

## MM 45: Nanomaterials - Nanospheres &amp; Fibres

Time: Wednesday 16:30–17:45

Location: H26

MM 45.1 Wed 16:30 H26

**Fabrication of transparent metal electrodes by nanosphere lithography** — ●ESER METIN AKINOGLU, ANTHONY MORFA, and MICHAEL GIERSIG — Freie Universität Berlin, Department of Physics, Berlin, Germany

Electrodes providing sufficient transparency and conductivity are important for high performance optoelectronic applications such as thin-film solar cells and light emitting diodes. Periodically perforated metal films provide a tunable basis to achieve high transparency while maintaining a low sheet resistance by simply changing the geometrical dimensions of the metal grid.

Nanosphere lithography is an inexpensive method to fabricate tunable transparent metal electrodes. This technique utilizes a self assembled and hexagonally close packed monolayer of colloidal polystyrene submicron particles as a lithography mask. Annealing and reactive ion etching in an oxygen plasma is used to modify the mask. Metal is then deposited and the resultant metal nanostructure shapes and dimensions are determined by the mask's negative image.

In this presentation we discuss results from transparent silver electrodes produced in this way. We demonstrate structural, electronic and optical properties of our gratings with SEM, AFM, four-point probe and optical measurements. Sheet resistances as low as 3 Ohm/Sq and an average transmissivity of 70% was achieved. Percent transmission values up to 82% are predicted by a simple geometric model promising competitiveness with transparent conductive oxides. Finally, these silver electrodes were incorporated into organic photovoltaic devices.

MM 45.2 Wed 16:45 H26

**C<sub>58</sub> solid materials: mechanical properties vs thermal stability** — SEYITHAN ULAS<sup>1</sup>, SVEN BUNDSCHUH<sup>2</sup>, CHRIS EBERL<sup>2</sup>, HENRIK HÖLSCHER<sup>3</sup>, ●ARTUR BÖTTCHER<sup>1</sup>, and MANFRED KAPPES<sup>1</sup> — <sup>1</sup>Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — <sup>2</sup>Institute of Advanced Materials and Material- and Biomechanics (IAM-WBM), KIT, Germany — <sup>3</sup>Institute of Microstructuring Techniques, KIT, Germany

Non-IPR C<sub>58</sub> cages as created by electron-impact induced fragmentation of IPR-C<sub>60</sub> fullerenes have been exploited as building blocks of new materials grown by applying low energy cluster beam deposition. The material fabricated at room temperature appears to be an amorphous wide-band semiconductor, RT-C<sub>58</sub>. Nanoindentation as applied to measure elastic modulus E and hardness H reveals values higher than those found for IPR-C<sub>60</sub> solids: E(RT)=14.1 GPa and H(RT)=1.23 GPa. This observation is rationalized in terms of the unique functionalization of C<sub>58</sub> cages by non-IPR sites which are responsible for the formation of covalently stabilized C<sub>58</sub> oligomers. Annealing the RT-C<sub>58</sub> films up to 1100 K results in a new material, HT-C<sub>58</sub>, which exhibits considerably modified electronic and vibrational properties. Such annealing activates the mobility of the initially vdWaals-stabilized cages and consequently maximizes their coordination degree (densification and strengthening by covalent interlinking). The related molecular transformations raise the overall mechanical hardness of the material: H(HT)=3.9 GPa, i.e. H(HT)=3 H(RT).

MM 45.3 Wed 17:00 H26

**Electrical properties of different kinds of multi-walled carbon nanotubes powders** — ●ABDELWAHAB HASSAN<sup>1</sup>, SILKE HAMPEL<sup>1</sup>, CHRISTIAN HESS<sup>1</sup>, ANATOLY ROMANENKO<sup>2</sup>, MANFRED RITSCHEL<sup>1</sup>, ALBRECHT LEONHARDT<sup>1</sup>, and BERND BUECHNER<sup>1</sup> — <sup>1</sup>IFW-Dresden, D-01171 Dresden, Germany — <sup>2</sup>Institute of Inorganic Chemistry, Novosibirsk 630090, Russia

Carbon nanotubes have attracted great interest due to their remarkable structure, electrical and mechanical properties. Among various

other properties of CNTs studied so far, the electrical transport properties are still unclear and needs a lot of attention. The electrical properties are strongly dependent on the structure of the nanotubes which varied with the quality of the CNTs. Different kinds of multi-walled carbon nanotubes MWCNT were synthesised by two CVD techniques (aerosol and fixed-bed CVD). The aim of this work is to study and compare the electrical properties as a function of synthesis condition and treatments of MWCNT powders. Morphologies of these MWCNTs are studied using Scanning Electron Microscopy and Transmission Electron Microscopy. The electrical measurements were separately carried out in two temperature ranges (4-294 K and 300-570 K) by four point technique. In the high temperature range 300-570 K, the conduction was found to be thermally activated and well described by Arrhenius type behaviour. However, in the low temperature range (4-294 K), the measured data gives a good fit to variable-range hopping (VRH) and the results are interpreted using Mott's (VRH) model. By using these models, various interesting electrical parameters have been calculated.

MM 45.4 Wed 17:15 H26

**Quantification of curvature effects in boron and carbon nanotubes: large errors in the zone-folding method** — ●HAGEN ECKERT<sup>1</sup>, VIKTOR BEZUGLY<sup>1,2</sup>, JENS KUNSTMANN<sup>1,3</sup>, and GIANAU-RELIO CUNIBERTI<sup>1,2</sup> — <sup>1</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — <sup>2</sup>Division of IT Convergence Engineering, POSTECH, Pohang 790-784, Republic of Korea — <sup>3</sup>Department of Chemistry, Columbia University, New York NY 10027, USA

The zone-folding method is a widely used technique for computing the electronic structure of carbon nanotubes as well as of other type nanotubes. Within this method the electronic dispersion of a nanotube is calculated from that of the corresponding 2D sheet (e.g. graphene). In this talk the problem of curvature based discrepancy between direct calculations from the tubular structure and from the related 2D sheets is examined. [1] Curvature effects of boron and carbon nanotubes of different diameters and chiralities are systematically quantified using the density functional based tight-binding method. The difference between both calculation methods can also be considered as the error of the zone-folding method. For each nanotube we quantify this error by calculating the standard deviation of the band energies and the maximal relative deviation between the derived ballistic currents. Our results indicate that quantitative predictions made using the zone-folding method may have non-negligible error.

[1] Bezugly, Eckert, Kunstmann, Kemmerich, Meskine, Cuniberti; submitted

MM 45.5 Wed 17:30 H26

**Ultrashort laser-pulse excitation of a (5,0) zigzag BN nanotube** — ●BERND BAUERHENNE, EEUWE ZIJLSTRA, and MARTIN GARCIA — Theoretische Physik - Universität Kassel - Heinrich-Plett-Str. 40, 34132 Kassel, Germany

BN nanotubes are isostructural to carbon nanotubes with boron and nitrogen atoms occupying the even and odd sublattices, respectively. In this work we investigate the laser excitation of a (5,0) zigzag BN nanotube using ab initio molecular dynamics simulations. We also analyse the mechanical properties of the nanotube in the laser-excited electronic state. We obtain a Young modulus of 920 GPa in the electronic ground state and show that this value decreases with increasing laser fluence. Our molecular dynamics simulations show that three optical phonon modes are simultaneously excited. We identify these three modes as the radial breathing mode, the radial buckling mode, and the longitudinal bond stretching mode. We demonstrate that it is possible to steer these excitation of the three modes by using a femtosecond-laser pulse train.