MM 41 Nanostructured Materials IV

Time: Friday 12:30–13:15 Room: IFW D

MM 41.1 Fri 12:30 IFW D

Electronic structure and properties of single-walled carbon nanotubes interacting with DNA bases — •Yong Kong and Huajian Gao — Max-Planck Institute for Metals Research, Heisenbergstr. 3, 70569 Stuttgart, Germany

Functionalization of carbon nanotubes (CNTs) has been extensively studied due to its potential in facilitating miniature electronic and optic devices for broad applications. Recently, Zheng et al. (Nature materials 2 (2003) 338; Science 302 (2003) 1545.) reported DNA-assisted dispersion and separation of CNTs. They found that bundled single-walled CNTs were effectively dispersed in water by their sonication in the presence of ssDNA and suggested ssDNA could bind to CNTs through π-stacking, resulting in helical wrap-ping to the surface. Very recently, CNT-based bio-nano-complex has been used to electrically detect protein and DNA (e.g. J. Am. Chem. Soc. 126 (2004) 3010.).

In order to advance the understanding of CNT-based bio-nano-system and further to predict/optimize the properties and performance of bio-CNT-complex based miniature devices, we conduct DFT-based ab initio calculations to investigate the interaction of DNA bases (A, T, C and G) with perfect and defective single-walled CNTs. DNA base-specific effects on electronic structure and electrical transport properties of single-walled CNTs with vacancy and stone-wales defects and with different chiralities are discussed on the basis of electronic structure and transport calculations. Our results suggests that the CNT-DNA base complex could be further exploited for applications such as DNA modulated molecular elec-tronics, molecular sensors and electronic DNA sequencing.

MM 41.2 Fri 12:45 IFW D

Analysis of phase contrast X-ray tomograms of nutshells: relating structure to properties — •Boris Breidenbach[1], Adrian Sheppard[2], Ulrike Wegst[3], and Klaus Mecke[1] — [1]Institut für theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — [2]Applied Mathematics, Australian National University, Canberra, Australia — [3]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Physical quantities of a porous materials, like elasticity and conductivity, depend on its chemical as well as structural properties. To examine the influence of structural properties only, chemically identical materials can be studied. Some biological materials, like wood and nutshells, mainly consist of cellulose, but the size and shape of fibers and pores is very different, as was found using various imaging techniques. Here we present the results of a study of nutshell properties using phase contrast X-ray tomography.

We determined the structure of six types of nutshells at a resolution of 0.3 μm to resolve the microscopic pore space. Parallel implementations of anisotropic diffusion and a region growing algorithm have been used to segment the data (typical size of 2000^3 voxels). Subsequently, we calculated the porosity and two-point correlation functions of the structures. In order to compare them to numerically and experimentally measured elasticity tensors, we also determined the complete set of Minkowski tensors which are motion covariant and allow for a characterization of anisotropic pore spaces.

MM 41.3 Fri 13:00 IFW D

CORRAX - A TI-FREE STAINLESS MARAGING STEEL INVESTIGATED BY 3 DIMENSIONAL ATOM PROBE — •Stefan Höring[1], Nelia Wanderka[1], Wolfgang Neumann[2], John Banhart[1], Harald Leitner[3], and Helmut Clemens[3] — [1]Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [3]Institut für Metallkunde und Werkstoffprüfung, Montanuniversität Leoben, Franz-Josef-Strasse 18, A - 8700 Leoben

Maraging steels are widely used for aerospace parts as well for tools and dies because of their good mechanical properties. Stainless maraging steels can be used as dies in the glass industry because of its good surface properties. The high strength of these steels is achieved by a precipitation hardening process. Typically these precipitates are in nanometer scale. An alloy with the technical name Corrax with the chemical composition 73.46 Fe-12.76 Cr-8.52 Ni-3.39 Al-0.79 Mo-0.58 Si-0.39 Mn-0.11 C (in at. %) was solution heat treated at 850 °C for 1/2 h and subsequently aged at 525 °C for 3 h, 10 h and 100 h. The microstructural evolution after annealing was studied by high resolution methods such as three dimensional atom probe (3DAP) and high resolution transmission electron microscopy (HRTEM). After 3 h annealing time small precipitates of nearly spherical morphology and of about 3-4 nm in diameter were formed. They are enriched in Ni and Al with an atomic ratio close to 1. While further heat treatment these precipitates grow to plates along one fixed direction.