

O 10: Nanostructures at Surfaces I

Time: Monday 10:30–13:00

Location: H45

O 10.1 Mon 10:30 H45

Realization of a single-atom transistor in silicon — ●MARTIN FUECHSLE, JILL A. MIWA, SUDDHASATTA MAHAPATRA, and MICHELLE Y. SIMMONS — Centre for Quantum Computation & Communication Technology, University of New South Wales, Sydney 2052, Australia

Scanning tunneling microscopy (STM) has been demonstrated to enable the positioning of individual atoms on metallic surfaces with unprecedented resolution [1]. However, the realization of atomic-scale logic circuits in silicon was hampered by the covalent nature of its bonds. While resist-based strategies allowed the formation of nanostructures on the silicon surface, truly atomic-scale devices, such as donor-based quantum computation devices [2], require the ability to position individual atoms within the silicon crystal with atomic precision. Here, we present a single-atom transistor based on an individual phosphorus donor patterned with a spatial accuracy of ± 1 lattice site within an epitaxial silicon environment. Using STM-based hydrogen lithography, the single impurity is deterministically placed between highly-doped transport electrodes. Low-temperature measurements confirm the presence of a single donor, the charge state of which can be precisely controlled with gate voltages. We find a charging energy that is similar to the value expected for isolated P donors in bulk silicon, previously only observed by optical spectroscopy. Our work presents an important step towards scalable donor-based quantum computer architectures.

[1] D.M. Eigler and E.K. Schweizer, *Nature* **344**, 524 (1990); [2] B.E. Kane, *Nature* **393**, 133 (1998).

O 10.2 Mon 10:45 H45

First-principles investigation of monoatomic and dimer Mn adsorption on noble metal (111) surfaces — ●FRANCISCO MUNOZ^{1,2}, ALDO ROMERO², JOSE MEJIA-LOPEZ³, and JOSE LUIS MORAN LOPEZ⁴ — ¹Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — ²Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — ³Fac. de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — ⁴Dep. de Física, Fac. de Ciencias, UNAM, Mexico D. F., Mexico

A DFT-based investigation of the adsorption of Mn single atoms and dimers on the (111) surfaces of Cu, Ag, and Au is presented. The electronic structure of the Mn adatom, chemisorbed in all inequivalent surface geometries, is analyzed. For all three substrates, the most stable geometry is a Mn atom chemisorbed in a threefold coordinated site. For the dimer, the least-energy configuration corresponds to the molecule lying parallel to the surface. In this geometry, both atoms are chemisorbed in threefold coordinated sites, but with different local symmetry. It is also found that the magnetic ground-state configuration is an antiferromagnetic arrangement of the Mn atoms; however, for the Ag substrate, the ferromagnetic state is close in energy. Furthermore, the Mn₂ molecule is chemisorbed with very similar energy on various geometries. To study the dynamical motion of the dimer components, we calculated the potential energy barriers for the Mn motion at the various surfaces. We conclude that the Mn dimer moves relatively freely for Ag, in contrast to Cu and Au.

O 10.3 Mon 11:00 H45

Nanopatterning of Cu(111)/Cu₂O by Focused Electron Beam Induced Processing — ●MARTIN DROST, FAN TU, ESTHER CARRASCO-BURGOS, MATTHIAS FRANKE, FLORIAN VOLLNHALS, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The fabrication of well-defined nanostructures on surfaces is an important goal in scientific research and technology. One can distinguish two general approaches: the bottom-up route, e.g., based on the self-assembly of molecules, and top-down methods like electron beam lithography to generate arbitrarily shaped structures. We target the combination of both by applying Focused Electron Beam Induced Processing (FEBIP) on a Cu(111)/Cu₂O surface to fabricate nanoscaled templates for the directed self-assembly of functional molecules. The interaction with the defined controlled electron beam induces chemical changes on the oxide surface on the nanometer scale. The feasibility of this approach was investigated by a combination of Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM) and

Auger Electron Spectroscopy (AES). Latest results will be presented and discussed.

