O 35: Nanostructures at Surfaces

Time: Tuesday 18:15-21:00

Location: Poster A

O 35.1 Tue 18:15 Poster A

Reactivity of Pt nanocluster arrays — •KARIN GOTTER-BARM, FLORIAN SPÄTH, UDO BAUER, CARINA BRONNBAUER, OLIVER HÖFERT, HANS-PETER STEINRÜCK, and CHRISTIAN PAPP — Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Graphene-supported nanocluster arrays are intriguing systems for the investigation of catalytic processes. We report on the reactivity of Pt nanoparticles deposited on graphene/Rh(111). High resolution XPS was employed to investigate the interaction with CO and SO₂ as well as the oxidation of CO. Three CO-induced species are observed in the C 1s core level spectra. These are assigned to CO adsorbed in on-top and bridge terrace sites and step sites in comparison with single crystal data. The step sites are occupied first during adsorption and show the highest desorption temperature, indicating that these are the most stable adsorption sites for CO. The oxidation of CO follows roughly pseudo first order kinetics. The activation energy determined from an Arrhenius analysis was found to be smaller than for stepped platinum crystals. The adsorption and reaction of SO₂ is monitored by measuring the S 2p core level, showing several SO_x (x = 1 - 3) species as intermediates and sulfur as final product on the surface.

This work was supported by SFB 953 "Synthetic Carbon Allotropes".

O 35.2 Tue 18:15 Poster A

Deposition of small clusters on oxide films and investigation of their mobility — •RAPHAEL FLOEGEL¹, CHRISTOPH SCHRÖDER¹, DOMINIK WOLTER¹, MATTHIAS BOHLEN¹, CONRAD BECKER², and HEINZ HÖVEL¹ — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, Germany — ²Aix-Marseille Université, CINaM, Marseille, France

Metal oxides have many applications (catalysis, microelectronics etc.). Al_2O_3 oxide films produced by oxidation of $Ni_3Al(111)$ can be used as a template for cluster growth. [1] They are characterised with Low-Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM).

Oxide films are also favourable for the study of deposited clusters because on the one hand the clusters are only marginally influenced by the substrate surface. On the other hand thin oxide films can still be characterised with STM. By the deposition of small mass selected clusters on the produced oxide films a systematic investigation of their mobility and coalescence depending on their size can be performed.

[1] S. Degen, C. Becker and K. Wandelt, Faraday Discuss., **125**, 343-356 (2004).

O 35.3 Tue 18:15 Poster A

FeNi nanoparticle preparation and deposition on W(110) — •HENDRIK BETTERMANN, MATTHIAS WERNER, and MATHIAS GET-ZLAFF — Institute of Applied Physics, University of Duesseldorf

Deposited clusters and nanoparticles are rather interesting objects not only from a fundamental point of view but also for technological applications due to their electronic and magnetic properties which show a strong dependence on particle size. Interactions between nanoparticles and substrate during and after deposition have an important influence on particle properties.

Our contribution is focused on Fe/Ni alloy nanoparticles of up to 5 nm in diameter.

We report on our initial results of a newly installed magnetron sputter aggregation source. Particles are mass/charge filtered in a quadrupole mass selector and deposited on a W(110) substrate. Size and structural properties are investigated by means of scanning tunneling microscopy (STM) under UHV conditions. We compare these results with those of larger nanoparticles of similar composition.

O 35.4 Tue 18:15 Poster A

Fabrication and characterization of silicon nanoparticles embedded in amorphous atomic layer deposited Al2O3 — •KLEMENS ILSE¹, JOHANNES ZIEGLER¹, ALEXANDER SPRAFKE¹, and RALF WEHRSPOHN^{1,2} — ¹Department of Physics, Martin-Luther University Halle-Wittenberg, Halle (Saale), 06120, Germany — ²Fraunhofer Institute for Mechanics of Materials IWM, Halle (Saale), 06120, Germany Due to their promising material properties and opportunities for integration into silicon planar technologies, silicon nanoparticles are subject of high interest for next-generation applications in microelectronics, photonics, photovoltaic, or nanobiotech industries. Common silicon nanoparticle fabrication techniques, such as ion implantation, magnetron sputtering or the superlattice approach include annealing steps with temperatures above 1000° C to enable formation and crystallisation of silicon nanoparticles. Typically, the obtained silicon nanocrystals are embedded in a matrix consisting of silicon dioxide or silicon nitride.

