# MM 58: Nanomaterials I

Time: Thursday 10:15–11:45 Location: IFW D

MM 58.1 Thu 10:15 IFW D

**Factors Influencing Melting and Solidification of In-Nanoparticles Embedded in an Al-matrix** — •Mostafa Mohamed, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics,Münster,Germany

Nano-crystalline Indium particles embedded in an Al-matrix are synthesized by rapid solidification. Calorimetry and electron microscopy was utilized to study the melting and solidification of In-nanoparticles with a diameter between 20-350 nm. The volume strains accompanying the transformation are accommodated partially by generation of dislocations and missing wedges of the nanoparticles. Thermal cycling leads to a reduction of the maximum overheating temperature, and an increase of the minimal solidification temperature. The three effects which can affect the equilibrium melting temperature of In-nanoparticles, change in volume during melting, differential thermal expansion of the nanoparticles and the matrix capillarity effect are discussed.

MM 58.2 Thu 10:30 IFW D

**Nanoparticles and Nanocomposite Thin Films Prepared by Gas Aggregation Source** — •Oleksandr Polonskyi, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Christian-Albrechts University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Nanocomposite thin films consisting of metal nanoparticles (NPs) in a dielectric organic or ceramic matrix have unique functional properties with numbers of applications. The metallic nanoparticles typically form via a self-organization during co-deposition of the metallic and matrix components. Various methods such as sputtering, evaporation, and plasma polymerization have been applied for the deposition of the matrix component, while the metallic component has mostly been sputter deposited. However, recently gas aggregation nanoparticle sources have attracted high interest in order to obtain independent control of filling factor and size distribution of the embedded metallic nanoparticles. In the present talk, the details about formation of nanoparticles and nanocomposites by means of gas aggregation method will be discussed. In addition, we report on the <<in-flight>> treatment of metallic nanoparticles, generated by gas aggregation method for novel nanostructure formation. Here, in particular, the attention will be paid to optical composites and silver containing biocompatible antibacterial coatings with tailored release rate.

MM 58.3 Thu 10:45 IFW D

**Formation of Co/SiO2 nanocomposites via dewetting of multilayer structures** — •Oleksandr Polonskyi, Justin Jetter, Carsten Hänel, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Christian-Albrechts University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Nanocomposite thin films with metallic nanoparticles embedded into dielectric matrix have attracted much attention for their interesting functional properties. In the current work, we focus on magnetic Co/SiO2 nanocomposites prepared via magnetron sputtering of Co-SiO2 multilayers and subsequent heat treatment, leading to formation of Co nanoparticles embedded in an SiO2 matrix via dewetting and self-organization. The influence of deposition parameters and heat treatment conditions on microstructure and properties of the resulting films was investigated. Structure and morphology of the samples were characterized by SEM and TEM. XPS was used to investigate the chemical composition of the deposited samples and for monitoring of the changes occurring during heat-treatment. Vibrating sample magnetometry (VMS) was applied for investigation of magnetic properties. The mechanism of the self-organized microstructural evolution will be discussed.

MM 58.4 Thu 11:00 IFW D

**Quantitative heat capacity measurements of Au nanoparticles using a nanocalorimeter** — •Emanuel Franke[1], David A. LaVan[2], and Cynthia A. Volkert[1] — [1]Inst. für Materialphysik, Uni Göttingen, 37077 — [2]MML, NIST, Gaithersburg, USA 20899

As sample length scales reach down to nanometers, and the surface influence becomes large, thermal properties such as the heat capacity change. The involved heat in such samples is very small and can only be measured via convent. calorimetry by pressing milligrams of sample material together, whereby the surface influence of the sample is reduced. However, nanoscale samples can be directly measured by MEMS-based differential nanocalorimeters which have sufficient res. to measure with nJ sensitivity. Nonetheless, it is well known that heat losses of the MEMS sensors may change in the presence of a sample, leading to large changes in the nanocalorimetric signal and quantitative determination of heat capacity. In this study, FEA is used to investigate the interplay of heat losses (rad. and cond.), sample properties (therm. emissivity and conductivity), and temp. distr. on the sensor. On the basis of this analysis, the influence of exp. issues (misaligned sample, amb. temp.) can be evaluated. Furthermore, the sample geometry could be adapted to minimize the influence of the sample prop. on the measurement. With this knowledge, the heat capacity of Au nanoparticles (1 nm to 20 nm) was measured from 30 K to 300 K with a heating rate of 18,000 K/s with a resolution of better than 1 nJ/K. Together with TEM investigations, this reveals an enhancement in the heat capacity at low temp. that decr. with incr. particle size.

MM 58.5 Thu 11:15 IFW D

**Stability of carbon nanotubes under hydrostatic pressure investigated by Monte Carlo simulations** — •Markus Hartmann — Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

Carbon nanostructures are a fascinating class of materials combining high stiffness with low weight and exceptional toughness that makes carbon a promising candidate for applications in structural mechanics. Understanding the mechanical properties of these structures on every length scale is of utmost importance to be able to exploit the full potential of these materials. Monte Carlo simulations are a perfect tool to gain an insight into the complex deformation behavior of carbon nanostructures like graphene [1], nanotubes [2] and fullerenes [3] on an atomic scale. In the presented work I will discuss investigations on the mechanical stability of carbon nanotubes under hydrostatic pressure. Carbon nanotubes of different sizes and chiralities will be investigated. The shape of the initially circular cross-section of the tubes will be monitored. Under increasing load it first ovalizes into an elliptic shape, upon further increase of the load the shape further evolves into a peanut-like shape. Finally I will discuss the effect of nanotube size on the critical collapse pressure.

[1] Hartmann et al., Europhys. Lett. 103, 68004 (2013)
[2] Sun et al., Proc. Appl. Math. Mech. 13, 7 (2013)
[3] Holec et al., Phys. Rev. B 81, 235403 (2010)

MM 58.6 Thu 11:30 IFW D

**Alternative substrate materials for silicene: $WSe_2$ and $MgX_2$ (X = Cl, Br, and I)** — •Udo Schwingenschlögl and Jiajie Zhu — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Silicene is the Si analogue of graphene with honeycomb structure and characteristic Dirac states, while being fully compatible with current Si-based nano-electronics. It can be prepared on metallic substrates, such as Ag(111), Ir(111) and $ZrB_2$(0001), but a strong interaction regrettably perturbes the electronic states. Semiconducting Si(111) and SiC(0001) substrates, on the other hand, require surface passivation due to dangling bonds, which complicates the preparation procedure. We employ first-principles calculations in order to identify alternative substrate materials, focussing on layered compounds, because a weak interaction with silicene is expected. Both $WSe_2$ and $MgX_2$ (X = Cl, Br and I) turn out to be interesting candidates. The effects of these substrates on the properties of silicene are analyzed and discussed with respect to technological requirements.

References:
- Journal of Materials Chemistry C **3**, 3946-3953 (2015)
- ACS Applied Materials & Interfaces **6**, 11675-11681 (2014)