O 10.4 Mon 11:15 H45

Electron quantization in arbitrarily shaped Au islands on MgO thin films — ●CHRISTIAN STIEHLER¹, YI PAN¹, WOLF-DIETER SCHNEIDER¹, PEKKA KOSKINEN², HANNU HÄKKINEN², NIKLAS NILIUS NILIUS^{1,3}, and HANS-JOACHIM FREUND¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — ²Departments of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, P.O. Box 35 (YFL), FI-40014 Finland — ³Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg, Germany

Electron quantization is a fundamental phenomenon that accompanies the transition from bulk metals to nanoclusters. The associated opening of a gap at the Fermi level crucially affects various properties of the nanostructure, e.g. its electrical and optical behavior and its performance in catalytic reactions [1]. By using low-temperature STM and STS, we have investigated the electronic structure of differently shaped 2D Au islands grown on MgO/Ag(001) thin films, concentrating on the size regime of the metal-insulator transition that occurs between 50-200 atoms in gold clusters. The observed symmetries and energy positions of quantum well states were rationalized by simple analytical models as well as by a density-functional-tight-binding approach that accounts also for structural disorder in the islands. Based on a statistically relevant number of single-cluster experiments, we derived general conclusions on the size of the HOMO-LUMO gap as a function of atom count and symmetry of the metal nanostructures.

[1] M. Valden, X. Lai, D. W. Goodman, *Science* **281**, 1647 (1998)

O 10.5 Mon 11:30 H45

Energy dependent nanoparticle deposition on a W(110) surface — WOLFGANG ROSELLEN, ●HENDRIK BETTERMANN, TORSTEN VELTUM, and MATHIAS GETZLAFF — Institute of Applied Physics, University Duesseldorf

Deposited clusters and nanoparticles are rather interesting objects not only from a fundamental point of view but additionally for technological applications due to their electronic and magnetic properties which depend strongly on the particle size. The structure determination after deposition is important because it significantly influences these properties. Our contribution is focused on magnetic 3d-nanoparticles on a W(110) substrate. After creation in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS) these particles are size selected by an electrostatic quadrupole. Mass selection and acceleration are possible because 50% of the particles are positively or negatively charged. Applying a voltage to the targeted substrate allows us therefore to change the deposition energy. Our investigations are carried out by means of scanning tunneling microscopy (STM). We will report on size and structural properties of Fe/Co particles at softlanding conditions at a kinetic energy below 1 eV per atom and compare it with accelerated and decelerated particles. We demonstrate that deceleration leads to reduced deformation whereas acceleration results in leaving the softlanding regime.

O 10.6 Mon 11:45 H45

Decoration of Co island edges on Cu(111) by Fe — ●JEISON A. FISCHER^{1,2}, SOO-HYON PHARK¹, MARCO CORBETTA¹, DIRK SANDER¹, and JÜRGEN KIRSCHNER^{1,3} — ¹Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — ²LFFS, Universidade Federal de Santa Catarina, Florianópolis, SC, Brazil — ³Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

We performed low temperature scanning tunneling spectroscopy (LT-STs) measurements on almost triangular bilayer Co islands on Cu(111), which were decorated along the rim by a nm wide Fe stripe. The sample was prepared by subsequent deposition of Co[1] and Fe at 300 K. We obtained energy resolved differential conductance maps for islands with different lateral size. We find that Fe decoration induces a vanishing of the well-established electronic rim state of Co [1, 2]. The Fe-decorated islands show a pronounced spatial modulation of the differential conductance within the Co core, which we ascribe to electron confinement. A quantitative analysis [3] identifies the characteristic length of confinement. It corresponds exactly to the geometrical height

of the triangular Co core, as derived from constant current topography STM images. The comparison between characteristic lengths of Fe-decorated-Co islands and pure Co islands establishes the electronic rim state as the relevant boundary for electron confinement of the latter. This leads to a smaller characteristic length for confinement in pure Co as compared to Fe-decorated islands. [1] Pietzsch et al. Phys. Rev. Lett. 96, 237203 (2006). [2] Oka et al. Science 327, 843 (2010) [3] Rodary et al. Phys. Rev. B 75, 233412 (2007)

