

## O 53: Nanostructures at surfaces: Dots, particles, clusters III

Time: Thursday 15:00–18:30

Location: SCH A215

O 53.1 Thu 15:00 SCH A215

**One-Dimensionally Ordered Metal Cluster Arrays on Carburized W(110)** — ●MAGDALENA BACHMANN, MARTIN GABL, NORBERT MEMMEL, and ERMINALD BERTEL — Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria

The growth of noble (Ag, Au) and transition metal (Co) nanodots on the carburized tungsten (15x12)C/W(110) surface is studied by scanning tunneling microscopy (STM). At elevated temperatures for all metals small clusters are observed which are arranged with the periodicity defined by the template structure (1.4 x 3.1 nm<sup>2</sup>). The same adsorption sites are occupied by transition and noble metal clusters. Apart from these similarities also marked differences exist, in particular at higher coverages, when more material is deposited than can be adsorbed on the favorable cluster adsorption sites in each unit cell. Close to room temperature excess cobalt atoms nucleate as "interstitial" Co clusters, whereas Ag forms double-layer islands overgrowing the nanodots. At elevated temperatures in case of Co monolayer-high islands are observed, filling the free space between the clusters, whereas in case of Ag a transport of excess Ag atoms to clean tungsten terraces takes place, resulting in regular cluster growth on carbon-covered patches. Obviously, for Co the difference in adsorption strength between the more and the less favourable sites within each unit cell is less pronounced. The present results for Au contradict to some extent a recent STM study by Varykhalov et al. [Phys. Rev. B 77, 035412 (2008)]. Reasons for these discrepancies will be discussed.

O 53.2 Thu 15:15 SCH A215

**Ag island and cluster growth and thermal stability on C<sub>60</sub> films** — ●LUKAS PATRYARCHA<sup>1</sup>, STEFANIE DUFFE<sup>1</sup>, MICHAEL MOSELER<sup>2,3,4</sup>, and HEINZ HÖVEL<sup>1</sup> — <sup>1</sup>Technische Universität Dortmund, Experimentelle Physik I — <sup>2</sup>Universität Freiburg, Fakultät für Physik — <sup>3</sup>Fraunhofer-Institut für Werkstoffmechanik, Freiburg — <sup>4</sup>Freiburger Materialforschungszentrum

In former experiments for Ag<sub>309</sub>/C<sub>60</sub>/HOPG and Ag<sub>309</sub>/C<sub>60</sub>/Au(111) a substrate dependent cluster stability was observed [1]. In order to compare with these data, here at T < 50 K Ag atoms with an effective coverage of 0.5 monolayers (ML) were evaporated on Au(111) functionalized with 1.5 ML C<sub>60</sub> and imaged with STM at 77 K. Cluster growth on 1 and 2 ML C<sub>60</sub> was observed directly after evaporation with STM at 77 K. After 45 min at 215 K most of the clusters grown on 1 ML decayed. The atomistic calculations for Ag<sub>309</sub>/C<sub>60</sub>/Au(111) [1] suggest that Ag atoms moved through 1 ML C<sub>60</sub> to the Au(111) surface and formed Ag monolayer islands below the C<sub>60</sub> film. Primary clusters with a height of about 1,3 nm and 1,7 nm were formed on 2 ML C<sub>60</sub> and stayed stable for 14 days at room temperature. In an additional experiment 4 ML Ag were evaporated. Also in this case no long-time stable clusters at T > 265 K on 1 ML C<sub>60</sub> were observed while clusters on 2 ML grew. By approximating the cluster shape with an ellipsoid a width-height-factor was calculated, so cluster growth effects and the change of the effective cluster coverage remaining on the surface after each annealing step could be identified.

[1] S. Duffe et al., submitted for publication

O 53.3 Thu 15:30 SCH A215

**X-ray evidence for mesoscopic relaxations in Cobalt nanoislands on Cu(001)** — OLEG MIRONETS<sup>1</sup>, ●HOLGER L. MEYERHEIM<sup>1</sup>, CHRISTIAN TUSCHE<sup>1</sup>, VALERY S. STEPANYUK<sup>1</sup>, EELENA SOYKA<sup>1</sup>, PAUL ZSCHACK<sup>2</sup>, HAWOONG HONG<sup>2</sup>, NICOLE JEUTTER<sup>3</sup>, ROBERTO FELICI<sup>3</sup>, and JÜRGEN KIRSCHNER<sup>1</sup> — <sup>1</sup>MPI f. Mikrostrukturphysik, D-06120 Halle (Germany) — <sup>2</sup>APS, Argonne National Laboratory, Argonne, IL 60439 (USA) — <sup>3</sup>ESRF, F-38043 Grenoble (France)