In this work, silicon nanoparticles were fabricated by low-pressure non-thermal plasma-processes and embedded in amorphous aluminium oxide produced by atomic layer deposition (ALD). Both processes were performed in a single reactor without any vacuum break in between and in a low temperature regime.

Here, characterization results concerning the crystallinity, photoluminescence, material composition, and particle size of the embedded silicon nanoparticles are presented and discussed.

O 35.5 Tue 18:15 Poster A Mass selected metal clusters on rare gas films: comparison with free beam data — •Christoph Schröder¹, Natalie Miroslawski¹, Dominik Wolter¹, Matthias Bohlen¹, Bernd von Issendorff², and Heinz Hövel¹ — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund — ²Albert-Ludwigs-Universität Freiburg, Physikalisches Institut, 79104 Freiburg

Mass-selected metal clusters were deposited on rare gas layers in order to investigate the electronic structure of the nanoparticles influenced by the surface. The electron states are analyzed with ultraviolet photoelectron spectroscopy (UPS), using a monochomatic argon discharge lamp with a photon energy of $h\nu$ =11.6 eV. As a reference we use UPS spectra of clusters measured in a free beam [1,2]. Using investigations of C₆₀ molecules on rare gas films, the quantitative comparison between the spectra for clusters in a free beam and deposited on rare gas is significantly improved.

[1] O. Kostko, PhD-thesis, Albert-Ludwig-Universität Freiburg (2007).

[2] H. Häkkinen, M. Moseler, O. Kostko, N. Morgner, M. A. Hoffmann and B. v. Issendorff, Phys. Rev. Lett. **93**, 093401 (2004).

O 35.6 Tue 18:15 Poster A Temperature dependent shape of deposited FeNi nanoparticles — •MATTHIAS WERNER, HENDRIK BETTERMANN, and MATHIAS GETZLAFF — Institute of Applied Physics, University of Duesseldorf Most of the properties of nanoparticles significantly depend on their size. For alloy systems the stoichiometry also plays an important role. In this contribution we report on the temperature dependent shape of size-selected deposited FeNi nanoparticles. This investigation is carried out by STM.

Fe50Ni50 Nanoparticles are produced by an arc cluster ion source (ACIS) and mass-filtered by an electrostatic quadrupole. The particles with diameters from 5 to 15 nm are deposited under UHV and softlanding conditions on a W(110) surface. They are tempered in situ by a resistive heater integrated in the manipulator. The heating process is varied in intensity and time. Melting point and variations close to it are observed to depend on the clusters' diameter. The influence of the anisotropy of the W(110) surface is also taken into consideration.

O 35.7 Tue 18:15 Poster A

Production and deposition of mass-selected iron clusters on MoS₂ **investigated with AFM** — •MATTHIAS BOHLEN, CHRISTOPH SCHRÖDER, DOMINIK WOLTER, and HEINZ HÖVEL — Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

In order to deposit iron clusters on various surfaces, we used a magnetron-sputter gas aggregation cluster source [1] and a semicontinuous time-of-flight mass selector [2]. For iron clusters the simulation of suitable target geometry was important. We deposited $Fe_{2000 \pm 36}$ clusters with different coverages, from 1% to 20% of a cluster-monolayer, on different samples. Using a cleaved surface of a MoS₂ crystal, atomically flat on microscopic areas but providing some bonding of the clusters, we were able to use atomic force microscopy (AFM) and verify a narrow cluster height distribution. The change of the cluster size due to contact with air is discussed.

