

## O 40: Particles and Clusters I

Time: Wednesday 15:45–17:15

Location: H38

O 40.1 Wed 15:45 H38

**Surface strain of Au clusters analysed by transmission electron holography** — ●RADIAN POPESCU<sup>1</sup>, ERICH MÜLLER<sup>1</sup>, DAGMAR GERTHSEN<sup>1</sup>, MATTHIAS WANNER<sup>1,2</sup>, MARCO SCHOWALTER<sup>3</sup>, ANDREAS ROSENAUER<sup>3</sup>, ARTHUR BÖTTCHER<sup>4</sup>, and MANFRED KAPPES<sup>4</sup> — <sup>1</sup>Laboratorium für Elektronenmikroskopie und Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe, Germany — <sup>2</sup>Forschungsinstitut für Pigmente und Lacke e.V., D-70569 Stuttgart, Germany — <sup>3</sup>Institut für Festkörperphysik, Universität Bremen, D-28359 Bremen, Germany — <sup>4</sup>Institut für Physikalische Chemie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We have carried out an accurate quantitative analysis of the dependence of the mean inner Coulomb potential (MIP) on the particles thickness for Au nano-clusters deposited on amorphous carbon (a-C) substrate taking into account the strain relaxation of the cluster surface atoms. It was shown that the high experimental cluster MIP values of about 80 V measured for the 0.5 nm Au clusters radii can be accounted for only by the strain of the surface atoms. The MIP value of Au volume atoms (atoms which have the Au-bulk coordination number) of  $V=32.1\pm 3.6$  V we have derived, is in good agreement with previous theoretical estimations of the Au bulk MIP values. The theoretical method developed here to calculate the MIP is not only applicable to the special case of Au clusters, but can be extended to any type of metallic materials.

O 40.2 Wed 16:00 H38

**Nanosecond and femtosecond laser photodesorption of NO from silver nanoparticles on a thin alumina film** — ●KI HYUN KIM<sup>1</sup>, DANIEL MULUGETA<sup>1</sup>, KAZUO WATANABE<sup>1</sup>, DIETRICH MENZEL<sup>1,2</sup>, and HANS-JOACHIM FREUND<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — <sup>2</sup>Technische Universität München, 85747 Garching, Germany

Nanosecond (ns) and femtosecond (fs) laser photodesorption (PD) of NO adsorbed on Ag nanoparticles supported on a thin Al<sub>2</sub>O<sub>3</sub> film has been studied by a mass selected time-of-flight method (MS-TOF) and by temperature programmed desorption. NO was adsorbed on 0.5-nm deposited Ag nanoparticles (~8 nm particle diameter) at 75 K, resulting in the formation of NO dimers. PD cross sections were calculated from the irradiance dependence of the total PD yield of NO fitted to a single exponential. With ns pulses (~5 ns) at  $h\nu=3.5$  eV in p-polarization, a PD cross section of  $5.6 \times 10^{-17}$  cm<sup>2</sup>, which is about 30 times larger than that on Ag(111), was obtained. Also, the NO mean translational energy (670 K) is larger than in that case. The enhancement is explained by resonant excitation of the Mie plasmon of the Ag nanoparticles at 3.6 eV.

With fs pulses (~100 fs) at  $h\nu=3.1$  eV in p-polarization, off-resonant from the Mie plasmon, a PD cross section of  $2.3 \times 10^{-16}$  cm<sup>2</sup> was obtained. The mean translational energy of NO was 540 K. The PD yield was proportional to the ~1.7th power of the laser fluence. A two-photon excitation process or a DIMET (desorption induced by multiple electronic transitions) may be involved in the PD with fs pulses.

O 40.3 Wed 16:15 H38

**In Situ Surface Enhanced Infrared Absorption Spectroscopy for the Analysis of the Adsorption and Desorption Process of Au Nanoparticles on the SiO<sub>2</sub>/Si Surface** — ●DOMINIK ENDERS<sup>1,2</sup>, TADAAKI NAGAO<sup>1,2</sup>, and TOMONOBU NAKAYAMA<sup>1,2</sup> — <sup>1</sup>National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan — <sup>2</sup>Nanoscale Quantum Conductor Array Project, ICORP, JST, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan

The adsorption and desorption of Au nanoparticles (AuNP) in colloidal D<sub>2</sub>O suspension on the SiO<sub>2</sub>/Si surface was investigated by in situ ATR-IR spectroscopy. With increasing surface density of AuNP the absorption of the vibrational modes of D<sub>2</sub>O and of the citrate molecules covering the AuNP increases due to surface enhanced infrared absorption (SEIRA). We show that the adsorption kinetics can be investigated by monitoring the molecular vibrational modes of D<sub>2</sub>O and the citrate molecules, and furthermore we clarify that the adsorption process can be described very well by a Langmuir-kinetics model. When exposing a saturated AuNP submonolayer to 2-aminoethanethiol/D<sub>2</sub>O

solution, the AuNP are removed from the surface and the IR absorption of the D<sub>2</sub>O vibrational modes become weaker again. Taking into account the time dependencies of the CH and the OD peaks, we propose a microscopic model explaining the mechanism of the desorption process.

