MM 37: Nanomaterials II

Time: Thursday 14:00–16:00 Location: IFW B

MM 37.1 Thu 14:00 IFW B

graphene, magnetism, hubbard, — •Jin-Jun Liang and Ping Huai — Shanghai Institute of Applied Physics, Shanghai, China

We investigate magnetic properties of defective graphene, using a modified Hubbard model of the pi electrons of the carbon atoms. Spin interaction between pi elections and dangling sp2 bond has been taken into consideration. Mean field approximation is employed in our calculation, in order to deal with very large fragment of graphene. Magnetism of graphene with different types of defects will be presented in this talk.

MM 37.2 Thu 14:15 IFW B

Metallic nanowire growth from solution using dielectrophoresis — •Alexander Nerowski[1], Markus Poetschke[2], Manfred Bobeth[2], Walter Weber[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01069 Dresden, Germany — [2]Institute for Materials Science, Dresden University of Technology, 01069 Dresden, Germany — [3]NamLab gGmbH, 01187 Dresden, Germany

A lot of effort has been made to manufacture metallic nanowires by top-down procedures as classical lithography. Metallic nanowire growth from solution represents a promising inexpensive bottom-up method working at room temperature. By applying an AC voltage, nanowires grow on a substrate between two electrodes in a solution containing metal complexes. Aiming at a controlled growth of straight and as thin as possible wires, the growth process is investigated both experimentally and theoretically. The nanowire itself, since it is conductive, is modeled as a half-sphere electrode. Our model includes the dielectrophoretic force on uncharged metal complexes as well as their diffusion in the solution. In particular, the growth velocity of the wire is found to depend only weakly on the applied voltage since the overall growth process is diffusion-controlled. Difficulties in comparing theoretical predictions and experimental observations due to poorly known material parameters are discussed. For reasonable parameter choices, the calculated nanowire growth velocity is in modest agreement with measurements.

MM 37.3 Thu 14:30 IFW B

Synthesis and characterization of Tin Oxide nanowires and nanobelts — •Ingo Paulowicz, Yogendra Kumar Mishra, Arnim Schuchardt, Viktor Hrkac, Lorenz Kienle, and Rainer Adelung — Christian Albrechts Universität Kiel, Technische Fakultät, Kaiserstraße 2, 24143 Kiel, Deutschland

Recent developments in the direction of semiconducting oxide nanostructures have provided new dimensions in energy harvesting and storage, battery materials, solar cells, flat panel displays and others in terms of miniaturization, response and cost effectiveness [1]. Beside zinc oxide, tin oxide is the second most important member in the class of metal oxide semiconductors. It is currently undergoing different processes of synthesis to produce cost effective electronics and other devices. Several complicated synthesis methods, starting from vapor liquid solid, have been used to synthesize 1-D nanostructures of tin oxide. In present work we report a very simple flame assisted versatile and cost effective technique for growing SnO2 nanorods, nanowires, nanobelts and their networks with macroscopic expansion on the cm scale. Growth and crystalline nature of nanorods were investigated by high resolution transmission electron microscopy, which revealed [100] and [101] growth and twin boundary propagation. Mechanical properties of tin oxide nanobelts and electrical properties of nanorods will be discussed.

Z. L. Wang et al., Adv. Mater. 15, 432 (2003), Annu. Rev. Phys. Chem. 55, 159 (2004).

MM 37.4 Thu 14:45 IFW B

Boron nanotubes: new players on the nano-field — •Viktor Bezugly, Jens Kunstmann, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01069 Dresden, Germany

The existence of pure boron nanotubes (BNTs) has been proposed more than ten years ago [1]. The BNTs are predicted to have a metallic conductivity independent of their diameter and chiral angle [1-3], in contrast to the well-studied carbon nanotubes. This property makes BNTs good candidates for nanometer-scale conducting elements of future electronic devices. Recent experimental work on BNTs [4] has provided the first evidence for their metallic behavior. Nevertheless, there are still many open questions on the physical properties of BNTs which need to be answered on both the theoretical and experimental sides. In our work we theoretically investigate the electronic structure and transport properties of large-diameter BNTs of different structures and chiralities. Our results are in agreement with recent experimental findings, and a method to control the electron transport in BNTs is proposed.