O 10.7 Mon 12:00 H45

Dynamics of Adsorbed EBID Precursors (W(CO)₆ and Co₂(CO)₈) and their Fragments — ●MUTHUKUMAR KALIAPPAN^{1,2}, HARALD JESCHKE¹, and ROSER VALENTI¹ — ¹Institut für Theoretische Physik, Max-von-Laue-Straße 1, 60438, Frankfurt am Main, Germany — ²muthukumar.kaliappan@gmail.com

We investigate the fundamentals of the growth process of nano composites in electron beam induced deposition (EBID) process using first principles molecular dynamics simulation. We compare the behavior of two carbonyl precursors (W(CO)₆ and Co₂(CO)₈) on two different SiO₂ surfaces (fully hydroxylated (FOH) and partially hydroxylated (POH)) that represent realistic EBID conditions. These precursors are commonly used to obtain tungsten and cobalt composites and our 20 ps simulations illustrates that these precursors are stable and mobile on the FOH surfaces behaving similar to the gas phase molecules. However, they fragment on POH surfaces upon their interaction with the surface active sites and tend to remain localized on their bonding sites. Apart from changes in the orientation, they show no tendency for the reformation of the parent precursor molecule. Vibrations of these adsorbed species are studied by computing their power spectrum from the trajectory that provides crucial information on the nature of adsorbed precursor fragments.

O 10.8 Mon 12:15 H45

Field equation for pattern formation on ion-beam eroded surfaces including redepositional effects — ●MARC OSTHUES, CHRISTIAN DIDDENS, and STEFAN LINZ — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

In the last decades various self-assembled spatially ordered nanopatterns on semiconductor surfaces generated by low-energy ion-beam erosion have been found in experiments. We have studied a modified damped Kuramoto-Sivashinsky equation as one representative continuum model for the formation of these surface patterns. Previous works [1,2] on modeling the redeposition mechanism taking place during the erosion process suggested that it is appropriate to take a linear and quadratic damping term into account. Using numerical simulations

and approximate analytical calculations, we show that the resulting field equation for the evolution of the surface morphology for normal ion incidence exhibits a variety of patterns, such as hexagonal dot and hole structures as well as ripple structures as a function of the parameters of the system.

[1] C. Diddens, S. J. Linz, unpublished

[2] N. Anspach, S. J. Linz, J. Stat. Mech., P06023 (2010)

O 10.9 Mon 12:30 H45

Continuum modeling of particle redeposition during ion-beam erosion — ●CHRISTIAN DIDDENS and STEFAN J. LINZ — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We have thoroughly investigated the effect of particle redeposition during ion-beam erosion for normal ion incidence within the framework a continuum model. The complicated highly non-local redeposition effect can be approximated in terms of the relative surface height with coefficients depending on the surface aspect ratio. For reasonable surface morphologies, our results are universal, i.e. do not qualitatively depend on the specific details of the sputter yield, preferred erosion directions or whether one or two lateral dimensions are considered. Furthermore, we show that an interplay of erosion, diffusion and redeposition is generically able to reproduce the hexagonally arranged nanodot patterns found in experiments with semiconductor targets.

O 10.10 Mon 12:45 H45

Supported Silver Nanoparticles for Catalytic Reactions: A RHEED Study — ●STEPHAN BARTLING, INGO BARKE, HANNES HARTMANN, and KARL-HEINZ MEIWES-BROER — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Size-selected Ag clusters deposited on amorphous alumina films can act as selective and efficient nanocatalysts for the partial oxidation of propylene [1]. In this contribution we present results for *in situ* reflection high energy electron diffraction (RHEED) from soft-landed Ag clusters in the size range of a few nm. The focus is placed on the alignment between particles and substrate that is driven by cluster-surface interaction. Whereas on highly ordered surfaces pronounced alignment was particularly found for small clusters [2], on thin Al₂O₃ layers deviations from a random orientation can only be observed for large Ag clusters (≤ 10 nm). The analysis of such spontaneous orientation along high-symmetry crystal directions parallel to the surface is assisted by *ex situ* AFM measurements.

[1] L.M. Molina et al., Catalysis Today **160**, 116 (2011)[2] A. Kleibert et al., Phys. Status Solidi B **247**, 1048 (2010)