

tic deformation could be studied in detail. This was the motivation for a nanomechanical approach to hydrogen embrittlement of metals using a novel in-situ electrochemical nanoindentation setup. In this work nanoindentation has been used to study the effect of hydrogen on deformation of small volumes for nickel and copper single crystals as two metals with different sensitivity to hydrogen embrittlement. Nickel is known to be prone to hydrogen embrittlement where there is no hydrogen embrittlement for copper. Electrochemical hydrogen charging reduces the load at which dislocations are nucleated (pop-in load) in nickel, while this results in no observable change in the pop-in load of copper single crystal as expected. The experimental results are analyzed using a thermodynamic model for homogenous dislocation nucleation. Based on these analyses, the activation energy for the onset of plasticity is believed to be reduced by the dissolved hydrogen in crystal lattice.

MM 8.5 Mon 16:30 H16

**Plasticity of thin polycrystalline metallic films: a discrete dislocation dynamics approach** — ●JOCHEN SENGER<sup>1</sup>, DANIEL WEYGAND<sup>1</sup>, OLIVER KRAFT<sup>1,2</sup>, and PETER GUMBSCH<sup>1,3</sup> — <sup>1</sup>IZBS, Universität Karlsruhe (TH) — <sup>2</sup>IMF II, Forschungszentrum Karlsruhe — <sup>3</sup>IWM, Fraunhofer Institut für Werkstoffmechanik, Freiburg

Recent experimental observations (Spolenak et al, PRL 90, 096102, 2003) showed that the stress distribution in polycrystalline thin metal films upon thermal cooling or heating can be quite inhomogeneous. Stress variations were observed between grains and even within grains. To study such stress distributions, a parallel discrete dislocation dynamics (DDD) tool is employed, based the tool described in Weygand et al., Mod. Sim. Mater. Sci. Eng. 10 (2002) 437. The parallelization is achieved using OpenMP for shared memory platforms. The concept is based on a common data structure, where the individual calculation tasks are distributed among the CPUs. The main computational tasks, the interaction calculation between dislocation and the evaluation of

the boundary conditions are performed on multiple CPUs and a very good scaling is achieved. The parallelized version of the DDD code is applied to the simulation of the small scale plasticity of polycrystalline thin films. The dislocation microstructure evolution and the resulting stress distributions are analysed and compared experiments and single grain simulations. If the calculated stresses of the multi grain simulations are averaged over areas corresponding to the experimental resolution, excellent agreement is found for stress amplitudes in simulation and experiment.

MM 8.6 Mon 16:45 H16

**Modulated lateral force microscopy: an AFM tool for analysis and modification of polymer surfaces** — ●HEINZ STURM — BAM VI.25, Federal Institute for Materials Research, Unter den Eichen 87, D-12205 Berlin

Scanning Probe Microscopy, here Scanning Force Microscopy in the contact mode, is widely used not only to examine the 3-dimensional surface topography, but also to evaluate nano-mechanical surface properties. This contribution focuses on the tip-surface interaction due to a shear deformation, i. e., friction. During forward and backward scan with a given scanning (shear) velocity, the cantilever lateral bending (torsion) is a measure for the lateral force. Unfortunately, both scan directions must be acquired and subtracted to separate the topography cross-talk from the friction image. Superimposing a lateral displacement between tip and surface via a dither piezo, the shear deformation is sinusoidally modulated. Images of amplitude and phase shift of the dynamic cantilever torsion within a frequency range from 30 kHz up to 60 MHz are presented. Due to the fact that friction is always a dynamic process, we prefer to call this technique "Modulated Lateral Force Microscopy" (MLFM) instead of just "Dynamic Friction Microscopy". The dependence of the modulated friction from the normal force between tip and lever can be described with the Johnson-Kendall-Roberts model.

