Formation of dendritic metallic nanowires — •Nitesh Ranjan[1], Hartmut Vinzelberg[2], and Michael Mertig[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Recently, we reported an electrical-field-controlled growth process for the directed bottom-up assembly of one-dimensional palladium nanowires between micro-fabricated electrodes [1]. The wires, grown from an aqueous palladium salt solution by dielectrophoresis, had a thickness of only 5-10 nm and a length of up to several micrometers. The growth process was found to depend largely on the deposition conditions like the strength and the frequency of the applied AC field and the concentration of the metal salt solution. Here, we report the formation of thin, but straight and dendritic metallic nanowires, obtained in the low-frequency regime. The morphology of the wires was characterized by scanning force microscopy (SFM), scanning electron microscopy and transmission electron microscopy. SFM investigations revealed that the palladium nanowires grown over the glass and silicon substrates have a typical thickness of about 25 nm. Room temperature I-V measurements show them to be Ohmic in nature with a resistance of about 80 kOhm. Low-temperature measurements show the phenomenon of zero bias anomaly. The investigated growth method is capable of controllable in-place formation of complex circuit patterns for future nanoelectronics. [1] Nitesh Ranjan, Hartmut Vinzelberg, Michael Mertig, Small 2, 1490 (2006).

MM 26.3 Wed 10:45 IFW B

A structure-induced metal-insulator transition in thin MoS nanowires — Igor Popov[1], Gotthard Seifert[1], and •Sibylle Gemming[2] — [1]Theoretische Chemie, TU Dresden, D-01062 Dresden, Germany — [2]Forschungszentrum Dresden-Rossendorf, P.O.Box 510119, D-01314 Dresden, Germany

Transition metal chalcohalides MX2 can form a wealth of diverse nanostructures, which range from large octahedral and fullerene-like hollow clusters and cylindrical nanotubes close to the nominal composition M:X = 1:2 to smaller, two-dimensional platelet-shaped clusters under sulfur excess and to one-dimensionally elongated nanowires under sulfur-deficient conditions. All of those structures exhibit specific electronic properties that differ from the ones of the pure bulk and open up a large application spectrum, that includes the lubricant aspect, but extends to catalysis and electronic transport. One-dimensionally delocalized electronic states provide the basis for the higher activity, reactivity and conductivity in such nanostructures. One-dimensional MX wires are composed of a central metallic wire coated by a sulfur and/or halide shell. They exhibit a very high structural regularity, hence, ballistic conductivity may be obtained in such structures. DFT calculations showed that wires can act as electromechanical switches, because they undergo a symmetry-dependent metal-insulator transition upon twisting [Nano Lett.,10.1021/nl801456f; Nano Lett., 2008, 8, 3928-3931].

MM 26.4 Wed 11:00 IFW B

Conductivity and shot noise in graphene at high bias voltages — •Aurelien Fay[1], Romain Danneau[1,2], Fan Wu[1], Matti Tomi[1], Julien Wengler[1], and Pertti Hakonen[1] — [1]Low Temperature Laboratory, Helsinki University of Technology, Espoo, Finland — [2]Institut für Nanotechnology, Forschungszentrum Karlsruhe, and Physikalische Institut, Universität Karlsruhe, Karlsruhe, Germany

The conductivity and the shot-noise in graphene contain both interesting informations on the transport properties of the Dirac fermions. By measuring these two quantities, we have shown that the transport in Graphene could be ballistic [1]. The interaction between optical phonons and charge carriers in graphene can suppress this ballistic transport and, therefore, dramatically changes the conductivity and the Fano factor.

We have increased the electron-phonon coupling in graphene by subjecting the graphene sample at high bias voltages [2]. At a relative low bias, we have measured a linear dependence of the conductivity as a function of the bias voltage. This has been recently pointed out by E. Sonin [3]. In the high bias regime, the decrease of the conductance and the drop of the Fano factor could both be explained by the interaction between optical phonons and charge carriers.

[1] R. Danneau *et al.*, Phys. Rev. Lett. **100**, 196802 (2008).
[2] W.K. Tse *et al*, Appl. Phys. Lett. **93**, 023128 (2008)
[3] E. B. Sonin, Phys. Rev. B **77**, 233408 (2008).

MM 27: Interfaces I

Time: Wednesday 11:30–12:45 Location: IFW B

MM 27.1 Wed 11:30 IFW B

Grain boundary migration by molecular-dynamics simulation — •Jian Zhou, Volker Mohles, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, Aachen

Molecular dynamics simulations have been used to study grain-boundary migration of three series ([001], [011], [111]) of twist grain boundaries (GBs) in copper. An orientation-correlated force being able to drive flat GBs with different misorientations was applied to all twist GBs. The temperature dependence of the GB mobility was determined over a wide misorientation range. It is found that there is an obvious reduction in activation enthalpy with respect to GB migration when the temperature rises to a certain point for many high-angle and high-energy GBs. This reduction could be attributed to the structural change in GBs, such that different GB migration mechanisms become active. Moreover, GB structures were characterized by common neighbor analysis at low temperature. For low-angle GBs, a network of screw dislocations were traced, and it was found that this structure is relatively stable during the GB migration process. For high-angle GBs, in contrast, much more complicated and spatially extended GB structures were observed, which move mainly by a collective shuffle mechanism.

MM 27.2 Wed 11:45 IFW B

Phase-field modelling of foam microstructure evolution — •Frank Wendler, Eduard Stirner, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Moltkestr. 30, 76133 Karlsruhe, Germany

Foam is a cellular materials with large variety of applications ranging from metal or polymer foams to cosmetics. After generation, a foam is a liquid with a complex rheological behaviour, dominated by surface free energy minimisation towards configurations of local equilibrium. We adapt a general multi phase-field model to describe this evolution step, important for the mechanical properties of a solidified foam material. Starting with a volume preserving Allen-Cahn model for incompressible dry foams with negligible liquid fraction (e.g. soap froth), a pressure dependant term is added to the functional of the free energy. This allows for the treatment of bubbles filled with a compressible gas. Assuming homogeneous pressures related to an equation of state a consistent model of boundary evolution can be given. The results approve that pressures within single bubbles are related to interface curvature according to the Young-Laplace equation. Simulations of bubble clusters and foam structures in 2D and 3D are presented, including the examination of pressure variations as a process step to optimize structure and accelerate equilibration. Finally, the treatment of wet foams with a non-negligible fraction of liquid, concentrated along the Plateau borders is given. Numerical evaluation of surface energies and dynamics show that it is not necessary to completely resolve the diffuse interface, which enables the simulation on larger length scales.

MM 27.3 Wed 12:00 IFW B

Simulations of surface energy driven processes at structured substrates — •Marcus Jainta and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

We introduce a new method based on a phase-field model to simulate the behaviour of multiple phase regions at given non-moving obstacles with sharp interfaces in terms of new boundary conditions. We discuss the results for different surface energies of the simulated microstructures and bubbles. In addition, we consider adhesion forces in the presence and absence of fluid flow. The simulation results of liquid droplets on structured surfaces are compared with experiments related to the Lotus effect. Finally we discuss the numerical method and implementation of the new boundary conditions.