O 40.4 Wed 16:30 H38

**Dealloying effects in rotating CuAu nanoclusters - A molecular dynamics study** — ●H. NEUBAUER and S.G. MAYR — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Dealloying effects in rotating liquid CuAu clusters are investigated with the help of classical molecular dynamics simulations using embedded atom method (EAM) potentials. We employ the model system, CuAu, to investigate the phenomenon as a function of cluster size and composition, i.e. for CuAu, Cu<sub>3</sub>Au and CuAu<sub>3</sub>. In addition to well-established surface energy related effects, we find an enrichment of Au on the surface due to centrifugal forces. An ellipsoid deformation of the cluster occurs, while Au forms a bulge around the rotating cluster. Disturbances occurring during rotational movement, such as thermal fluctuations or oscillations, are found to counteract the dealloying process by mixing the constituents; for long enough times a stationary state is reached. We acknowledge the SFB 602 - TP B3 for financial support.

O 40.5 Wed 16:45 H38

**The local tunnelling conductance on cobalt clusters at semiconductor surfaces** — ●KRISTIAN SELL, ARMIN KLEIBERT, VIOLA VON OEYNHAUSEN, and KARL-HEINZ MEIWES-BROER — Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock

We present scanning tunnelling spectroscopy (STS) and microscopy (STM) measurements on isolated cobalt nanoparticles with diameters ranging from 2 to 12 nm after *in-situ* deposition on Ge(001). The mass-filtered clusters have been deposited under soft-landing conditions ( $E_{\text{kin}}/\text{atom} < 0.5\text{eV}$ ) using an arc cluster ion source (ACIS).

In the present range of particle sizes the tip folding plays a great role. With the help of a "blind reconstruction method" it is possible to approximate the shape of the tip [1]. After a respective deconvolution of the STM images faceted particles become visible. According to their equilibrium shape - being a truncated octahedron in the case of fcc cobalt - hexagonal and quadrangular facets appear in the images [2]. STS is sensitive to occupied and unoccupied states near the Fermi level and reveals the existence of distinct states in the tunnelling conductivity of the substrate as well as on the clusters. Thus, the richly structured density of states of the germanium surface serves as STM/STS condition test [3]. The tunnelling conductivity measured on the cobalt nanoparticles Ge(001) will be discussed in detail.

[1] J.S. Villarrubia, J. Vac. Sci. Technol. B 14, 1518 (1996), [2] M. Jamet, Phys. Rev. Lett. 86, 4676 (2001), [3] K.-L. Jonas, Appl. Phys. A 82, 131-137 (2006)

O 40.6 Wed 17:00 H38

**Resonant Raman Scattering on Functionalized Carbon Nanotubes** — ●MATTHIAS MÜLLER<sup>1</sup>, JANINA MAULTZSCH<sup>1</sup>, CHRISTIAN THOMSEN<sup>1</sup>, DAVID WUNDERLICH<sup>2</sup>, and ANDREAS HIRSCH<sup>3</sup> — <sup>1</sup>Inst. für Festkörperphysik, TU Berlin — <sup>2</sup>Zentralinst. für Neue Materialien und Prozesstechnik, Univ. Erlangen-Nürnberg, Fürth — <sup>3</sup>Inst. für Organ. Chemie, Univ. Erlangen-Nürnberg, Erlangen

We report Raman measurements on carbon nanotubes functionalized with diverse alkenes and various degrees of functionalisation. Selective reactions of the different tube species (metallic or semiconducting) due to the availability of electrons near the Fermi level were first reported by Strano et al.[1]. Our work focuses on resonant Raman scattering of the radial breathing mode (RBM) concerning the preferred addition of the nucleophile to metallic tubes as suggested by Graupner et al.[2].

Assigning the chiral indices of the tubes by means of the so-called Kataura plot[3] we can study the influence of functionalisation on the transition energies of either metallic and semiconducting tubes in detail. Data of the high energy (HEM)- and defect-mode (D-mode) will also be discussed.

[1] M. Strano et al., Science 301, 1519 (2003) [2] R. Graupner et al., J. Am. Chem. Soc. 128, 6683 (2006) [3] J. Maultzsch et al., Phys Rev