 H. Haberland, M. Mall, M. Moseler, Y. Qiang, Th. Reiners, Y. Thurner, J. Vac. Sci. Technol. A 12, 2925 (1994).

[2] B. von Issendorff, R.E. Palmer, Rev. Sci. Instru. **70**, 4497 (1999).

O 35.8 Tue 18:15 Poster A

3d metal nanoparticles deposited on graphene — •WOLFRAM GILBERT, TORSTEN VELTUM, HENDRIK BETTERMANN, and MATHIAS GETZLAFF — Institute of Applied Physics, University of Düsseldorf

In the past few years graphene gained the attention of scientists due to its unique mechanical and electrical properties. In addition to this, fabrication and deposition of nanoparticles on a substrate is of great interest for studies, e.g. as model catalysts. In this contribution we compare the properties of nanoparticles deposited on graphene with those on a 3d metal thin film.

A thin metallic film is epitaxially grown by electron beam evaporation on a W(110) single crystal under ultra-high vacuum conditions. To achieve a structurally ordered monolayer graphene on the ferromagnetic substrate we use chemical vapour deposition with propylene. The structure of this system is characterized in-situ by means of scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED).

The nanoparticles are produced by a continuously working arc cluster ion source (ACIS), mass-selected by an electrostatic quadrupole $(\Delta m/m=10\%)$ and subsequently deposited on the target surface under soft landing conditions. The structural analysis of the nanoparticles is carried out by STM.

O 35.9 Tue 18:15 Poster A Deposition of mass selected clusters produced with the THErmal CLuster Apparatus (THECLA) — •ANDREAS GRUHN, STEFANIE ROESE, JENS-CHRISTIAN MEYER, DAVID ENGE-MANN, and HEINZ HÖVEL — Fakultät Physik / DELTA, TU Dortmund, Germany

The clusters in THECLA are produced in a supersonic nozzle expansion [1][2]. In this case the clusters have a mass distribution and a narrow velocity distribution. A typical cluster consists of $(2.5\pm^{2.8}_{1.7})\cdot 10^2$ atoms and has a velocity of $1.3 \cdot 10^3 \,\mathrm{m}$. It is a matter of particular interest to have a mass selected cluster beam. In the source the clusters are partially ionized. The ion current is increased by a hot-cathode plasma ionisation [3]. Because of their charge, the cluster ions can be mass selected by deflection in a transverse electric field. The ion current is measured with a moveable Faraday cup. After deposition on substrates, the clusters can be characterized by atomic force microscopy (AFM) and transmission electron microscopy (TEM). The quality of mass selection is determined by comparing the results and the mass spectrum of the source. Based on the measurements and simulations, the ion optics is optimized. The goal is to achieve maximum quality of the mass selection with a sufficient high ion current. This allows more accurate measurements of properties depending on the cluster size.

 O. F. Hagena, Z. Phys. D 20, 425 (1991).
H. Hövel et al., Phys. Rev. B 48, 18178 (1993).
I. M. Goldby et al., Rev. Sci. Instrum. 68, 3327 (1997).

O 35.10 Tue 18:15 Poster A

Contamination induced defect formation during Chemical Vapor Deposition of graphene and the formation of silicon dendrites — •UMUT KAMBER¹, CEM KINCAL¹, BARIŞ YAĞCI², ÖZGÜR BIRER², and OĞUZHAN GÜRLÜ¹ — ¹Istanbul Technical University, Istanbul, Turkey — ²Koç University, Istanbul, Turkey

