MM 33: Nanomaterials II - Tubular nanostructures

Time: Tuesday 15:45–17:45 Location: IFW A

MM 33.1 Tue 15:45 IFW A

Synthesis, characterization and electrical properties of copper coated multi-walled carbon nanotubes — •Abdelwahab Hassan, Silke Hampel, Eslam Ibrahim, Christian Hess, Albrecht Leonhardt, and Bernd Büchner — Leibniz-Institute for Solid State and Materials Research (IFW-Dresden), D-01171 Dresden, Germany

In the recent years, carbon nanotubes (CNTs) have received considerable attention as new materials for a variety of potential applications due to their interesting properties. As well as, CNT- can be reinforced metal matrix composites (MMCs).The coating of CNTs with metal and metal oxide is fundamentally important for applications of CNTs in nanoelectronic device, gas sensor and composite materials, etc. As well as coating of CNTs lead to a significant improvement of interfacial bond between CNTs and metal matrix. Therefore, in the present contribution, a novel route to synthesize copper/multi-walled carbon nanotubes (MWCNTs) was developed using a chemical electroless plating process after the radio frequency (RF) plasma treatment of the CNTs. Plasma treatment of MWCNTs surface was carried out in various gaseous atmospheres, namely Ar, H2 and N2 to improve copper adhesion. N2 plasma treatment showed better surface activation of the MWCNTs. This study investigated the effect of plasma treatment time, flow rate and RF power to improve the copper coating. The morphology of MWCNTs were studied by TEM, SEM, Raman spectroscopy, XPS as well as X-ray diffraction (XRD). The measurements of electrical conductivity of uncoated and copper coated MWCNTs were measured by four-point method in temperature range 300-573 K.

MM 33.2 Tue 16:00 IFW A

Growth of periodic arrays of perpendicularly aligned multi-walled carbon nanotubes — •Eser Metin Akinoglu, Anthony John Morfa, and Michael Giersig — Freie Universität Berlin, Department of Physics, Berlin, Germany

Multi-walled carbon nanotubes (MWCNTs) are promising nano materials with unique properties such as their extraordinary mechanical strength and their electrical conductivity. Using a combination of nanosphere lithography (NSL) for catalyst nano-patterning and plasma enhanced chemical vapor deposition (PECVD) for perpendicularly aligned growth we can produce different MWCNT systems. NSL utilizes a hexagonally close packed monolayer of submicron polystyrene spheres (PSS) as a lithography mask for metal deposition. A periodic array of triangular shaped metal islands remains after chemically removing the PSSs. The size and distance in between the metal islands can be tuned by enlarging or shrinking the hexagonal unit cell which can be tuned through the used PSS size. In the PECVD of MWCNTs a vapor-liquid-solid growth process is used where nickel acts as a catalyst and as a protective helmet during ion bombardment for perpendicular MWCNT growth. By changing the catalyst pretreatment, plasma conditions, growth temperature, gas composition and growth time of the PECVD process we can vary the MWCNT growth kinetics yielding vastly different results in terms of shape, size and crystalinity. In this presentation we show the optimization of parameters for MWCNT growth and discuss potential bio and energy applications such as antimicrobial surfaces and field emitter arrays.

MM 33.3 Tue 16:15 IFW A

Investigation of the antimicrobial activity of well-dispersed multiwalled carbon nanotubes (MWCNT) — •Maryam Khazaee[1], Dan Ye[1], Anindya Majumder[1], Larysa Baraban[1], Jörg Opitz[1,2], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Fraunhofer Institute IZFP Dresden, 01109 Dresden, Germany — [3]Division of IT Convergence Engineering, POSTECH, Pohang, Korea

Antimicrobial activity of well-dispersed MWCNTs with an average diameter of 10 nm was investigated by analyzing the growth curves of Escherichia coli (E.coli) population in surfactant-modified MWCNTs and polymer-modified MWCNTs in Luria Bertani (LB) broth. MWCNTs can be dispersed in ionic surfactants like sodium dodecyl sulfate (SDS), sodium dodecylbenzenesulfonate (SDDBS), sodium cholate (SC), dodecyltrimethylammonium bromide (DTAB) and decyltrimethylammonium bromide (CTAB), as well as in a non-ionic polymer-polyvinylpyrrolidone (PVP). Good dispersion of surface functionalized MWCNTs was observed by UV-Vis spectroscopy and microscopic techniques. Biocompatibility of these surfactants was estimated by analyzing the growth curves of E. coli population in both surfactant-LB broth and polymer-LB broth. SDDBS and PVP, which showed the least toxicity towards the E. coli cells, were selected to study the interaction of well-dispersed MWCNTs by these materials with bacteria. Observation of the deformed E.coli cell membranes using SEM confirms the antimicrobial activity of MWCNTs.

