MM 36: Nanomaterials I: Excess Volume and Confinement

Time: Wednesday 11:45–12:45 Location: H 0107

MM 36.1 Wed 11:45 H 0107

Redistribution of Excess Volume by Mechanical Deformation in Nanocrystalline Alloys — •Michael Johannes Deckarm, Timo Tscharntke, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, D-66123 Saarbrücken

Nanocrystalline (NC) alloys with grain sizes at the low end of the nanoscale ($\approx$ 10nm) are characterised by a large volume fraction of grain boundaries ($>$ 25%), contributing to dramatically increased total excess volume and energy compared to conventional materials. We try to shed light on the interplay between these excess quantities and the altered mechanical properties of NC metals. Using a combination of X-ray diffraction, length and density measurements to detect direction-dependend and absolute excess volume changes before and after uniaxial compression, enabled us to compare our findings qualitatively with the predictions made by Bachurin and Gumbsch in (1). They simulated (MD-simulation) uniaxial deformedation of NC Pd and deduced an anisotropic redistribution of the grain boundary excess volume and an anisotropic change of Young's modulus. In contrast, we found no evidence for excess volume redistribution but rather an excess volume annihilation along the direction of compression. A possible reconciliation might be related to viscoelastic recovery processes.

(1) D. V. Bachurin, P. Gumbsch, Physical Review B, 85, (2012), 085407 1-9, doi:10.1103/PhysRevB.85.085407

MM 36.2 Wed 12:00 H 0107

Defects and structural anisotropy of HPT- and ECAP-deformed Ni studied by difference dilatometry — •Jaromir Kotzurek[1], Anton Hohenwarter[2], Simon Trubel[3], Christian Neubauer[1], Sergiy Divinski[3], Wolfgang Sprengel[1], Gerhard Wilde[3], Reinhard Pippan[4], and Roland Würschum[1] — [1]Institute of Materials Physics, Graz University of Technology — [2]Department of Materials Physics, University of Leoben — [3]Institute of Materials Physics, University of Münster — [4]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences Leoben

Difference dilatometry is used to study the excess volume associated with defects which are induced by high-pressure torsion (HPT) and equal-channel angular pressing (ECAP). Based on our recent studies of grain-boundary excess free volume in HPT-deformed Ni [1], issues of structural anisotropy and method of deformation are in the focus of the present studies. Both HPT- and ECAP-deformed nickel show an anisotropic defect annealing behavior prior to the onset of recrystallization, which can be associated with an anisotropic grain shape caused by the deformation. Anisotropic length change is also found after uniaxial post-deformation of HPT-Ni, indicating that the anisotropy is not caused by residual stresses. Financial support by the FWF Austrian Science Fund is appreciated (project P25628-N20).

[1] E.-M. Steyskal et al, Phys.Rev.Lett., **108** (2012) 055504

MM 36.3 Wed 12:15 H 0107

Charakterisierung der Nanoporen in mit Ionic Liquid beladenem Silica Gel über die Messung der Positronenlebensdauer — •Christian Herold — Technische Universität München, München, Deutschland

In diesem Beitrag werden Messungen an unterschiedlichen Silica Gel Proben vorgestellt, die mit einem Ionic Liquid (IL) beladen sind. Supported Ionic Liquid Phase (SILP) Materialien besitzen großes Potential für Anwendungen sowohl in Wissenschaft als auch in Industrie, u.a. als Katalysatoren. Mittels Positronen-Annihilations-Lebensdauer-Spektroskopie (PALS) war es uns möglich, das mittlere Volumen der Nanoporen im Silica Gel zu bestimmen. Dieses freie Volumen wird durch die Beladung mit IL und/oder Wasser drastisch reduziert. Bei einer Beladung mit 70 Volumenprozent IL ist das mittlere Porenvolumen gegenüber reinem Silica Gel um ca. 60% verringert.

MM 36.4 Wed 12:30 H 0107

Local sublattice symmetry breaking in graphene with centrosymmetric deformations — Martin Schneider[1], Daiara Faria[2], •Silvia Viola Kusminskiy[1], and Nancy Sandler[3] — [1]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universitaet Berlin, Deutschland — [2]Universidade Federal Fluminense, Rio de Janeiro, Brasil — [3]Ohio University, Ohio, United States

A generic deformation of a graphene sheet causes inhomogeneous strain which results in an effective, non-uniform pseudomagnetic field acting on the Dirac fermions. This can provide an alternative route to confine and control charge carriers in graphene. We investigate the electronic properties of a graphene sheet in the presence of an out-of-plane deformation with centro-symmetric geometry, for which the pseudomagnetic field presents trigonal symmetry. We address the question of confinement of electrons due to this deformation, using a scattering formalism based on the continuum description of graphene. In particular we study the local density of states (LDOS) of the electronic carriers, and show that this type of deformation causes a noticeable imbalance in the distribution of charge density between the two graphene inequivalent sublattices even for small deformations. We perform exact numerical calculations and show that the results are well described within an analytical, perturbative approach for small deformations. We discuss our results in view of recent experimental findings.