Chemical Vapor Deposition (CVD) is an effective method used for producing graphene on copper foils. During CVD process Cu foils are heated up to 1200 K in a quartz tube under the flow of a mixture of hydrogen and argon. In order to grow graphene methane is let in to the tube for a short while with a very small flow rate compared to argon or hydrogen. Depending on the temperature during growth, flow rates of each gas, as well as on heating and cooling rates, the quality of graphene is affected. In our work we encountered silicon contamination on some of the sample batches. We have made systematic preparations and measurements in order to understand the reason of such contamination. Depending on the existence of graphene the shapes and sizes of such contaminants were observed to vary. The formation of point like and dendritic silicon-oxide islands on graphene and their manipulation by means of localized etching will be presented. O 35.11 Tue 18:15 Poster A Investigation of the geometric structure of small deposited Au clusters. — IVAN BAEV¹, TORBEN BEECK¹, •DENIZA CHEKRYGINA¹, STEPHAN KLUMPP¹, MICHAEL MARTINS¹, STEPHAN ROTH², PARASMANI RAJPUT³, GONZALO SANTORO², SARATHLAL KOYILOTH VAYALIL², and WILFRIED WURTH^{1,2} — ¹Physics Department, University of Hamburg, D-22761, Hamburg, Germany — ²DESY, D-22607, Hamburg, Germany — ³3Atomic & Molecular Physics Division, Bhabha Atomic Research Center, Trombay, 400085, Mumbai, India

The investigation of new materials is nowadays propelled by the possibility to create size selected clusters of any desired materials. With the improvement of new 3rd generation synchrotron sources it should be possible to measure the geometric structure of clusters as small as several atoms in size. So far studies using spectroscopic techniques have focused on electronic and magnetic properties of small deposited metal clusters which could show new promising physical and chemical properties.

In this work we present a development towards disentangling structural effects from pure electronic effects as function of cluster size, with a main goal to investigate the geometry of deposited Au clusters on a Si wafer stabilized with an Al cap layer. In our work we are going to use grazing incidence small angle x-ray scattering (GISAXS) and x-ray absorption spectroscopy (EXAFS) to achieve this goal.

This work is supported by a PIER innovation grant.

O 35.12 Tue 18:15 Poster A Scanning photoelectron microscopy of high-temperature- $C_{sx}C_{68}$ — •JÜRGEN WEIPPERT¹, SEYITHAN ULAS¹, SHARALI MALIK², MATTEO AMATI³, LUCA GREGORATTI³, MAYA KISKINOVA³, and ARTUR BÖTTCHER¹ — ¹Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — ³ESCA microscopy beamline Elettra - Sincrotrone Trieste, ScPA Area Science Park, 34149 Basovizza-Trieste, Italy

Surface morphology of the non-IPR fulleride $Cs_x C_{68}$ grown via codepositing Cs and mass-selected C_{68}^+ in UHV has been studied by scanning photoelectron microscopy (Escamicroscopy). $Cs_x C_{68}$ survives heating up to $T^* \approx 1000K$ and shows a high thermal stability (related IPR fullerides: decomp. $\approx 800K$). The C1s- and Cs4d-based images revealed Cs-rich islands as striking species surrounded by planar Cs-poor areas. The islands are created by thermally activated segregation of Cs atoms emerging from the subsurface region. Whereas C1s and Cs4d XP spectra taken from the Cs-poor regions show ionic bonds stabilizing the $Cs_x^{+a} C_{68}^{-b}$ compound the chemical state of the elements constituting the Cs-rich islands are photoactive: Initially Cs4d band exhibits four components (69 – 81eV), and C1s band consists of two components (281 – 286eV). This structure evolves under illumination ($hv \approx 500eV$) towards the pattern of ionic -C-Cs bonds.