MM 33.4 Tue 16:30 IFW A

Investigation of the antimicrobial activity of well-dispersed multiwalled carbon nanotubes (MWCNT) — •Maryam Khazaee[1], Dan Ye[1], Anindya Majumder[1], Larysa Baraban[1], Jörg Opitz[1,2], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Fraunhofer Institute IZFP Dresden, 01109 Dresden, Germany — [3]Division of IT Convergence Engineering, POSTECH, Pohang, Korea

Comparative dispersion capability of ionic surfactants like Sodium dodecyl sulfate (SDS), Sodium dodecylbenzenesulfonate (SDDBS), Sodium cholate (SC), Dodecyltrimethylammonium bromide (DTAB) and Decyltrimethylammonium bromide (CTAB) and a non-ionic polymer- Polyvinylpyrrolidone (PVP) was examined to disperse MWCNTs. The surface functionalized dispersed MWCNTs with average diameter of 10 nm were investigated using microscopic techniques. Among these surfactants, SDDBS and DTAB provided maximum and minimum dispersion susceptibility, respectively. Furthermore, different concentrations of PVP showed good capabilities for MWCNTs dispersion. Biocompatibility of these surfactants and polymer was estimated by analyzing their optical density (OD) growth curves after treating them with E.coli. SDDBS and PVP which showed the least toxicity, were selected to study their biocompatible interaction with well dispersed MWCNTs. Observation of the deformed E.coli cell membranes confirm the antimicrobial activity of MWCNTs.

15 min break

MM 33.5 Tue 17:00 IFW A

Unveiling the atomic structure of single-wall boron nanotubes — •Jens Kunstmann[1,2], Viktor Bezugly[2,3], Hauke Rabbel[2], and Gianaurelio Cuniberti[2,3] — [1]Department of Chemistry, Columbia University, 3000 Broadway New York, NY 10027, USA — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

Despite recent successes in the synthesis of boron nanotubes (BNTs), the atomic arrangement of their walls has not yet been determined and many questions about their basic properties do remain. Here, we unveil the dynamical stability of BNTs by means of first-principles molecular dynamics simulations. We find that free-standing, single-wall BNTs with diameters larger than 0.6 nm are thermally stable at the experimentally reported synthesis temperature of 870 degrees Celsius and higher. The walls of thermally stable BNTs are found to have mixed triangular-hexagonal morphologies. The latter could develop into a new structural paradigm in boron chemistry.

MM 33.6 Tue 17:15 IFW A

From metal to semiconductior: an *ab initio* study of chemically functionalized boron nanotubes — •Viktor Bezugly[1,2], Hermut Michael Zopf[1], Jens Kunstmann[1,3], and Gianaurelio Cuniberti[1,2,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Center for Advancing Electronics Dresden, TU Dresden — [3]Department of Chemistry, Columbia University, 3000 Broadway, New York — [4]Dresden Center for Computational Materials Science, TU Dresden

Nanotubes of elemental boron have been synthesized in recent years [1]. In contrast to carbon nanotubes (CNTs), boron nanotubes (BNTs) are metallic independent of their diameter and chirality and have higher conductivity than metallic CNTs [1,2]. In our DFT investigations we show how chemical functionalization of single-walled BNTs can tune the basic electronic properties from metallic to semiconducting. The effect can be achieved by atoms or functional groups which have a par-

ticular chemical bonding interactions with BNTs. Our result indicate that functionalization of BNTs offers chirality independent control of the electronic structure of the nanotubes, which is paramount for industrial applications.

[1] F. Liu *et al.*, *J. Mater. Chem.* **20**, 2197 (2010); J. Liu, Z. Iqbal, *MRS Online Proc. Lib.* **1307** (2011) DOI: 10.1557/opl.2011.320.

[2] V. Bezugly *et al.*, *ACS Nano* **5**, 4997 (2011).

MM 33.7 Tue 17:30 IFW A

Electronic structure calculations of modified diamondoids — •Bibek Adhikari and Maria Fyta — Institute for Computational Physics, Stuttgart, Germany

Diamondoids are diamond like cage structure with hydrogen terminations, which have tremendous potential for nanotechnological applications. We focus on alteration and structural modifications of diamondoids by doping these molecules with various elements. We perform density functional theory based calculations to reveal the electronic properties of these doped diamondoids. We plan to investigate the position of the dopants with respect to the cage structure for lower as well as higher diamondoids and reveal the stability and structural characteristics with respect to different doping sites. We next turn to the study of selective functionalization of these molecules. We functionalize two sites of the same diamondoid with a thiol and amine group, respectively. In the end, we discuss the effect of functionalization of self-assembled diamondoid monolayers. The aim is to selectively tune the optical and electronic properties of diamondoids with dopants and/or functionalization groups in view of their novel nanotechnological applications.