O 31: Nanostructures at surfaces: Dots, particles, clusters, arrays II

Time: Tuesday 11:15–13:15 Location: WIL C107

O 31.1 Tue 11:15 WIL C107

Electrochemical preparation of Co-Ag nanostructured materials for GMR applications — •José Manuel García — University of Barcelona, Barcelona, Spain

Although giant magnetoresistance (GMR) phenomenon was discovered in sputtered Fe/Cr multilayers, some years later other configurations (i.e. granular films or nanowires) as well as other systems (i.e. Co/Cu, CoFe/Ag) were found to exhibit this property. Among those systems the Co-Ag system seems to be a good candidate as magnetoresistive material, because sharp magnetic/non-magnetic interfaces are expected in view of the total immiscibility between the two metals shown by the phase diagram. On the other hand, electrodeposition is a technique that day by day is gaining positions among the mainly employed physical methods for the preparation of thin films. This is due to the fact that electrodeposition shows some advantages over the physical techniques: versatility, selectivity, higher deposition rates and higher thicknesses, among others.

This work focuses on the preparation of different kinds of Co-Ag nanostructured materials with giant magnetoresistance. Granular films, multilayers and nanowires were prepared taking profit of the versatility of electrodeposition. Co(Core)-Ag(Shell) nanoparticles were also prepared but by a chemical method. The interest was to compare the properties of the Co-Ag materials obtained under the different configurations. In all cases, the experimental conditions were optimized in order to obtain the highest magnetoresistance values as possible and trying to share light on the mechanism responsible of GMR.

O 31.2 Tue 11:30 WIL C107

F-center in a MgO-surface and MgO-bulk — •Daniel Berger and Paul-Gerhard Reinhard — Lehrstuhl für theoretische Physik II, Erlangen

A quantum-mechanical/molecular-mechanical (QM/MM) hierarchical model was applied to investigate electronic and optical properties of color centers in the insulating MgO material. F-centers situated directly at the surface as well as deeper inside had been studied and compared with previous results where available.

The color centers discussed here are oxygen vacancies filled by two electrons. The two electrons of such an F-center were treated quantum mechanically applying time-dependend DFT at the level of the local-density approximation. The DFT equations were solved in spacial grid representation. The hosting MgO lattice is described in the framework of the Gaussian Shell Model (GSM) at a classical level with appropriate ion-ion potentials within the lattice and pseudo-potentials for the interaction with the QM electrons. The dynamical polarization of the substrate ions is taken into account for the material in a vicinity of the defect, typically covering 2-4 shells of ions.

The density distribution of the defect electrons are in fair agreement with results from ab-initio calculations, while lattice relaxation is overestimated. Moreover, surface deformation through the color center shows a systematic dependency from the size of the active zone. The optical response shows marked resonance peaks whose properties change dramatically with the layer.

O 31.3 Tue 11:45 WIL C107

Catalytic Pt Nanoparticles on GaN Surfaces: In-situ Characterization of Nanoparticle-Support Interaction via High-pressure Synchrotron XPS — •Susanne Schaefer[1], Sonja Wyrzgol[2], Ian Sharp[1], Andreas Jentys[2], Detre Teschner[3], Axel Knop-Gericke[3], Johannes Lercher[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalysis Research Centre, Technische Universität München, Garching, Germany — [3]Fritz-Haber-Institut, Max-Planck-Gesellschaft, Berlin, Germany

Pt nanoparticles on GaN surfaces are investigated as a model system for the electronic control of catalytic reactions at the surface of a wide band gap semiconductor. In the synchrotron XPS study reported here, the electronic interaction of platinum nanoparticles with GaN surfaces was investigated with regard to semiconductor band bending as well as the chemical state of the nanoparticles due to charge transfer processes. Four nanoparticle geometries were tested on both, n-type and p-type GaN surfaces. All samples were measured at room temperature under vacuum and at 200°C, under oxygen, under hydrogen, under hydrogen/ethene (reaction gas, mixture 10:1), and in vacuum after gas exposure. Generally, the nanoparticles exhibited three Pt species, with varying relative intensities, depending on the nanoparticle geometry and substrate doping. From the presented results, we conclude a strong substrate-nanoparticle interaction, which depends on the GaN doping and band bending, as well as on the generation of electron-hole pairs under intense synchrotron illumination.

O 31.4 Tue 12:00 WIL C107

Dimensional Nanometrology with Grazing Incidence Small Angle X-ray Scattering (GISAXS) — •Jan Wernecke, Michael Krumrey, Levent Cibik, Stefanie Marggraf, and Peter Müller — Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin

Reliable methods for dimensional characterisation of structures in the nanometer range are now a necessity in many fields of industry and science, e.g. for next-generation EUV lithography, new photovoltaic devices or magnetic nanoparticles. The method we have chosen for measurements of statistically averaged structural properties of nanostructured surfaces is GISAXS. This is a versatile technique to probe statistic properties such as mean particle size, spacial distribution and roughness of nanostructured surfaces and nanoparticle assemblies on top of or buried in bulk material. The GISAXS experiments were performed at the Four-Crystal Monochromator (FCM) beamline in the laboratory of PTB at BESSY II using the SAXS setup of the Helmholtz-Zentrum Berlin (HZB). This presentation will give a short overview of the instrumentation and the capabilities of the laboratory to perform dimensional nanometrology with GISAXS and will show first experimental results. Gratings for EUV lithography have been investigated in terms of coating layer thickness, roughness, grating period and blaze angle. Furthermore, dimensional properties of Au nanoparticles on silicon substrate were determined. The obtained particle sizes were in good agreement with SAXS measurements of these particles in liquid suspension.