References: [1] I. Boustani, A. Quandt, E. Hernandez, A. Rubio, J. Chem. Phys. 110, 3176 (1999); [2] J. Kunstmann, A. Quandt, Phys. Rev. B 74, 035413 (2006); [3] N.G. Szwacki, C.J. Tymczak, Chem. Phys. Lett. 494, 80 (2010); [4] F. Liu, C. Shen, Z. Su, X. Ding, S. Deng, J. Chen, N. Xu, H. Gao, J. Mater. Chem. 20, 2197 (2010).

MM 37.5 Thu 15:00 IFW B

Charging Gold Nanoclusters in Ionic Liquids — •Alexander Held and Michael Walter — FMF Uni Freiburg, Germany

Structures at the nanometer scale show quantized charging effects that can be observed by differential pulse voltammetry experiments. The charge dependent cluster capacitance of gold nanoclusters in the ionic liquid BMImBF4 is investigated using density functional theory (DFT) simulations. The DFT results can be understood via a semiclassical model describing the effect of a polarity inversion of the BMImBF4 double layer on the charge dependent cluster capacitance. These models also explain features seen in recent experimental data.

The DFT calculations have been carried out using the state of the art projector augmented wave method on a real space grid with the GPAW [1] implementation.

[1] https://wiki.fysik.dtu.dk/gpaw/

MM 37.6 Thu 15:15 IFW B

Atomistic simulations of nano-scale impact on phonon modes of Ge — •Daniel Sopu[1], Jani Kotakoski[2], and Karsten Albe[1] — [1]Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]Division of Materials Physics, University of Helsinki, P.O.Box 42, 00014 Helsinki, Finland

Using molecular dynamic simulations, we have studied the phonon density of states of different nano-structures like nanoparticles, nanocrystals, embedded nanoparticles and nanoglasses. We investigate the vibrational properties of Germanium as an example for a covalently bonded material using two different interatomic potentials. By comparing the vibrational properties of the nanostructures to single crystalline and bulk amorphous structures, significant deviations have been found. For each structure individually, the predominating finite-size effect was identified. We developed a complete description of size effects on phonon density of states in terms of disorder, phonon confinement due to the particle, and surface stress.

MM 37.7 Thu 15:30 IFW B

Molecular dynamics study of diffusion-induced recrystallisation — •Sebastian Manuel Eich, Michael Kasprzak, and Guido Schmitz — Institute of Material Physics, University of Muenster, Germany

Diffusion-induced recrystallisation (DIR) was investigated in thin film Au-Cu and Ni-Pd interdiffusion couples. Characteristic concentration levels are observed inside newly formed grains instead of the expected continuous Ficks diffusion profiles. This effect seems to be related to elastic mismatch strain in the diffusion zone. Experimental results reveal a relationship between characteristic compositions and the ideal shear strength of metals. Within the diffusion zone, the characteristic compositions are always adjusted so that a maximum stress of about 70% of the ideal shear strength is established. In our model, we use molecular dynamics based on embedded-atom potentials (EAM) to study the process of DIR in gold-copper diffusion couples. We simulate the stress development in thin (3-6 nm) copper layers fixed to a substrate. Step by step, copper atoms are replaced by gold. We observe a linear increase in stress with gold concentration until a critical level is reached and spontaneous relaxation and break of coherency take place. Using different conditions (temperature, external pressure ...), we are

able to confirm that the maximum stress is close to, but always lower than the ideal shear strength in the dominant slip system.

MM 37.8 Thu 15:45 IFW B

High-temperature thermal stability of nanocrystalline iron — •Jules M. Dake and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Nanocrystalline materials promise enhanced properties, but the realization and application of such materials is limited by their thermal stability. The large specific grain-boundary area leads to a strong driving force for grain growth, which can, in some cases, occur at or even below room temperature [1]. When atoms of a second species with an appreciable segregation enthalpy are introduced, they should, in theory, reduce the grain-boundary energy and thus the driving force. Exactly this has been reported for numerous binary systems, as summarized in [2]. Our investigations of binary Fe alloys show similar results up to a temperature of $\sim 900°$C. Above this limit, however, stability is suddenly lost. *In situ* XRD results appear to incriminate the α-to-γ transformation. Direct observation of the microstructure by FIB microscopy reveals a growth morphology similar to that of recrystallization or abnormal grain growth.

[1] M. Ames *et al.*, *Acta Mater.* **56** (2008) 4255–4266.
[2] J. R. Trelewicz and C. A. Schuh, *Phys. Rev. B* **79** (2009) 094112.