

## O 89: Metal Substrates: Epitaxy and Growth

Time: Friday 9:30–12:30

Location: MA 041

O 89.1 Fri 9:30 MA 041

**Real time observation of multiphoton photoemission and surface second harmonic generation during the growth of Fe on Cu(001)** — ●CHENG-TIEN CHIANG, AIMO WINKELMANN, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale), Germany

We observed simultaneously the multiphoton photoemission and second harmonic generation (SHG) at 3.1 eV incident photon energy during the growth of Fe on Cu(001). The well-known intensity variations observable in medium energy electron diffraction measurements of Fe/Cu(001) were correlated with the variations of the SHG signal. Using SHG as a reference, we assign the different phases of the Fe growth to the observed photoemission spectra. With this approach, we obtain the work function variations as a function of film thickness from the photoemission spectra. For the first 4 monolayers (ML) of Fe deposited on Cu(001), a non-monotonic variation of the work function is observed, with a decrease of 0.14 eV for 1 ML Fe. This value is consistent with theoretical calculations [1]. In correspondence to the work function variations, a resonant three-photon photoemission (3PP) feature oscillates in intensity as a result of the fixed relationship between the vacuum level and an intermediate image potential state. From the exponentially decaying part of 3PP signal we can estimate the inelastic mean free path of electrons with kinetic energy of 4 eV above the Fermi level to be about 10 Å.

[1] S. Achilli *et al.*, J. Phys.:Condens. Matter **19**, 305021 (2007)

O 89.2 Fri 9:45 MA 041

**The buried Ni/Cu(001) interface at the atomic scale** — ●HOLGER L. MEYERHEIM<sup>1</sup>, DIRK SANDER<sup>1</sup>, NIKOLAY NEGULYAEV<sup>1</sup>, VALERI S. STEPANYUK<sup>1</sup>, RADIAN POPESCU<sup>1</sup>, IONA POPA<sup>2</sup>, and JÜRGEN KIRSCHNER<sup>1</sup> — <sup>1</sup>MPI-Halle, Weinberg 2, D-06120 Halle (Germany) — <sup>2</sup>ESRF, BP 220, F-38043 Grenoble (France)

We present a combined surface x-ray diffraction and theoretical analysis of the buried Ni/Cu(001) interface structure after deposition of 3 and 5 monolayers of Ni at room temperature. Highly accurate reflection intensities along the integer order crystal truncation rods were collected at the beamline ID3 of the ESRF in Grenoble (France). The analysis reveals interface mixing where  $27 \pm 10\%$  of top layer Cu-atoms are exchanged by Ni. In addition, a 0.13 Å inward relaxation of top layer Ni-atoms is determined. Atomic scale simulations reveal a kinetic pathway for the Ni/Cu-exchange process and explain the observed limited degree of intermixing. A disperse distribution of Ni within the Cu surface with a preferential Ni-Ni separation of 3-4 nearest neighbor distances is found [activation energy for exchange ( $E_b$ ) equal to 0.65 eV]. Intermixing is spatially confined to two atomic layers adjacent to the interface in agreement with experiment. The calculations also provide an explanation for the markedly different behavior of intermixing reported for Fe-Cu(001) interface, where Fe forms embedded clusters in the Cu surface [1].

[1] D.D. Chambliss and K.E. Johnson, Phys. Rev. B **50**, 5012 (1993)

O 89.3 Fri 10:00 MA 041

**SXRD study at both sides of a temperature induced surface phase transition on Sn/Cu(001)** — ●JESUS MARTINEZ-BLANCO<sup>1</sup>, VICTOR JOCO<sup>2</sup>, CARLOS QUIROS<sup>3</sup>, PILAR SEGOVIA<sup>2</sup>, and ENRIQUE G MICHEL<sup>2</sup> — <sup>1</sup>Fritz Haber Institut, Berlin, Germany — <sup>2</sup>Universidad Autonoma de Madrid, Spain — <sup>3</sup>Universidad de Oviedo, Spain