Surface x-ray diffraction (SXR) combined with scanning tunneling microscopy (STM) and molecular dynamics (MD) calculations provides evidence that monolayer thick Co nanoislands on Cu(001) experience large relaxations called mesoscopic misfit (MM). In small Co islands consisting of several tens of atoms only, the average bond length is reduced to 2.40-2.45 Å (bulk: 2.51 Å). The SXR analysis is based on the determination of the Co-adlayer position on Cu(001) by probing the intensity distribution along the crystal truncation rods [1]. In contrast to the case of large islands (>>100 atoms), where Co-atoms reside in hollow sites separated by 2.56 Å, Co-atoms in mesoscopic misfitted islands also occupy positions off the hollow sites. The MM

is identified by giant static disorder of the Co-atoms representing the distribution of adsorption sites around the hollow site position. MD calculations are in excellent agreement with the SXR derived results.

[1] O. Mironets, H. L. Meyerheim, C. Tusche, V.S. Stepanyuk, E. Soyka, P. Zschack, H. Hong, N. Jeutter, R. Felici, and J. Kirschner, Phys. Rev. Lett. 100, 096103 (2008)

O 53.4 Thu 15:45 SCH A215

**Effect of confined surface electrons on atomic motion on nanoislands** — ●LARISSA NIEBERGALL<sup>1</sup>, ALEXEY S. SMIRNOV<sup>2,3</sup>, NIKOLAY N. NEGULYAEV<sup>2</sup>, WOLFRAM HERGERT<sup>2</sup>, ALEXANDER M. SALETSKY<sup>3</sup>, and VALERI S. STEPANYUK<sup>1</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — <sup>2</sup>Physics Department, Martin-Luther-University, 06099 Halle, Germany — <sup>3</sup>Faculty of Physics, Moscow State University, 119899 Moscow, Russia

Several fascinating phenomena occur if surface electrons are confined to closed nanostructures [1-3]. The first experimental investigation of the quantum confinement of surface electrons on nanoscale islands on (111) noble metal surfaces by means of STM has been performed by Li et al. [3]. These studies revealed the validity of the confinement picture down to the smallest of island sizes. Here, the quantum confinement of surface electrons on top of nanoscale islands and around them is studied by means of the first-principles Korringa-Kohn-Rostocker Greens function method [4]. Our kinetic Monte Carlo simulations reveal that confinement-induced electronic states around and on top of nanoislands significantly affect atomic diffusion [4]. Formation of empty zones and orbits of adatom motion is shown. We demonstrate that the quantum confinement dramatically influences the growth process of nanoislands at low temperatures [4].

1. N. N. Negulyaev et al., Phys. Rev. Lett. 101, 226601 (2008)
2. V. S. Stepanyuk et al., New J. Phys. 9, 388 (2007)
3. J. Li et al., Phys. Rev. Lett. 80, 3332 (1998)
4. A. S. Smirnov et al., Phys. Rev. B 78 041505R (2008)

O 53.5 Thu 16:00 SCH A215

**Reduction of the critical temperature in ultrathin superconducting lead nanocrystals** — CHRISTOPHE BRUN<sup>1</sup>, I-PO HONG<sup>1</sup>, FRANÇOIS PATTHEY<sup>1</sup>, I .YU. SKLYADNEVA<sup>2,3</sup>, R. HEID<sup>4</sup>, P. M. ECHENIQUE<sup>2,5</sup>, K. P. BOHNEN<sup>4</sup>, E. V. CHULKOV<sup>2,5</sup>, and ●WOLFDIETER SCHNEIDER<sup>1</sup> — <sup>1</sup>Ecole Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — <sup>2</sup>Donostia International Physics Center (DIPC), 2018 San Sebastian/Donostia, Basque Country, Spain — <sup>3</sup>Inst. Strength Physics and Mat. Sci., 634021, Tomsk, Russia — <sup>4</sup>Forschungszentrum Karlsruhe, Inst. f. Festkörperphysik, D-76021 Karlsruhe, Germany — <sup>5</sup>Departamento de Fisica de Materiales and Centro Mixto CSIC-UPV/EHU, Facultad de Ciencias Quimicas, 20080 San Sebastian/Donostia Basque Country, Spain

The energy gap of superconducting Pb nanocrystals grown on a Si(111) substrate was probed *in situ* layer-by-layer between 5 to 60 monolayers by low-temperature scanning tunneling spectroscopy. The critical temperature  $T_c$  was found to decrease from its bulk value as a function of inverse island thickness, in quantitative agreement with *ex situ* magnetic susceptibility measurements, however, in stark contrast to previous scanning probe results. *Ab initio* density functional calculations of the electron-phonon coupling constant support the experimental findings and show that the decrease of  $T_c$  mainly originates from a concomitant decrease of the electronic density of states at the Fermi level.

