# MM 51: Nanomaterials - Nanocrystalline & Porous Materials I

Time: Thursday 10:15–11:30 Location: H25

MM 51.1 Thu 10:15 H25

**Molecular dynamics simulations of free volume redistribution in metallic nanoglasses** — •Omar Adjaoud and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt, Germany

Nanoglasses are formed with glassy regions separated by interfacial areas which are called glass-glass interfaces. These interfaces influence many properties of nanoglasses such as mechanical properties. The structure arrangement at the interfaces produces excess free volume. The nanoglasses properties depend on the structure and density of their interfaces. Therefore, a detailed study of the structure and density of glass-glass interfaces is required to understand nanoglasses properties.

In the present study, we have performed molecular dynamics (MD) simulations to model excess free volume and structure of glass-glass interfaces in a metallic glass (MG) Cu64Zr36 and a MG Pd80Si20 which is a representative of metal-metalloid systems. The interactions between the atoms are described by embedded atom model. The free volume was created by randomly diluting a sphere of 1 nm radius in the simulation box of 5.8x5.8x5.8 nm dimensions for different densities with respect to the bulk glass density. For each density the system was monitored in MD runs by following the density redistribution throughout the sample with time. As a second set of simulations, a cluster of four glassy spheres of 5 nm diameter were created to form a free volume between them. The evaluation of the free volume was followed by MD simulations. The results are compared to experimental observations.

MM 51.2 Thu 10:30 H25

**Investigation of the grain boundarie excess free volume in nanocrystalline $Pd_{90}Au_{10}$ under plastic deformation** — •Michael J. Deckarm, Jonas Heppe, Björn Lechthaler, Christian Braun, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

In as-prepared nanocrystalline (nc) materials, grain boundaries (gb) are usually in a local nonequilibrium configuration, reflecting the preparation history. A two-stage recovery process of as prepared nc Pd90Au10 has been found [1]: First a reduction of the excess free volume at lower temperatures followed by grain growth at higher temperatures. Thus by careful annealing the nanocrystalline specimen below the onset temperature of grain growth, it is possible to locally equilibrate the gb by reducing their excess free volume but avoiding grain growth. As a result, the change of the free volume in the gb can be deduced by density measurements. Moreover, using calorimetry we can determine the excess enthalpy resulting from plastic deformation of the equilibrated samples, so obtaining the relation between stored excess enthalpy and excess free volume. Combining the results from XRD, density and thickness measurements, we find that deformation is accompanied by reduction of excess free volume.

[1] A. Tschöpe, R. Birringer and H. Gleiter; Calorimetric Measurements of the Thermal Relaxation in Nanocrystalline Platinum; Journal of Applied Physics (USA). Vol. 71, no. 11, pp. 5391-5394. 1 June 1992

MM 51.3 Thu 10:45 H25

**Stabilization of Nanocrystalline Iron by Segregation of Carbon at the Grain Boundaries** — •Marie Christine Trynogga[1], Andreas Herz[2], Yuzeng Chen[3], Christine Borchers[1], and Reiner Kirchheim[1] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]TU Ilmenau, FG Werkstoffe und Elektrotechnik, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau — [3]State Key Lab of Solidification Processing, Northwestern Polytechinical Univeristy, Xi'an, China

A nanocrystalline iron-carbon alloy was produced by high-energy ball milling to experimentally confirm the *defactants* (**def**ect **act**ing ag**ents**) concept, which was introduced in [1]. For this system the *defactants* concept predicts that the carbon atoms act as segregating solute atoms, i.e. the carbon is enriched at the grain boundaries and significantly reduces the grain boundary energy. So the formation of grain boundaries is favoured, stabilizing the grain boundaries leading to a nanocrystalline structure.

Iron powder was mixed with graphite reaching carbon concentrations of up to 4.3 wt.%. The samples were produced by high-energy ball milling. The microstructure was investigated by X-ray diffraction (XRD) and transmission electron microscopy (TEM). It was observed that the $\alpha$-iron structure persists and the grain size decreases with increasing carbon concentration. This dependence follows from the *defactants* concept connected with a simple mass balance of carbon in a closed system.

[1] R. Kirchheim, Acta Materialia 55 (2007) 5129 and 5139

MM 51.4 Thu 11:00 H25

**Solid solution strengthening in nanocrystalline Pd-Au alloys** — •Andreas Leibner[1], Manuel Grewer[1], Christian Braun[1], Jonas Heppe[1], Jochen Lohmiller[2], Patric Gruber[2], and Rainer Birringer[1] — [1]Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2 2, 66123 Saarbrücken — [2]Karlsruher Institut für Technologie, Institut für Angewandte Materialien, Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen

It is well known that nanocrystalline (nc) materials show enhanced mechanical properties depending on their grain size. In binary alloys, solute drag enhances the stability of the nanoscale microstructure. However, systematic studies on the influence of solute content on the mechanical response of nc alloys with constant grain size are still scarce. Here we report on the influence of gold concentration on the strength of nc Pd-Au with 10nm-sized grains. The samples were prepared by inert gas condensation and tested in shear-compression-specimen (SCS) geometry. While all Pd-Au compositions show the typically increased strength due to grain refinement, the overall trend is a fairly linear strength decrease with rising gold concentration. In contrast, Vickers hardness measurements on arc melted coarse grained Pd-Au alloys exhibit classical solid solution hardening.

MM 51.5 Thu 11:15 H25

**Following the deformation processes of nanocrystalline PdxAu1-x by the combination of in-situ straining and ACOM-TEM** — •Aaron Kobler[1,2], Christian Kübel[1], and Horst Hahn[1,2] — [1]Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany — [2]Technische Universität Darmstadt (TUD), 64287 Darmstadt, Germany

Understanding the deformation mechanisms in nanocrystalline (nc) metals and alloys is crucial for improving their performance and stability as needed for technical applications. Most of our current understanding stems from in-situ deformation experiments on bulk nc materials using XRD. However, it is difficult to understand the local processes based on bulk measurements. The local processes are traditionally investigated using classical BF/DF-TEM. Recently, ACOM-TEM is used instead of BF/DF-TEM as it identifies the crystallographic orientation of all crystallites and detects all CSL special boundaries within the imaged area. We have implemented the ACOM-TEM (NanoMegas) on a FEI Tecnai-F20 in micro-probe (up) STEM mode, that allows us to acquire (fast) STEM reference images. We combined ACOM-TEM imaging with in-situ straining inside the TEM using Hysitron's TEM Picoindenter using steps of increasing strain. First investigations were conducted on magnetron sputtered Au samples. Deformation of this film inside the TEM allowed us to follow the continuous process of grain growth and grain rotation in nc Au with increasing strain. New results on the influence of alloying content in PdxAu1-x on the deformation mechanisms will be discussed.