## MM 9: Liquid and amorphous materials III

Time: Monday 14:45–15:45

Location: H4

MM 9.1 Mon 14:45 H4

**Liquid phase demixing and growth in Cu-based alloys** — ●MATTHIAS KOLBE<sup>1</sup>, JIANRONG GAO<sup>2</sup>, JIUZHOU ZHAO<sup>3</sup>, LORENZ RATKE<sup>1</sup>, and DIETER HERLACH<sup>1</sup> — <sup>1</sup>DLR, Institut für Materialphysik im Weltraum, Linder Höhe, 51170 Köln — <sup>2</sup>Key Lab of Electromagnetic Processing of Materials, North Eastern University, Shenyang 110004, China — <sup>3</sup>Institute of Metal Research, CAS, Shenyang 110016, China

Cu-based alloys as Cu-Cr, Cu-Co, Cu-Nb and Cu-Fe exhibit a flat liquidus in the binary phase diagram. This property is often associated to metastable phase separation in the region of the undercooled melt: When the metastable miscibility gap is entered, the homogeneous alloy separates into a Cu-rich and a Cu-poor liquid. The undercooled melt solidifies rapidly and the metastable liquids are frozen in. Microstructure analysis of the solidified material allows the determination of properties of the metastable liquids. We studied phase separation and phase growth of the metastable Co-rich L1 phase in Co-84at%Cu by electromagnetic levitation (EML) and drop tube experiments. In addition, samples have been processed and solidified in the TEMPUS facility during parabolic flights under low gravity conditions. Compared to processing in EML on ground, the fluid flow is reduced in TEMPUS by an order of magnitude. The solidified microstructures show the influence of cooling rate and of the different convection levels in the liquid on phase growth. The results are discussed within current models of liquid phase growth.

MM 9.2 Mon 15:00 H4

**Negative entropy of mixing in computer simulated bulk glass forming AlxNi1-xZr60 melts** — MOHAMMED GUERDANE and ●HELMAR TEICHLER — Inst. f. Materials Physics, University of Göttingen, D-37077 Göttingen

For multi-component random systems, the ideal solution model predicts positive entropy of mixing, reflecting the increase of configuration space by exchange of chemically different particles. Glass forming melts are usually far from being random. Regarding this, AlxNi1-

xZr60 is known to have marked short- and intermediate-range order. The former is characterized by icosahedral neighbour cages around Al- and by trigonal-prismatic ones around Ni-atoms, the latter by chain arrangements of Al- and of Ni-cages (M. Guerdane and H. Teichler, PRE 65, 014203 (2001)). Here the question arises whether in AlxNi1-xZr60 melts the entropy of mixing is positive, due to a gain in configuration space by particle exchange, or negative, due to a decreased density of low-energy states in the complex liquid at mid-concentrations. Concerning this, we report molecular dynamics results for AlxNi1-xZr60 melts based on the adiabatic switching approach. They show strong negative entropy of mixing along the quasi-binary line, i.e., predominance of enthalpic over entropic effects in this bulk glass forming liquid. (Supported by DFG SPP 1120 \*Phase Transformations in Multi-Component Melts\*.)

MM 9.3 Mon 15:15 H4

**Primary crystallization reaction in Al-Y-Fe glasses containing low melting point nanoparticles** — ●NANCY BOUCHARAT<sup>1</sup>, HARALD RÖSNER<sup>2</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe, P.O.B. 3640, 76021 Karlsruhe, Germany

Many rapidly quenched Al-rich alloys partially devitrify via a primary crystallization reaction, which results in the development of a high number density of homogeneously dispersed Al-nanocrystals. Although several experimental results are consistent with the formation of nucleation sites during rapid quenching via homophase catalysis, the nature and the origin of the nucleation sites is not yet completely resolved. To assess the role of the as-quenched state in the nanocrystallization process, 1at.% Pb or 1at.% In, respectively were substituted for Al in an Al-Y-Fe glass prior to rapid quenching. The microstructure of the respective products consists of a homogeneous dispersion of nanocrystalline Pb particles or In-enriched regions within an amorphous Al-Y-Fe matrix. In both cases, the primary crystallization is strongly shifted to lower temperatures compared to the reaction in the inclusion-free sample. While likely mechanisms have been proposed