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[1], Daniel Weygand[1], Oliver Kraft[1,2], and Peter Gumbsch[1,3] — [1]IZBS, Universität Karlsruhe (TH) — [2]IMF II, Forschungszentrum Karlsruhe — [3]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[1], Jianrong Gao[2], Jiuzhou Zhao[3], Lorenz Ratke[1], and Dieter Herlach[1] — [1]DLR, Institut für Materialphysik im Weltraum, Linder Höhe, 51170 Köln — [2]Key Lab of Electromagnetic Processing of Materials, North Eastern University, Shenyang 110004, China — [3]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[1], Harald Rösner[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — [2]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 num-ber density of homogeneously dispersed Al-nanocrystals. Although sev-eral 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

to explain the catalytic effect of Pb inclusions on the nanocrystallization process, the analyses on the In-containing sample give new evidence that the inclusions generate a modification of the local structural arrangement of the amorphous matrix promoting the retention of quenched-in nuclei during the quenching process.

MM 9.4 Mon 15:30 H4

Microstructure and properties of glassy NdCoAl alloys with Ga and Nb additions — •Mihai Stoica[1], Mihaela Buschbeck[2], Annett Gebert[2], Ludwig Schultz[2], Albrecht Wiedenmann[3], Olivier Perroud[3], Shankar Wenkataraman[1], Simon Pauly[1], and Jürgen Eckert[1] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — [2]IFW Dresden, Institute for Metallic Materials, P.O. Box 270016, D-01171 Dresden, Germany — [3]Hahn-Meitner Institute Berlin, Glienickerstr. 100, D-14109 Berlin, Germany

The glass forming ability and structure upon fast cooling were investigated for Nd60Co30Al10 with Ga and Nb additions. The investigated alloys contained 1, 3 and 5 at. % of Ga or Nb. From every composition different samples were produced. The melt spinning apparatus was used to make glassy ribbons 4 mm wide and 0.03 mm thick and by copper mould casting rods with diameters of 1 and 2 mm were cast. The structure of the samples was investigated by means of X-ray diffraction and electronic microscopy and the thermal stability by differential scanning calorimetry (DSC). In order to rule out the effect of composition and cooling conditions, the microstructure and thermal behaviour of master alloys with and without Ga and Nb additions were also checked. The paper will discuss the microstructure formation for different samples, as a function of two parameters: the composition and the cooling rate. The work was supported by the German Science Foundation (DFG) via the DFG priority program *Phasenumwandlungen in mehrkomponentigen Schmelzen*.

MM 10: Liquid and amorphous materials IV

Time: Monday 16:15–17:30 Location: H4

MM 10.1 Mon 16:15 H4

Structure and electronic transport of *a*-Ni$_x$(Ti$_{50}$Al$_{50}$)$_{100-x}$ — •Jan Rauchhaupt, Thomas Raubold, and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

An approach to understand the development of any crystalline structure from the initial disordered state is to investigate stabilization processes in amorphous phases as precursors of any ordered structure. Amorphous thin films are ideal to do so because they exist in just one phase, can be prepared in exactly the right composition and the development of their structure and electronic transport properties dependent on the composition and temperature are easy to measure. In order to minimize their global energy many different alloys organize themselves under the influence of a resonant interaction between the valence electrons as one subsystem and the static structure as the other one. These resonances were observed in many systems, from simple metals and semiconductors to ionic glasses and TM-containing alloys (TM=transition metal). We discuss the results of the measurements as a hybridization effect of the Al-p-electrons with the empty d-states of the TM. Amorphous ternary alloys of Ni, Ti and Al were prepared in situ at T=4 K in a HV-cryostate and were annealed up to the crystalline state. The static structure, by means of electron diffraction, the resistivity and the thermopower were measured as a function of temperature and composition. Additionally quantitative *White Lines* measurements were performed to prove the predicted hybridization effects.