O 53.6 Thu 16:15 SCH A215

**Gas Sensitivity in Nanoporous Crystalline Metal Oxides: Dependence on Coordination Number** — ●JULIA DRAEGER<sup>1</sup>, MARKUS ULRICH<sup>1</sup>, CLAUS-DIETER KOHL<sup>2</sup>, STEFANIE RUSS<sup>3</sup>, and ARMIN BUNDE<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik III, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen — <sup>2</sup>Institut für Angewandte Physik, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen — <sup>3</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We use a percolation model to study numerically and analytically the influence of gas adsorption on the conductance of thin films of nanoporous crystalline metal oxides. We model the layers by a network of intergranular contacts with conductances that depend on the

amount of adsorbed gas molecules. For a given layer thickness, average grain size and coordination number we estimate the critical gas concentration  $N_c$  below which the nanoporous structure is insulating due to the absence of a percolating cluster of conducting grains. Above  $N_c$ , which decreases strongly with the coordination number, the conductance increases rapidly. In order to obtain a low threshold  $N_c$ , it is advantageous to consider films consisting of several monolayers with low coordination number.

O 53.7 Thu 16:30 SCH A215

**Metal-organic networks as templates for Fe and Co nanostructures** — ●UTA SCHLICKUM<sup>1</sup>, REGIS DECKER<sup>1</sup>, FLORIAN KLAPPENBERGER<sup>2</sup>, GIORGIO ZOPPELLARO<sup>3</sup>, SVETLANA KLYATSKAYA<sup>3</sup>, MARIO RUBEN<sup>3</sup>, JOHANNES BARTH<sup>2</sup>, and HARALD BRUNE<sup>1</sup> — <sup>1</sup>Institut de Physique des Nanostructures, EPF-Lausanne, Switzerland — <sup>2</sup>Physik Department E20, Technische Universität München, Germany — <sup>3</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany

Recently we demonstrated the capability to form extremely regular metal-organic honeycomb nanomeshes using linear dicyanide molecules in combination with Co atoms on Ag(111). The size of the network unit cell can be adjusted by the length of the employed linear molecular bricks [1]. In this contribution we present a new approach to steer the growth of metal-nanostructures using these metal-organic networks as templates. When depositing Fe or Co atoms onto the template, the metal atoms adsorb exclusively on top of the metal-organic network avoiding the open hexagonal cavities. In addition, the nucleation sites for Fe clusters can be shifted from the organic ligands towards the metal coordination nodes by changing the deposition temperature. Therefore, by tuning the honeycomb mesh size and the deposition temperature we can control the adsorption sites, the shape and the spacing of the small metal-clusters.

[1] U. Schlickum et al., Nano Lett. 3813 (2007)

O 53.8 Thu 16:45 SCH A215

**Silver cluster growth on highly oriented molecular films** — ●GÜNTHER WEIDLINGER<sup>1</sup>, LIDONG SUN<sup>1</sup>, MICHAEL HOHAGE<sup>1</sup>, SINA GUSENLEITNER<sup>2</sup>, STEPHEN BERKEBILE<sup>2</sup>, MICHAEL RAMSEY<sup>2</sup>, and PETER ZEPPEFELD<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Straße 69, A-4040 Linz — <sup>2</sup>Institut für Physik, Fachbereich Experimentalphysik, Karl-Franzens-Universität Graz, Universitätsplatz 5, A-8010 Graz

Para-sexiphenyl (p-6P) was deposited on the Cu(110)-(2x1)O surface at room temperature under UHV conditions. The structure of the (2x1)-reconstructed substrate served as a template for the growth of a highly ordered molecular film. The sequential deposition of p-6P films was monitored by means of Reflectance Difference Spectroscopy (RDS) showing a high optical anisotropy at the HOMO-LUMO transition energy, which is characteristic for the growth of a well-oriented molecular layer. Following the growth of this molecular layer, Ag clusters were prepared on the p-6P film by means of physical vapor deposition. The cluster growth can be monitored by the RD signal related to the particle plasmon resonance of the Ag clusters. Ex-situ AFM studies of these samples reveal that the Ag clusters are distributed homogeneously on the p-6P layer. Furthermore, photoelectron emission spectroscopy measurements show that the p-6P features are absent in the corresponding spectra, indicating that the Ag clusters are on top of the p-6P layer.