The crystalline structure of 0.5 monolayer of Sn atoms adsorbed on Cu(001) has been studied by surface X-ray diffraction (SXRD) measurements. This surface undergoes a temperature-induced phase transition at 360 K from a single domain ( $\sqrt{2} \times \sqrt{2}$ )R45° phase at high temperature to a two rotated domains ( $3\sqrt{2} \times \sqrt{2}$ )R45° phase at low temperature. A full data set including in-plane reflections, superstructure rods and crystal truncation rods was measured for each phase. The optimization method employed for fitting the experimental data for both the high and low temperature phases is a type of genetic algorithm called Differential Evolution, used in this work for the first time to extract crystallographic information from SXRD data. For the low temperature phase, our results confirm the removing of every third row of copper in the alloyed top layer. For the high temperature phase, the overall dependence of the measured structure factors with the perpendicular momentum transfer is similar to the values extracted from

the low temperature phase, suggesting a disordered nature for the high temperature phase. We propose a detailed model for this phase and for the nature of the thermal induced disorder. We discuss possible mechanisms to keep the local structure across the phase transition and the nature of the high temperature disordered phase.

O 89.4 Fri 10:15 MA 041

**Ripple growth and - orientation during grazing incidence deposition of Cu/Cu(001)** — ●HERBERT WORMEESTER, FRITS RABBERING, GEORGIANA STOIAN, RAOUL VAN GASTEL, and BENE POELSEMA — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands

We have studied the consequences of oblique incidence deposition for the morphology of the growth-front for a "prototypical" system Cu/Cu(001). Previous electron diffraction measurements showed that deposition at grazing incidence leads to the evolution of ripples, oriented perpendicular to the plane of incidence of the atom beam. New experimental results with high resolution low energy electron diffraction and STM will be presented. The ripple formation has also been studied with kMC simulations, which support and predicted experimentally observed changes in ripple orientation at later stages in growth. The relevant activation barriers for intra- and interlayer diffusion processes in these simulations have been tuned to describe quantitatively(!) experimentally observed morphologies in a wide range of temperatures (150-300 K) and coverages (up to 40 ML). A change in ripple orientation from perpendicular to parallel to the plane of incidence has been detected around a coverage of 40 ML at a temperature of 250K and a polar deposition angle of 80°. At 230K and at more grazing incidence this orientation transition has been found to occur at a much earlier stages in growth. This change in ripple orientation is related to the Super Poisson roughening of the growth front.

O 89.5 Fri 10:30 MA 041

**Initial growth of Cu on Cu(001) by in-situ pulsed laser deposition at low temperatures** — ●ANDREAS DOBLER and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

In previous studies we have characterized the initial growth of Cu on Cu(001) by pulsed-laser deposition (PLD) near room temperature by scanning tunneling microscopy (STM). In order to extend the temperature range to lower temperatures, we designed a setup which permits direct deposition onto the sample in the STM at pressures of  $1.5 \times 10^{-10}$  mbar. The distance between the ablation target and the sample is 270 mm and the incidence angle is 60° relative to the sample normal. The deposition rate is  $2.5 \times 10^{-5}$  atomic layers per pulse at a fluence of 3.5 J/cm<sup>2</sup>.

We present first results on the initial growth of Cu on Cu(001) using the in-situ PLD setup. At the large incidence angle, sputtering holes appear on the surface due to the high kinetic energies of the deposited particles. We analyzed the densities of monolayer and vacancy islands at different temperatures and laser fluences and compared the results to thermal deposition measurements at identical conditions. Self-sputtering can be reduced by lowering the fluence and applying a magnetic field which eliminates ions of the ablation plume.

O 89.6 Fri 10:45 MA 041

**What causes the high island densities in pulsed laser deposition?** — GEORG RAUCHBAUER, FLORIAN WIMMER, ANDREAS BUCHSBAUM, GERHARD BETZ, PETER VARGA, and ●MICHAEL SCHMID — Inst. f. Allg. Physik, TU Wien, Österreich

Pulsed laser deposition (PLD) is a method for growing thin films that combines nonthermal particle energies (typically 30 to 200 eV) with ultrahigh-vacuum compatibility. Compared to thermal deposition, PLD-grown films show a significantly higher island density and improved layer-by-layer growth. These features were attributed to either the high instantaneous particle flux or the high particle energies. Using scanning tunneling microscopy (STM), we have studied the nucleation and growth of Pt and Co on Pt(111) by PLD and we show that the high particle flux is not sufficient to explain the island densities observed. Experiments at low temperature, where adatom motion is frozen, and molecular dynamics simulations show that particle energies of  $\approx 100$  eV are sufficient to create small adatom clusters by "failed

sputtering". These clusters serve as nucleation centers and explain the differences between thermal deposition and PLD. We propose that the same mechanism is effective in sputter deposition.

