

MM 49: Nanomaterials II

Time: Thursday 11:45–13:00

Location: H 1029

MM 49.1 Thu 11:45 H 1029

Control of residual less noble element content during dealloying — ●ZHEN QI¹ and JÖRG WEISSMÜLLER^{1,2} — ¹Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany — ²Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Nanoporous metal prepared by the corrosion of an alloy can take the form of monolithic, millimeter-sized bodies containing approximately 10^{15} nanoscale ligaments per cubic millimeter. Applications have been suggested, for instance in catalysis, sensing and actuation. Although the process of dealloying has seen many studies, the underlying processes remain to be clarified in more detail. Here we explore the structure size and residual Ag content in AgAu alloys during electrochemical dealloying. We study different dealloying potentials and a series of alloys including specifically solid solutions that are dilute in Au. A major finding is that nanoporous samples with large content of residual Ag can be prepared. This is surprising in view of the overpotential required for bulk dealloying. The overpotential exceeds the variation of the Ag Nernst potential through the alloy series, suggesting that equilibrium thermodynamics of the bulk alloy alone cannot explain the arrest of the corrosion at finite Ag content. The data set acquired in our study will provide a data base for verifying models of the corrosion process that include capillary terms as well kinetic aspects such as adatom diffusion and vacancy island nucleation.

MM 49.2 Thu 12:00 H 1029

Strengthening of Au-Au bonds in small gold clusters by adsorbing noble gases — ●LUCA M. GHIRINGHELLI, SERGEY LEVCHENKO, and MATTHIAS SCHEFFLER — Fritz Haber Institute, D-14195, Berlin

In state-of-the-art experiments for the vibrational spectra of metal clusters in the gas phase, photodissociation spectroscopy is performed on clusters complexed with noble gas (RG) atoms, where a RG atom is usually expected to form a weak van der Waals bond. By employing DFT (PBE functional with selected comparisons to PBE0, and to MP2 and CCSD(T) calculations), we surprisingly find a partially covalent bond of *neutral* dimers with RG. For RG = Ar, Kr, Xe one or two RG atoms can bind in a linear molecule with Au₂. While both Hirschfeld and Mulliken analyses show a small electron transfer from the RG to Au₂, the Au-Au bond *shortens* and the Au-Au stretch frequency increases. This is inconsistent with the expected effect of electron transfer to the antibonding orbital of the dimer. Electron-density (n) differences between the bonded systems and the isolated fragments show an accumulation of n between RG and the neighboring Au atom, and between the gold atoms. The analysis of the projected density of states reveals that, although only non-bonding orbital interactions and no charge transfer occurs between RG and Au₂, the d -electrons of Au₂ are redistributed due to the interaction with RG in such a way that the Au-Au σ_s bond is strengthened.

MM 49.3 Thu 12:15 H 1029

Boron Nanotubes: Structural Stability and Electronic Properties — ●VIKTOR BEZUGLY, JENS KUNSTMANN, and GIANAURELIO CUNIBERTI — Institute for Materials Science and Max Bergman Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

The transport properties, work functions, electronic structure, and structural stability of boron nanotubes with different radii and chiralities are investigated theoretically [1]. As the atomic structure of boron nanotubes and the related sheets is still under debate, three probable structural models are considered. For comparison with recent transport measurements [2], the intrinsic conductance of ideal nanotubes with large diameters is determined. All considered boron

nanotubes are highly conductive, irrespective of their lattice structures and chiralities, and they have higher conductivities than carbon nanotubes. Furthermore, the work functions of the three sheets and the corresponding large-diameter nanotubes are determined. It is found that the value of the nanotubes obtained from one model sheet agrees well with the experiment in contrast to the other two models. The energetic stability of nanotubes with diameters >2 nm approaches that of the corresponding boron sheets. However, for smaller diameters the relative stabilities change significantly.

[1] V. Bezugly, J. Kunstmann, B. Grundkoetter-Stock, T. Frauenheim, T. Niehaus, G. Cuniberti, ACS Nano **5**, 4997 (2011).

[2] F. Liu, C. Shen, Z. Su, X. Ding, S. Deng, J. Chen, N. Xu, H. Gao, J. Mater. Chem. **20**, 2197 (2010).

MM 49.4 Thu 12:30 H 1029

Structural and electrical properties of silicon/silicon dioxide nanostructures grown by decomposition of SiOx for photovoltaic applications — ●MAURIZIO ROCZEN¹, MARTIN SCHADE², THOMAS BARTHEL¹, JAN AMARU TÖFFLINGER¹, ABDELAZIZE LAADES³, MICHAEL BLECH³, ENNO MALGUTH¹, HARTMUT LEIPNER², LARS KORTE¹, and BERND RECH¹ — ¹HZB, Institut für Silizium-Photovoltaik, Berlin, Germany — ²MLU, IZM, Halle, Germany — ³CiS, Erfurt, Germany

For the application as nanodot hetero-emitter the self organized growth of Si/SiO₂ nanostructures by decomposition of sub-stoichiometric SiOx layers is investigated as well as the structural and electrical and properties of the nanodot system. The SiOx layers are deposited by PVD and CVD techniques onto crystalline Si (c-Si) wafers. The O/Si ratio is obtained by XPS and EDX measurements. XPS shows that decomposition of SiOx is completed after annealing the films at 900 °C. The growth of crystalline Si nanodots is shown in HRTEM images and confirmed by Raman spectroscopy. The size and density of the nanostructures is controlled by the applied annealing temperature and oxygen content. Oxygen rich films show a blue shifted photoluminescence signal which might be related to quantum size effects. Hydrogen concentration of CVD deposited SiOx decreases with increasing oxygen with direct influence on the charge carrier lifetime. The current density through the c-Si/SiOx system decreases with increasing oxygen content. AFM current mapping show a reduction of percolation paths. Doped SiOx induces a band bending of 730 meV in the substrate.

MM 49.5 Thu 12:45 H 1029

Luminescence Properties of Cer-doped Yttrium Aluminum Garnet (YAG:Ce) Nanoparticles - Absolute Quantum Yields and Influence of Particle Size — ●MARTIN KAISER¹, CHRISTIAN WÜRTH¹, UTE RESCH-GENGER¹, MARK VORSTHOVE², and ULLRICH KYNAST² — ¹BAM Federal Institute for Materials Research and Testing, Berlin, Germany — ²University of Applied Sciences, Münster, Germany

Yttrium aluminum garnet (YAG) doped with Ce³⁺ (YAG:Ce) is a green-yellow emitting phosphor widely used in the rapidly expanding market of white light LEDs for converting the blue emission of (In,Ga)N-Chips into white. Its advantages compared to other materials include a high photostability and a high luminescence quantum yield (QY) of up to 95 %.

Here, we present measurements of the QY and luminescence lifetimes of a series of YAG:Ce particles of varying sizes ranging from 20 nm to a few micrometer using a new custom designed integrating sphere setup traceably calibrated. The ultimate goal is to understand the influence of the surface-to-volume ratio and the Ce³⁺ dopant concentration on the photophysical properties of these materials. Our measurements reveal that the QY and decay kinetics are clearly affected by particle size. Low temperature time-resolved measurements were performed to gain a deeper understanding of the decay kinetics.