O 53.9 Thu 17:00 SCH A215

**Modification of SrTiO<sub>3</sub> single-crystalline surface after plasma flow treatment** — ●ALEXANDR A. LEVIN<sup>1</sup>, NIKOLAY A. KULAGIN<sup>2</sup>, TORSTEN WEISSBACH<sup>1</sup>, TILMANN LEISEGANG<sup>1</sup>, ENRICO LANGER<sup>3</sup>, and DIRK C. MEYER<sup>1</sup> — <sup>1</sup>Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Kharkiv National University for Radioelectronics, av. Shakespeare 6-48, 61045 Kharkiv, Ukraine — <sup>3</sup>Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany

Surface of pure and transition metal-doped SrTiO<sub>3</sub>(STO) single crystals before and after hydrogen plasma-flow treatment (energy of 5...20 J/cm<sup>2</sup>) is investigated by wide-angle X-ray diffraction (WAXRD), fluorescence X-ray Absorption Near Edge Structure (XANES) and scanning electron microscopy (SEM) techniques. Plasma treatment results in the formation of a textured polycrystalline layer at the surface of the single-crystalline samples with different orientation. The formation of the quasi-ordered structures consisting of nanoscale-sized pyramids is observed by SEM. XANES evidences the change of the valency of the

part of Ti<sup>4+</sup> to Ti<sup>3+</sup> due to the plasma treatment. The data obtained together with results of X-ray spectroscopy measurements [1] gives evidences of the change of stoichiometry of the STO samples resulting in a change of their physical properties after plasma treatment [2].

[1] N.A. Kulagin, A.A. Levin, E. Langer, D.C. Meyer, I. Doichinovich, Ya. Purich. Crystallography Reports 53 (N6) (2008) 1061-1067 [2] J.-C. Krupa, N.A. Kulagin. Physics of Laser Crystals. Kluwer Academic Publisher. Brussels, 2003

O 53.10 Thu 17:15 SCH A215

**Generation of phononic temperature waves during short pulse laser nanostructuring experiments on metals** — ●DMITRY IVANOV and BAERBEL RETHFELD — Technical University of Kaiserslautern, Physics Department, Erwin Schroedinger Str. 46, 67663 Germany

In this work we demonstrate the generation of phononic temperature waves in short pulse (pico- and femto-seconds) laser nanostructuring experiments on a metal surface. The existence of such waves was predicted based on numerical calculations with the atomistic-continuum model. This model describes the kinetics of transient nonequilibrium laser-induced processes at the atomic level and fast electron heat conduction in continuum. The analysis of obtained numerical data allowed to deduce the macroscopic parameters of observed thermal waves. The description of wave-like behavior within the frames of the diffusion equation is considered and the comparative analyzes between the continuum and the atomistic-continuum calculations is presented. The characteristic time of thermal wave relaxation was found to be on the level of 50 ns.

O 53.11 Thu 17:30 SCH A215

**Thermodynamics and sintering kinetics of Pt-Rh nanoalloys from lattice Monte Carlo simulations** — ●JOHAN POHL, MATHIAS NALEPA, and KARSTEN ALBE — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Pt-Rh nanoparticles play an important role as catalytically active material in many devices, but an in depth understanding of the thermodynamics and kinetics of this nanoalloy is, however, still lacking.

We have therefore studied the thermodynamics and kinetics of Pt-Rh nanoparticles in the framework of a bond-order simulation mixing model. First, the bulk phase-diagram is calculated that includes ordered low-temperature phases as predicted from first-principles calculations. Next, the role of finite-size effects for the phase stability in nanoparticles is investigated by semi-grand canonical Monte-Carlo simulations and thermodynamic integration, while order parameters of the finite and bulk phases are discussed. Finally, the model is extended to account for the kinetics of vacancy and surface diffusion.

Simulations of the sintering process of free particles of different sizes as well as sintering on a substrate with varying metal-substrate interaction are presented and compared with results from sintering theory.

