

MM 24: Nano structured materials II

Time: Wednesday 16:45–18:15

Location: H4

MM 24.1 Wed 16:45 H4

Atomistic simulation of carbon nanostructures in electronic nonequilibrium — ●HARALD O. JESCHKE¹, ALDO H. ROMERO², TRAIAN DUMITRICA³, and MARTIN E. GARCIA⁴ — ¹Institut für Theoretische Physik, Universität Frankfurt, Germany — ²CINVESTAV Querétaro, Querétaro, México — ³Department of Mechanical Engineering, University of Minnesota, USA — ⁴Theoretische Physik, Universität Kassel, Germany

We analyze the response of carbon nanostructures to laser induced nonequilibrium by performing molecular dynamics simulation on time dependent potential energy surfaces. We observe that typical defects in carbon nanotubes become instable upon excitation of electron hole pairs, and the nanotubes heal. We also find that the excitation of coherent phonons can be exploited in capped carbon nanotubes to achieve a clean separation of the nanotube cap and body. In a broad investigation of the stability of single wall nanotubes upon laser irradiation we find interesting dependencies on nanotube diameter and on the laser pulse parameters.

MM 24.2 Wed 17:00 H4

Radial distribution function as a tool to analyse nanotubes chiralities — ●PEDRO OJEDA¹, MAURICIO TERRONES², HUMBERTO TERRONES², DARIN HOFFMAN³, THOMAS PROFFEN³, ANTHONY CHEETHAM⁴, and MARTIN GARCIA¹ — ¹Theoretische Physik FB 18, Universitaet Kassel — ²Advanced Materials Department, IPICT, SLP, Mexico — ³Manuel Lujan Jr. Neutron Scattering Center, Los Alamos, NM 87545, USA — ⁴Materials Research Laboratory, University of California, Santa Barbara, CA 93106-5121, USA

The radial distribution function (RDF) of different single walled carbon nanotubes (SWCNTs) has been calculated showing characteristic patterns. Features related to diameter, chirality and doping in these nanostructures are analyzed. We also investigate the induced chirality of two samples, prepared with the chemical vapor deposition (CVD) method and the high pressure Co conversion (HIPCo) procedure, respectively, by comparing the experimental RDF signal obtained from the neutron scattering technique with the RDFs of our simulations. We found armchair and zigzag nanotubes in the sample, but we cannot discard the presence of other chiralities. We believe that this is a useful method to study chiralities induced by different methods of production. Data up to $Q = 30 \text{ \AA}^{-1}$ were used in the Fourier transform, giving a high real space resolution of $\Delta r \sim 0.2 \text{ \AA}$.

MM 24.3 Wed 17:15 H4

A general approach to control the radius and the chirality of nanotubes — ●JENS KUNSTMANN¹, ALEXANDER QUANDT², and IHSAN BOUSTANI³ — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — ²Institut für Physik der Ernst-Moritz-Arndt-Universität Greifswald, Domstraße 10a, 17489 Greifswald — ³Bergische Universität Wuppertal, FB C Mathematik und Naturwissenschaften, Gaußstraße 20, 42097 Wuppertal

The success of future nanotechnologies will strongly depend on our ability to control the structure of materials on the atomic scale. For nanotubes it turns out that one of their structural parameters - the chirality - may not be controlled during synthesis. We explain the basic reason for this defect and show that novel classes of nanotubes like boron nanotubes, related to sheets with anisotropic in-plane mechanical properties, may overcome these problems. Our results further suggest that extended searches for nanomaterials similar to pure boron will allow for one of the simplest and most direct ways to achieve structure control within nanotechnology.

MM 24.4 Wed 17:30 H4

Molecular dynamics simulation of the formation of iron-platinum clusters — ●NORBERT LÜMMEN¹ and THOMAS KRASKA² — ¹Institute for Physics and Technology, University in Bergen, Norway — ²Institute for Physical Chemistry, University Cologne, Germany

The formation of iron-platinum clusters from the vapour phase is investigated by molecular dynamics simulation. The metal interaction is modelled by an embedded atom potential method. Argon is added

as carrier gas for removing the condensation heat from the system.

The first step of the particle formation is homogeneous nucleation. We found that in the iron-platinum system pure platinum nucleation takes place to a certain extent. We attribute this effect to the difference in cohesive energies of the two substances leading to heat transfer from platinum clusters to iron atoms which makes it less likely for them to condense at the same time due to their high temperature. This observation is in agreement with experimental results on the palladium-platinum system in the literature.

The proceeding growth process comprises surface growth, coalescence and agglomeration. The analysis of the atomic order shows that the disordered tetragonal face centred structure dominates. In order to obtain the ordered L1₀ structure we have run sinter simulations with different temperature programs applied to the carrier gas argon. Furthermore different cluster sizes ranging from 3 nm to 3.5 nm are analysed with respect to the structure formation. At the current state the onset of L1₀ formation can be observed.

MM 24.5 Wed 17:45 H4

Platinum deposition on polyethylene films investigated by molecular dynamics — ●THOMAS KRASKA and ROBERTO ROZAS — Institute for Physical Chemistry, University Cologne, Luxemburger Str. 116, 50939 Köln, Germany

The growth mechanisms of platinum clusters on and in a polyethylene film is investigated by molecular dynamics simulation. This system has been chosen as a model system with a relatively simple polymer. Platinum is modelled by the embedded atom method and polyethylene by a united atom model with flexible bonds, angle potential, and torsion potential for the intramolecular two-, three-, and four-body interactions. The intermolecular interaction is modelled by a Lennard Jones potential. Furthermore argon is added as carrier gas which removes heat from the vapour phase by collision with the platinum atoms and the polymer surface. An equilibrated polyethylene film is set in the middle of a rectangular box. The gas phase volume of the box is filled with platinum and argon atoms. Once the simulation is started clusters form in the vapour phase as well as on and in the polyethylene film.

Simulations at different platinum vapour phase densities are analysed with respect to the growth mechanism. General agreement is found with metal/polymer systems investigated experimentally in the literature. At higher platinum supersaturation less platinum diffuses into the polymer film. This is due to homogeneous nucleation the vapour phase leading to large clusters, which less likely diffuse into the polymer.

MM 24.6 Wed 18:00 H4

Balancing the White Light Shade of Dual-Color Emitting Nanocrystals — ●SERGIY MAYILO¹, SAMEER SAPRA², THOMAS KLAR¹, ANDREY ROGACH¹, and JOCHEN FELDMANN¹ — ¹Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians Universität München, Germany — ²Physical Chemistry Group, Technische Universität Dresden, Germany

Semiconductor nanocrystals (NCs) are highly fluorescent with fluorescence quantum efficiencies as high as 80%, being ideal candidates for use in white light emitting devices. Simple mixing of red, green and blue emitting NCs may lead to undesirable changes in color during the lifetime of the device due to different temporal stabilities of the components. Here we present the generation of white light from core-shell-shell CdSe/ZnS/CdSe NCs [1]. These particles have two emission lines: blue (500 nm) from the CdSe shell and orange (612 nm) from the CdSe core. The ZnS layer is used as a spacer between the two emitting regions. The shade of the white light can be controlled during synthesis by varying the thickness of the CdSe shell. The relative intensities of both emission lines are also determined by intra-nanocrystal energy transfer. When the colors are well matched the resulting emission appears as pure white light. The synthesized NCs have 30% quantum efficiency.

[1] S. Sapra, S. Mayilo, T.A. Klar, A.L. Rogach, J. Feldmann, Bright white light emission from semiconductor nanocrystals: by chance and by design, *Advanced Materials* (in press)