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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 routh 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.

## O 54: Nano-optics of metallic and semiconducting nanostructures (experiments II)

Time: Thursday 15:00–18:30 Location: SCH A216

O 54.1 Thu 15:00 SCH A216

**Negative-index bi-anisotropic photonic metamaterial by direct laser writing and silver shadow evaporation** — •Michael S. Rill[1], Christine E. Kriegler[1], Michael Thiel[1], Georg von Freymann[1,2], Stefan Linden[1,2], and Martin Wegener[1,2] — [1]Institut für Angewandte Physik and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe (TH), Wolfgang-Gaede-Str. 1, 76131 Karlsruhe — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, 76021 Karlsruhe, Germany

Metamaterials are artificially fabricated structures composed of sub-wavelength metallic building blocks ("photonic atoms") that show – unlike natural substances – magnetism at optical frequencies [1].

Here, we present a novel blueprint of a negative-index metamaterial [2]. Our structure is realized using 3D direct laser writing, $SiO_2$ atomic layer deposition and silver shadow evaporation. The comparison of measured linear optical spectra with theory shows good agreement and reveals a negative real part of the refractive index $n$ at around 3.85 $\mu$m wavelength – despite the fact that the metamaterial structure is bi-anisotropic [3,4] due to the lack of inversion symmetry along its surface normal.

[1] V.M. Shalaev, Nature Photon. **1**, 41 (2007).