O 53.12 Thu 17:45 SCH A215

**Surface enhanced Raman scattering of polymer molecules** — MANUEL GONÇALVES and ●OTHMAR MARTI — Universität Ulm - Inst. für Experimentelle Physik, Albert-Einstein-Allee 11, 89069 Ulm, Deutschland

Localized surface plasmons may enhanced the near-fields several orders of magnitude. The near-field enhancement depends strongly on shape and material of the metallic nanostructure. These enhancements permit to obtain Raman spectra of few of single molecules. However, spectral fluctuations and blinking were observed for single molecules adsorbed on metallic nanoparticles.

Surface enhanced Raman scattering (SERS) has been observed on polymer films, cast on silver nanostructures. Polymers as polybutadiene (PB), polybutadiene-block-polyisoprene (PB-b-PIP), poly(methyl methacrylate) (PMMA), and the elastomer polydimethylsiloxane (PDMS) were investigated. These materials present low fluorescence when illuminated with laser light of wavelength  $\lambda = 532$  nm, comparing to dye-molecules as Rhodamine 6G, usually used in SERS measurements. On the other hand, polymer molecules have long chains and may have many orientations close to rough metal surface. Therefore, averaged SERS spectra are expected for films. Nevertheless, SERS spectra with spectral fluctuations and blinking were observed.

The highest Raman enhancements occur at the edges and corners of the metallic particles. The near-field enhancements obtained from FEM based calculations confirm the experimental observations.

O 53.13 Thu 18:00 SCH A215

**Energy dissipation during hyperthermal deposition of non-IPR fullerenes on HOPG** — STEFAN-SVEN JESTER, DANIEL LÖFFLER, PATRICK WEIS, ●ARTUR BÖTTCHER, and MANFRED KAPPES — Institut für Physikalische Chemie, Universität Karlsruhe, 76131 Karlsruhe, Germany

Low energy cluster beam deposition, LECBD, has been used to generate thin films comprising monodisperse non-IPR fullerenes,  $C_n$ ,  $50 < n < 60$ , on HOPG. The topography of the resulting  $C_n$  films has subsequently been studied by AFM. Deposition experiments were carried out at hyperthermal incident kinetic energies,  $E_0$  (1-40 eV) and elevated surface temperatures  $T_s$  (300-700 K). Initial sticking of  $C_n$  cages is governed by the lateral density of step edges, which act as pinning and nucleation centers for migrating cages. Thus, in the early deposition stages, the surface exhibits large areas of empty terraces, while the step edges themselves are well-decorated. The terraces in turn become decorated by dendritic  $C_n$  islands in later deposition stages. Both, the mean size of these 2D islands and the mean distance between nearest islands,  $\delta$ , scale with the size of the terraces. When increasing the primary kinetic energy, the fractal-like islands become smaller and less dendritic in shape. The mean initial sticking coefficient decays exponentially with increasing  $E_0$ . Instead of the dendritic islands generated at room temperature, densely packed islands terminated by smooth rims are observed at elevated temperatures. The findings are rationalized by a model which describes the friction-conditioned energy losses in the sliding movement of the cages on terraces.

O 53.14 Thu 18:15 SCH A215

**Pt dimers landing on Cu(001): an *ab initio* approach** — ●GEORGE PAL, GEORG LEFKIDIS, and WOLFGANG HÜBNER — Fachbereich Physik, Technische Universität Kaiserslautern, P.O.Box 3049, 67653 Kaiserslautern, Germany

We present real-space first-principles calculations for the adsorption of not only one but also two Pt clusters on a non-magnetic Cu(001) substrate. Considering that the interaction of adsorbates on surfaces is a local phenomenon, a representation of the substrate by a large cluster of 74 Cu atoms allows one to treat the electronic structures of both systems, i.e., the adsorbate and the surface, on equal footing. Using highly correlated quantum chemistry, we investigate different scenarios of soft-landing of Pt dimers on the substrate, for which we also optimize the Pt-Pt distance, and we compute the electronic excited states, which yields the optical absorption spectrum, on top of the electronic configuration at equilibrium geometry.

By analyzing the absorption spectra and the electronic densities of states we are able not only to characterize the interactions between the adsorbates and the substrate, but also to identify the surface-mediated interactions among the dimers. The latter is very important for technological applications since in experimental setups metallic substrates can alter the properties of the adsorbates, thus leading to new physics.

[1] Y. Pavlyukh, J. Berakdar and W. Hübner, Phys. Rev. Lett. **100**, 116103 (2008)

[2] G. Pal, G. Lefkidis and W. Hübner, submitted to J. Phys. Chem.