MM 10.2 Mon 16:30 H4

FeNbB bulk metallic glass with high boron content — •Mihai Stoica[1], Khalil Hajlaoui[2], Jayanta Das[1], Jürgen Eckert[1], and Alain Reza Yavari[2] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — [2]LTPCM-CNRS, I.N.P. Grenoble, 1130 Rue de la Piscine, BP 75, F-38402 University Campus, France

Fe-based alloys able to form magnetic bulk metallic glasses (BMGs) are of the type transition metal – metalloid and often contain 5 or more elements. Usually, the metalloid content is around 20 atomic %. Very recently, the Fe66Nb4B30 alloy was found to be able to form BMG by copper mold casting technique, despite its high metalloid content. Several composition with boron contents around 30 at. % or even higher were calculated since 1993 as possible compositions of the remaining amorphous matrix after the first stage of nanocrystallization of Finemet-type Fe77Si14B9 glassy ribbons with 0.5 to 1 atomic % Cu and a few percent Nb addition. Melt-spun ribbons of all calculated compositions were found to be glassy. The composition of the ternary Fe-based BMG investigated in the present study resulted as an optimization of all possibilities. The alloy is ferromagnetic with glass transition temperature Tg = 845 K, crystallisation temperature Tx = 876 K, liquidus temperature Tliq = 1451 K and mechanical strength of 4 GPa. The coercivity of as-cast samples is very low, around 1.5 A/m. The present contribution aims at discussing the thermal stability, mechanical and magnetic properties of the Fe66Nb4B30 BMG.

MM 10.3 Mon 16:45 H4

Microstructure of rapidly quenched amorphous Ni100-2xNbxYx alloys — •Norbert Mattern[1], Uta Kuehn[1], Thomas Gemming[1], Guenter Goerigk[2], and Juergen Eckert[1] — [1]Leibniz-Institut IFW Dresden, Helmholtzstr.20,01069 Dresden — [2]Haysylab at DESY,Notkestr.85,22603 Hamburg

Two-phase amorphous Ni-Nb-Y alloys can be prepared by rapid quenching from the melt[1]. The structure formation takes place in the phase separated undercooled liquid. Recent experimental and thermodynamical assessment of the Ni-Nb-Y phase diagram shows an extension of miscibility gap in the melt of the monotectic binary Nb-Y system up to 60 at% Ni content into the ternary Ni-Nb-Y system.The microstructure of the as-quenched ribbons consists of two amorphous regions Nb-enriched and Y-enriched exhibiting features of self-similarity with a size distribution from micrometer dimensions down to several nanometers. Small-angle X-ray diffraction confirms the fractal microstructure. For Ni contents > 60at% (critical composition) a "homogeneous" amorphous microstructure is observed by transmission electron microscopy (TEM) in accordance with thermodynamic calculations which are based on the regular solution model for the liquid. On the other hand, small-angle X-ray diffraction data indicate clearly chemical inhomogeneities within the nm-range. From the inhomogeneous amorphous precursors ultrafine nanocrystalline microstructure can be formed upon annealing as the first step of crystallization.

[1]N. Mattern, U. Kuehn, A. Gebert, T. Gemming, M. Zinkevich, H. Wendrock, L. Schultz, Scripta Mater., 53 (2005) 271

MM 10.4 Mon 17:00 H4

Cold rolling induced amorphization and nanocrystallization processes studied by positron lifetime and 2-dimensional Doppler broadening measurements — •Wolfgang Lechner[1], Werner Puff[1], Herbert Rabitsch[1], Gerhard Wilde[2], and Roland Würschum[1] — [1]Institut für Materialphysik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria — [2]Institut für Materialphysik, Universität Münster

In order to contribute to an atomistic understanding of the interfacial structure and processes during amorphization and nanocrystallization, the present work deals with studies of interfacial free volumes by means of positron-annihilation-spectroscopy. In addition to positron lifetime spectroscopy, coincident Doppler broadening of the positron-electron annihilation photons is applied as novel technique for studying the chemistry of interfaces. To study the amorphization process, pure foils of Cu and Zr with a nominal composition of $Cu_{60}Zr_{40}$ were mechanically intermixed by cold rolling. Starting from the constituent pure metals, a nanoscale multilayer structure of elemental layers and amorphous interlayers develops in an intermediate state of folding and rolling, where free volumes with a Zr-rich environment occur that are presumably located in the hetero-interfaces between the various layers or in grain boundaries of the Cu-layers. To analyze the nanocrystallization reaction that occurs in marginal glass formers, pure foils of Al and Sm with a composition of $Al_{92}Sm_8$ were produced by the above-mentioned synthesis route. Specific modifications of free volumes and their chemical environment could be observed for various strain levels.