

## HL 25 C/diamond

Time: Tuesday 18:00–19:00

Room: POT 151

HL 25.1 Tue 18:00 POT 151

**Electronic and optical properties of boron-doped nanocrystalline diamond** — ●WOJCIECH GAJEWSKI<sup>1</sup>, JOSE GARRIDO<sup>1</sup>, KEN HAENEN<sup>2</sup>, OLIVER WILLIAMS<sup>2</sup>, and MARTIN STUTZMANN<sup>1</sup> — <sup>1</sup>Walter Schottky Institute, - TU München, Am Coulombwall 3, 85748 Garching — <sup>2</sup>Institute for Materials Research, University of Hasselt, Wetenschapspark 1, 3590, Belgium

We report the optical and electronic properties of boron-doped nanocrystalline diamond (B-NCD) thin films, grown on quartz substrates by CH<sub>4</sub>/H<sub>2</sub> plasma CVD. Diamond thin films with a thickness below 200 nm and with boron concentrations ranging from 0 to 5000 ppm have been investigated. Hall effect measurements confirmed the expected p-type conductivity. The conductivity of B-doped NCD samples with low boron concentration in the gas phase strongly depends on temperature. The carrier concentration in the temperature range from 400K to 700K is thermally activated. At higher boron doping, the conductivity and the carrier concentration are no longer temperature dependent, and the samples exhibit quasimetallic properties. The Hall mobility shows no clear temperature dependence. As expected, the higher the carrier concentration, the lower the mobility. Spectrally resolved photocurrent measurements have revealed a strong dependence of the photosignal on the surface termination. Major differences occur in the energy range 3.5 - 5.4 eV. The influence of grain boundaries and surface states on the electronic transport and optical properties will be discussed.

HL 25.2 Tue 18:15 POT 151

**Thin films of metallic carbon nanotubes and their optical spectra** — ●SABINE BLATT<sup>1</sup>, FRANK HENNRICH<sup>1</sup>, HILBERT V. LÖHNEYSEN<sup>2,3</sup>, and RALPH KRUPKE<sup>1</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe — <sup>2</sup>Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — <sup>3</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe

The exceptional electrical and structural properties of single-walled carbon nanotubes (SWNTs) open up a wide range of future applications provided that metallic and semiconducting nanotubes can be separated on a large scale. The separation through dielectrophoresis makes use of the different electric field-induced polarizabilities of the two types leading to a separation in ac electric fields [1, 2]. This method allows for the first time to produce thin films of only metallic SWNTs and to measure their optical absorption spectra [3]. Recent experiments address the dependence of the separation yield on the type and the concentration of the surfactant used to disperse the nanotubes and on the conductivity of the dispersion. For a better understanding of the dielectrophoretic forces finite elements simulations are performed additionally.

[1] Krupke, R.; Henrich, F.; v. Löhneysen, H.; Kappes, M. M. *Science* 2003, 301, 344-347 [2] Krupke R.; Henrich F.; Kappes M. M.; v. Löhneysen H. *Nano Lett.* 2004, 4, 1395-1399 [3] Krupke, R.; Linden, S.; Rapp, M.; Henrich, F. *cond-mat/0508418*

HL 25.3 Tue 18:30 POT 151

**Chemical functionalization of ultrananocrystalline diamond thin films with aromatic molecules** — ●S.Q. LUD<sup>1</sup>, M. DANKERL<sup>1</sup>, J. HERNANDO<sup>1</sup>, M. STEENACKERS<sup>2</sup>, R. JORDAN<sup>2</sup>, P. BRUNO<sup>3</sup>, D.M. GRUEN<sup>3</sup>, P. FEULNER<sup>4</sup>, J.A. GARRIDO<sup>1</sup>, and M. STUTZMANN<sup>1</sup> — <sup>1</sup>Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany — <sup>2</sup>Lehrstuhl für Makromolekulare Stoffe, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany — <sup>3</sup>Materials Science Department, Argonne National Laboratory, Argonne, Illinois 60439, USA — <sup>4</sup>Physics Department E20, Technische Universität München, James-Franck-Strasse, 85748, Garching, Germany

We present a novel approach for the surface functionalization of ultrananocrystalline diamond films via grafting of high-reactive 4-nitrobiphenyl-4-diazonium cations. The grafting process is associated with the cleavage of dinitrogen followed by the binding of the remaining radicals to the surface, forming a stable and covalent C-C bond. X-ray photoelectron spectroscopy, ac impedance spectroscopy, atomic force microscopy and cyclic voltammetry have been used to investigate the structure and surface coverage of the organic overlayer. We have further explored the electrochemically controlled conversion of the surface nitro group to an amino group. The resulting surface offers a reliable surface chemistry

for subsequent modification in contrast to the non-reactive nitro group. With this approach, an addressable coupling of biological molecules to an inert and inorganic solid substrate, with considerable importance for biosensing tasks, can be explored.

HL 25.4 Tue 18:45 POT 151

**Simulations of Novel Nanoporous Carbon Materials** — ●JOHAN M. CARLSSON and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

Carbon is one of the most versatile elements in nature and Nanoporous carbon (NPC) constitutes yet another class of carbon materials that exhibit unusual properties. NPC has the ability to catalyze dehydrogenation reactions, but the actuating chemical reaction steps are still unclear. This uncertainty is also due to the fact that the atomic structure of NPC depends on the preparation conditions. TEM experiments suggest that NPC derived from hydrocarbons has the form of crumpled graphene sheets with a significant amount of non-hexagonal rings in the structure. We have therefore carried out an extensive study to characterize NPC. Our density-functional theory (DFT) calculations reveal that the atomic relaxation transforms defects into combinations of non-hexagonal rings, which we identify as the “motifs of NPC”. These motifs lead to strain and local buckling of the structure. They also induce defect states close to the Fermi level, leading to that some of them being charged, which may facilitate molecule dissociation. These motifs can then be combined to build models of new carbon materials. A random distribution of the motifs leads to the formation of a NPC material while an ordered configuration of the motifs can instead form new, graphene like, carbon structures based on non-hexagonal rings, similar to the Haecelites. Our calculations indicate that both NPC and the generalized Haecelites can have a heat of formation comparable to other metastable carbon materials such as nanotubes.