O 35.13 Tue 18:15 Poster A Does the band structure picture hold for Si Nanocrystals of few nm in size? — Prokop Hapala, •Ante Šiljić, Pavel Jelínek, Pingo Mutombo, Katerina Kusova, and Ivan Pelant — Institute of Physics of the ASCR, v.v.i. Cukrovarnicka 10, Prague 6, Czech Republic

There has been a long-standing discussion on whether or not an electronic band structure concept. i.e. energy-to-wavevector dispersion, can be assigned to zero-dimensional objects such as quantum dots (nanocrystals) (see e.g. [1]). To answer this question, we developed a general method [2], which allows reconstruction of electronic band structure of nanocrystals from ordinary real-space electronic structure calculations. We combine the method with fully relaxed large-scale Density Functional Theory calculations of a realistic Si nanocrystals of up to 3 nm in size with different surface passivations including hydrogen, hydroxyl and methyl groups [3]. To demonstrate character of the band structure of Si nanocrystals, we calculate band dispersion along the Γ -X direction to compare it with a bulk counterpart. Based on this comparison, we conclude that the band structure concept is applicable to silicon nanocrystals with diameter larger than ~ 2 nm with certain limitations. In addition we will discuss impact of polarized surface hydroxyl groups or geometric distortion on momentum space selection rules important for light emission.

- [1] M. S. Hybertsen, Phys. Rev. Lett. 72, 1514 (1994)
- [2] P. Hapala, et al., Phys. Rev. B 87, 195420 (2013)
- [3] K. Kůsová et al., ACS Nano 4, 4495 (2010)

O 35.14 Tue 18:15 Poster A

SiOx nanoparticles generation in the gas phase by pulsed DC magnetron sputtering — •OLEKSANDR POLONSKYI, EGLE VASILI-AUSKAITE, THOMAS STRUNSKUS, and FRANZ FAUPEL — Institute for Materials Science, Chair for Multicomponent Materials, Christian-Albrechts University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Nanoparticles and their composites have received an increasing attention in the last few decades due to their unique chemical, physical, mechanical, electrical, and optical properties, which provide hosts of potential applications in modern technology. Si-based nanomaterials are in particular interest. In this work we utilize such called gas aggregation cluster sources (GAS), based on the magnetron sputtering, for fabrication of SiOx nanoparticles. We observed that a low concentration of oxygen is necessary to admix for the cluster formation process. It was shown that a gas aggregation source based on pulsed reactive DC magnetron sputtering gives rise to a high increase in deposition rate of nanoparticles compared to continuous operation. The focus of the contribution is on nanoparticles size control and cluster growth and transport mechanism in the GAS. The influence of experimental conditions (Ar pressure/flow, discharge parameters, oxygen admixture) on nanoparticles size was investigated. The prepared nanoparticles were characterized with regard to chemical composition, morphology and optical properties.

O 35.15 Tue 18:15 Poster A Teaching the growth of nanostructures and Ostwald ripening in a master course chemistry — •JAN PHILIPP MEYBURG and DETLEF DIESING — Universität Duisburg-Essen

Growth of nanostructures and processes as ageing and ripening of grown nanostructures are fundamental for the understanding of processes in catalysis, for instance. The authors show a computer experiment based on a kinetic Monte Carlo simulation. The computer experiment describes both phenomena, growth and ripening applied to the homoepitaxial growth of silver on a Ag(111) surface. Using DFT data for the activation energy of diffusion and lateral pair interaction energies the computer experiment simulates the island formation during the nanostructure growth in the regime of low coverages $\theta \approx 0.1$. If the adsorption processes are switched off, the dendritic to hexagonal shapes of the nanostructures change to larger sphere like structures due to sole surface diffusion as typical for Ostwald ripening. A selection of the first student results is shown. These results are compared with STM experiments [1,2] for growth and ripening on (111) surfaces. [1] E. Cox et al. Phys. Rev. B, 71:115414, 2005 [2] K. Morgenstern et al., Phys. Rev. Lett., 76:2113, 1996.

