathin insulating layers are the key to circumvent those two requirements. Therefore, we have studied the growth of ultrathin sodium chloride (NaCl) films with various layer thickness on different metallic substrates by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at low temperatures (8K and 80K). We could show that the evaporation of NaCl on Au(110) leads to the growth of NaCl islands of different height. The first two layers are showing a (1x4) superstructure rectangular to the missing-row reconstruction of the Au(110) surface. Incomplete growth structures like holes in the islands as well as the third sodium chloride layer show the well-known rectangular edge geometry. With the aid of DFT-calculations a first structure model could be found to explain the observed superstructure.

O 31.6 Mon 18:15 P1C

Surface structure and chemical composition of the Te covered Au₇₅Ag₂₅(111) surface — ●TOBIAS KIRSCHBAUM, TILMAN KISSLINGER, LUTZ HAMMER, and M. ALEXANDER SCHNEIDER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

When depositing chalcogenides on clean transition metal surfaces the adsorbates coordinate substrate atoms to form a surface alloy or other surface structures [1,2]. The situation is unclear if a binary alloy functions as substrat. There, the chalcogenide has a variety of possibilities to bind within the surface and might be able to induce stoichiometries in the subsurface that differ from the bulk.

Here we present an investigation of the clean and Te covered Au₇₅Ag₂₅(111) surface by means of room-temperature scanning tunneling microscopy (STM) and low-energy-electron diffraction (LEED). The clean Au₇₅Ag₂₅(111) surface is that of a disordered substitutional alloy. Our LEED-IV analysis ($R = 0.064$) proves an enrichment in silver in the second layer to $\approx 50\%$, whereas the other layers stay nearly bulk-like within the errors. Upon deposition of 1/3 ML Te at 90 K and annealing to at least 473 K a $(\sqrt{3} \times \sqrt{3})R30^\circ$ -structure forms. STM shows a honeycomb-like arrangement. A LEED-analysis confirms that this is a pure AgTe overlayer at hcp positions on a nearly bulk-like Au₇₅Ag₂₅(111) crystal.

[1] Jiaqi et al., Surf. Sci., **669**, 198, 2018

[2] Liu et al., J. Phys. Chem. Lett., **10**, 1866, 2019

O 31.7 Mon 18:15 P1C

Scanning tunneling microscopy study of submonolayer growth of Mn_xAu_{1-x} on Cu(001) — ●ISMET GELEN¹, TAUQIR SHINWARI¹, YASSER A. SHOKR^{1,2}, EVANGELOS GOLIAS¹, and WOLFGANG KUCH¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — ²Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt

Mn_xAu_{1-x} exhibits many antiferromagnetic (AFM) phases. Mn₂Au is one of them that has a high Néel temperature (≈ 1600 K) and, due to its noncentrosymmetric spin structure and metallic nature, is an interesting AFM material for spintronic applications. Here, we

study the growth of $\text{Mn}_x\text{Au}_{1-x}$ in the submonolayer (sub-ML) regime on Cu(001) by medium- and low-energy electron diffraction (MEED, LEED), Auger electron spectroscopy (AES), and scanning tunneling microscopy (STM). Different Mn concentrations ($x \approx 0.7-0.9$) and different thicknesses ($\approx 0.2-1.1$ ML) were studied, as monitored by AES. Mn and Au were coevaporated by electron bombardment on Cu(001) at

room temperature (RT). The growth of thicker films showed MEED intensity oscillations up to around 9 ML. The LEED images display substrate patterns for thicknesses < 0.5 ML, while they display a $c(2 \times 2)$ structure for thicker sub-ML films. We observe $\text{Mn}_x\text{Au}_{1-x}$ islands on Cu(001) for all sub-ML films with island sizes between $\approx 5 \times 5$ and 30×30 nm².