O 89.7 Fri 11:00 MA 041

**Double layer growth of Ru on Pt(111) - the contributions of strain and metal-metal bonds** — ●PETRA M. ERNE<sup>1</sup>, ANDRÁS BERKÓ<sup>1,2</sup>, ANDREAS BERGBREITER<sup>1</sup>, HARRY E. HOSTER<sup>1</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Permanent Address: Institute of Surface Chemistry and Catalysis, University of Szeged, H-6701-Szeged, Dóm tér 7, Hungary

As found in previous STM-studies, vapor deposition of Ru onto Pt(111) leads to the formation of double layer islands of rather small lateral dimensions [1,2], similar to the behavior reported for Co/Cu(111) [3]. In order to clarify whether this behavior is mainly due to the lattice mismatch between Pt(111) and the hexagonally packed Ru(0001) surface, or whether the main reason is a much stronger local Ru-Ru interaction as compared to the Ru-Pt intermetallic bond, we carried out Ru growth experiments on pseudomorphic Pt/Ru(0001) monolayer islands and films, where lattice mismatch effects should play no role. The results indicate that the differences between the Ru-Pt bond and the Ru-Ru bond are the dominating effects.

[1] Poster O 55.61

[2] H. Hoster, T. Iwasita, H. Baumgärtner, W. Vielstich; Phys. Chem. Chem. Phys. 3; 2001, 337.

[3] J. de la Figuera, J.E. Prieto, C. Ocal, R. Miranda; Surf. Sci. 307-309; 1994; 538.

O 89.8 Fri 11:15 MA 041

**Atomic ensembles in Au<sub>x</sub>Pt<sub>1-x</sub>/Pt(111) surface alloys - linking a quantitative STM study with DFT calculations** — ●ANDREAS BERGBREITER<sup>1</sup>, HARRY E. HOSTER<sup>1</sup>, YOSHIHIRO GOHDA<sup>2</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Institute for Theoretical Chemistry, Ulm University; D-89069 Ulm, Germany

The knowledge of the available adsorption sites on catalyst surfaces is essential for the understanding of their adsorption and catalytic properties. 2D alloys, in which intermixing is confined to the surface, are excellent model systems to study correlations between the atomic distribution and the adsorption or reaction behavior. Based on high-resolution STM imaging with chemical contrast, the atomic distribution in Au<sub>x</sub>Pt<sub>1-x</sub>/Pt(111) surface alloys is characterized by a segregation into homoatomic aggregates. This can be rationalized by an effective repulsion between unlike atoms in the outermost layer, which is supported also by DFT calculations. Using a 2D lattice gas Hamiltonian, we are able to simulate the atomic distribution via a Metropolis Monte-Carlo (MC) algorithm [1]. The effective interaction parameters for the Hamiltonian were derived from DFT-calculated energies for different ordered Au<sub>x</sub>Pt<sub>1-x</sub>/Pt(111) slabs. The measured surface densities of different atomic ensembles, as counted in the STM data, and the MC generated distribution agree well, even though only pairwise interactions are considered in the Hamiltonian.

[1] A. Bergbreiter et al.; Phys. Chem. Chem. Phys. 9, 2007; 5127.

O 89.9 Fri 11:30 MA 041

**Zn/Pd(111) - Adlayer versus Alloy Formation: An Investigation by Low-Energy Ion Scattering** — ●WERNER STADLMAYR and NORBERT MEMMEL — Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria

The system Zn/Pd(111) has recently attracted attention due to its relevance for methanol steam reforming. However, conflicting growth modes were reported in XPS studies [1] and TPD/CO-titration investigations [2], respectively. While the former work postulates the onset of alloy formation already slightly above room temperature, the latter work excludes alloy formation below 600 K. We apply low-energy ion scattering spectroscopy with monolayer sensitivity to clarify this issue. [1] A. Bayer, K. Flechtner, R. Denecke, H.P. Steinrueck, K.M. Neyman, N. Roesch, Surf. Sci. 600, 78 (2006). [2] H. Gabasch, A. Knop-Gericke, R. Schloegl, S. Penner, B. Jenewein, K. Hayek, B. Kloetzer, J. Phys.