O 35.16 Tue 18:15 Poster A

Hydrogenation of doped silicon clusters — •CHRISTINE BÜLOW¹, VICENTE ZAMUDIO-BAYER¹, ARKADIUSZ LAWICKI¹, GEORG LEISTNER¹, KONSTANTIN HIRSCH¹, BERND VON ISSENDORFF², and TOBIAS LAU¹ — ¹Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — ²Physikalisches Institut, Universität Freiburg, Freiburg, Germany

Silicon is the most widely used semiconductor for various applications. Due to the demand of miniaturization of electronic devices there has been a high interest to study silicon nanoparticles. Small 3d-transitionmetal doped silicon clusters show a distinct behavior of their magnetic properties: While in exohedrally doped species the dopant exhibits almost atomic spin magnetic moments, endohedrally doped silicon clusters loose the spin polarization of the metal dopant atom. This quenching is coordination driven and several theoretical investigations predict that hydrogen passivation can restore the magnetic moment of the dopant. Additionally, hydrogen passivation stabilises the clusters.

In this work we present two different methods to produce free hydrogen passivated silicon clusters in the gas phase using a magnetron sputtering source. Hydrogenation is either done by introducing hydrogen into the plasma of the magnetron or by physio- or chemisorption in a collision cell. The cluster composition is analysed in a time-of-flight mass spectrometer. We discuss the mass spectra of these two different preparation methods.

O 35.17 Tue 18:15 Poster A Protein-Assisted Assembly of Nanoparticles on Nanoparticles: Toward Plasmonic Nanoclusters — •Roland Höller, ANDREAS FERY, and MUNISH CHANANA — Department of Physical Chemistry II, University of Bayreuth, 95440 Bayreuth, Germany

Metallic core-satellite nanoclusters are highly interesting for their potential applications in the fields of surface-enhanced Raman spectroscopy (SERS), light harvesting, and optical metamaterials due to their ability to support localized surface plasmons and thus allowing to manipulate electromagnetic fields at the nanoscale.[1] Many strategies have been developed to assemble colloidal plasmonic nanoparticles into metal-metal core-satellite nanoclusters using small alpha-omega endfunctionalized molecular linkers, viruses, and DNA.[2] However, most of these approaches for nanocluster fabrication are either limited to 2D structures on substrates or arduous and expensive in synthesis. In this work, we present a novel protein-assisted nanoparticle assembly method, which is simple, inexpensive and upscalable, yielding highly stable and well-defined plasmonic core-satellite nanoclusters with small interparticle distances. The morphology of the nanoclusters was characterized using TEM and SEM. The optical properties were studied at the ensemble level and single cluster level by means of UV-Vis spectroscopy and dark-field optical microscopy and spectroscopy.

[1] Fan et al., Science 2010, 328, 1135.

[2] a) Gandra et al., Nano Letters 2012, 12, 2645; b) Li et al., Small 2012, 8, 3832; c) Sebba et al., Nano Letters 2008, 8, 1803.

O 35.18 Tue 18:15 Poster A Interaction of Palladium with Ultrathin Ionic Liquid films — •BENJAMIN MAY, FLORIAN RIETZLER, HANS-PETER STEINRÜCK, and FLORIAN MAIER — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Profound knowledge of the interfaces between ionic liquids (ILs) and catalytically active transition metals is highly relevant in heterogeneous catalysis. In particular in SCILL (Solid Catalyst with Ionic Liquid Layer) systems, the IL layer allows modifying reactions by influencing solubility of reactants and/or selectivity of the catalyst (co-catalytic effect).[1]

X-ray photoelectron spectroscopy (XPS) was used in this study to obtain basic information on the interactions between an ionic liquid (IL) and palladium atoms and nanoparticles. To do this ultrathin films of the IL 1-ethyl-3-methylimidazolium trifluoromethanesulfonate were prepared on an Au(111) surface via IL physical vapor deposition[2] at different substrate temperatures. Pd was then thermally evaporated onto these frozen and liquid IL films. Interactions of IL and Pd as well as changes in IL film morphology were monitored by XPS.

This work was supported by the Cluster of Excellence Engineering of Advanced Materials.

- [1] U. Kernchen et al., Chem. Eng. Technol. 2007, 30, 985-994.
- [2] T. Cremer et al., Langmuir 2011, 27, 3662-3671.