O 31.5 Tue 12:15 WIL C107

Röntgenbeugungsuntersuchung von Ir-Nanopartikeln auf einer Graphen/Ir(111) Oberfläche — •Dirk Franz[1], Stefan Schumacher[2], Miguel Mantilla[3], Carsten Busse[2], Thomas Michely[2] und Andreas Stierle[1] — [1]AG Grenzflächen, Universität Siegen, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]MPI für Metallforschung Stuttgart, Germany

Eine Graphen/Ir(111) Oberfläche kann als Templat für den Wachstumsprozess von Iridium-Nanopartikeln genutzt werden, um diese in einer geordneten, regelmäßigen Weise anzuordnen [1]. Mittels chemischer Gasphasenabscheidung wurde Graphen auf einer Iridium (111) Oberfläche unter Ultrahochvakuumbedingungen aufgewachsen und in eine mobile UHV-Kammer für Röntgenbeugungsuntersuchung und Oberflächenpräparation transferiert. Die Ausbildung von Ir Nanopartikeln wurde während des Aufdampfens von Iridium in-situ durch Oberflächen Röntgenbeugung und Röntgenreflektionsmessungen an der Angstrom Quelle Karlsruhe (ANKA) charakterisiert. Die Messungen erlauben direkte Rückschlüsse auf die Orientierung, Größe und Form der Nanopartikel.

[1]: A. T. N'Diaye, S. Bleikamp, P. J. Feibelman und T. Michely, Phys. Rev. Lett. **97**, 215501 (2006)

O 31.6 Tue 12:30 WIL C107

Fabrication of plasmonic nanostructures for efficiency enhancement of silicon solar cells — •Stefan Griesing, Andreas Englisch, Uwe Schmitt, and Uwe Hartmann — Inst. of Experimental Physiks, Saarland University, P.O. Box 151150, 66041 Saarbrücken

Plasmonic scatterers cause an increase of the light-conversion efficiency of silicon solar cells due to the extended light path. Especially nanostructures with a diameter of more than 100nm scatter a large fraction of the incoming irradiation in the wavelength regime of 550nm to 1050nm. A technical challenge is the fabrication of large homogeneous areas of plasmonic nanostructures with a narrow size distribution. We report an approach in which this is realized by sputtering or thermal evaporation of silver thin films (5- 20nm thickness) and subsequent vacuum annealing. SEM images show that size, shape and density

of the particles are dependent on the annealing temperature and the mass thickness of the deposited layer. In addition, in-situ SEM measurements of the annealing process will be presented.

O 31.7 Tue 12:45 WIL C107

O2 and CO on noble metal clusters on C/W(110) templates — •Magdalena Bachmann, Norbert Memmel, and Erminald Bertel — Institute for Physical Chemistry, University of Innsbruck, Austria

Small noble-metal (especially Au) clusters on oxidic supports have gained a lot of attention in the last years due to their high activity and selectivity as catalysts for CO oxidation reaction. The importance of cluster-size effects and influence of the substrate material are still discussed controversially. We introduce two differently carburized W(110) surfaces (i.e. R(15x12)C/W(110) and R(15x3)C/W(110)) as templates for the growth of two different types of Au, Ag and Cu nanoclusters. Investigation of the adsorption properties of the reactants CO and O2 on these surfaces might yield illuminative results concerning the Au-catalyzed CO oxidation. In a first step towards this goal the influence of the reaction gases on the stability of the nano-clusters was investigated by scanning tunnelling microscopy. Differences and similarities concerning gas induced alterations on different types of clusters are discussed.

O 31.8 Tue 13:00 WIL C107

Physical and chemical properties of small supported coinage metal clusters — •Martin Amft[1], Natalia Skorodumova[1], Olle Eriksson[1], Sébastien Lebègue[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden — [2]Laboratoire de Cristallographie, Résonance Magnétique et Modélisations (CRM2, UMR CNRS 7036) Institut Jean Barriol, Nancy Université BP 239, Boulevard des Aiguillettes 54506 Vandoeuvre-lès-Nancy,France

We investigate, by means of ab-initio density functional theory calculations, the adsorption and catalytic activity of supported small coinage metal clusters.

Our focus lies on cluster-size effects, the influence of different support materials, e.g. metal oxides and graphene, mobility of the deposited clusters, and the co-adsorption of additional molecule species. In the case of adsorption on graphene, we especially account for van der Waals interactions by the vdW-DF and the PBE+D2 methods, and study the mobility and initial clustering processes of gold on this material.

In the case of metal oxide supports, we explain the experimentally found catalytic characteristics of Au_{1-4}/MgO(100) by studying their ability to (co-) adsorb CO and O_2 molecules and address the question whether the presence of H_2O influences the catalytic activity of small gold clusters on MgO towards CO oxidation.