Chem B 110, 11391 (2006).

O 89.10 Fri 11:45 MA 041

**Anomalous scaling of Cu-island dynamics on Ag(100)** — ●CHRISTOPHER ZAUM and KARINA MORGENSTERN — Institut für Festkörperphysik, Gottfried Wilhelm Leibniz Universität, Appelstr. 2, D-30167 Hannover, Germany

We deposited Cu-islands containing 10 to 500 atoms on a clean Ag(100) surface at room temperature and investigated diffusion and decay of these islands with a fast scanning tunneling microscope. Islands at sizes above 80 atoms per island are adsorbed in hollow-sites. Islands at sizes below 80 atoms per island are adsorbed in bridge-sites. Diffusion and decay behavior of the hollow-site islands is similar to the behavior of both Ag-islands on Ag(100) and Cu-islands on Cu(100). In contrast, the diffusivity and the decay time of the bridge-site islands are significantly higher than any previously measured values. This indicates a novel mechanism of diffusion.

O 89.11 Fri 12:00 MA 041

**DFT study of epitaxial graphene on Ru(0001)** — ●BIN WANG<sup>1</sup>, MARIE-LAURE BOCQUET<sup>1</sup>, STEFANO MARCHINI<sup>2</sup>, SEBASTIAN GÜNTHER<sup>2</sup>, and JOOST WINTTERLIN<sup>2</sup> — <sup>1</sup>Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, Lyon, France — <sup>2</sup>Department Chemie, Ludwig-Maximilians-Universität München, München, Germany

Graphene is a flat monolayer of carbon atoms with a honeycomb lattice, which has been a rising star in materials science for its unique electronic structure. It can also grow on surfaces if the lattice constants of the surface and of graphene match. In case of lattice mismatch, as in the case of metal surfaces like Ru(0001) [1] or Ir(111) [2], epitaxial growth leads to a moiré structure. We have investigated epitaxial graphene on a Ru(0001) substrate by means of large-scale density functional theory (DFT) calculations. We show that, contrary to other substrates, the graphene electronic structure displays massive local changes, alternatingly varying between a zero gap and a band gap of 2 eV. This result is caused by alternating weak and strong contact areas of the graphene on the Ru surface, correlated with a large geometric buckling of 1.5 Å over the 30 Å periodic moiré superstructure. The mismatching lattice between graphene and the substrate thus leads to a changing symmetry and electronic structure that both vary regularly on the nanometer scale. The results are in good agreement with recent STM experiments [1].

[1] Marchini S., Günther S. & Wintterlin J., Phys. Rev. B. 76, 075429 (2007) [2] N'Diaye A.T., Bleikamp S., Feibelman P. J. & Michely T., Phys. Rev. Lett. 97, 216501 (2006)

O 89.12 Fri 12:15 MA 041

**Incommensurate epitaxy of graphene on Ir(111)** — ●ALPHA N'DIAYE, JOHANN CORAUX, CARSTEN BUSSE, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln

Graphene can epitaxially be grown on Ir(111) by thermal decomposition of hydrocarbons. Due to the incommensurate lattices of graphene and the underlying Ir(111) surface, a large supercell moiré with a periodicity of 25 Å emerges. Despite the incommensurability of the two lattices, graphene grows well ordered on Ir(111) with the dense packed iridium [110] direction parallel to the [1120] of graphene.

We present two ways of preparing graphene on Ir(111). One method employs preadsorption of ethylene (C<sub>2</sub>H<sub>4</sub>) and subsequent thermal decomposition. This yields a high graphene island. The average island size can be controlled by temperature, while the coverage is fixed to about 20% of the surface area. Based on the analysis of the evolution of graphene flake size distribution with time and temperature, we propose the coalescence of graphene flakes as a coarsening mechanism.

The second method is based on continuous exposure of the hot Ir(111) surface to ethylene. At the chosen temperatures (between 970 K and 1320 K) ethylene decomposes on iridium, but not on graphene. This process is suited to covering the whole surface with one layer of graphene. Nucleation of graphene flakes takes place exclusively at step edges.

Epitaxial perfection increases with the domain size. The domain size is crucially dependent on the preparation temperature. At 1320 K this size exceeds the micrometer scale.