To investigate the influence of plastic deformation on the potential energy state of bulk metallic glasses, calorimetry and ultrasonic measurements are performed. Wide-band pulses of a bandwidth of 100 MHz are used to excite the 20 MHz transducer in order to get higher time-resolution. They are used to measure sound velocity as a function of plastic deformation. The results provide evidence of activated relaxations modes.

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[1] M. Kopycinska-Müller, A. Caron, S. Hirsekorn, U. Rabe, H. Natter, R. Hempelmann, R. Birringer and W. Arnold, Phys. Chem. 222, 471, (2008)

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**Quantification of free volume variations of Pd40Ni40P20 bulk metallic glass deformed by room temperature rolling** — •Yuanli Xu[1,2], Yue Zhang[1], Jixiang Fang[1], Horst Hahn[1], and Jiangong Li[2] — [1]Forschungszentrum Karlsruhe, Institut for Nanotechnology, Karlsruhe 76021, Germany — [2]Institute of Materials Science and Engineering, Lanzhou University, Lanzhou 730000, China

Mechanical and thermal properties of metallic glasses change significantly with increasing inhomogeneous deformation. This can be attributed to the introduction of localized excess free volume in shear bands. Therefore, the quantification of free volume is of importance for understanding of the structure of the shear bands and the corresponding changes in mechanical and thermal properties of metallic glasses. In the present work, the Pd40Ni40P20 (at.%) bulk metallic glass prepared by suction casting method was deformed to different strains by rolling at room temperature at a constant strain rate. Differential scanning calorimetry was employed to measure the variation of heat capacity with temperature for the undeformed and rolled Pd40Ni40P20 bulk metallic glass. The average value of the reduced free volume was quantitatively calculated from heat capacity for different strains. Compared with the undeformed Pd40Ni40P20 bulk metallic glass, about 23 % excess free volume was introduced into the rolled Pd40Ni40P20 bulk metallic glass at a strain exceeding 90%. These results may be helpful for understanding of the structure of the shear bands in the bulk metallic glasses and the properties of the deformed bulk metallic glasses.

MM 35.14 Wed 16:30 P4

**Liquid Cu-Ni-Fe: Molar volume and short range order.** — •Jürgen Brillo[1], Ivan Egry[1], Louis Hennet[2], Mirko Kehr[3], and Irina Pozdnyakova[2] — [1]Institut für Materialphysik im Weltraum, Deutsche Zentrum für Luft- und Raumfahrt, Linder Höhe, 51170 Köln — [2]CRMHT, CNRS, 1D, Ave. de la Recherche Scientifique, 45071 Orleans Cedex 2, France — [3]TU Chemnitz, Institut für Physik, Professur Röntgen- und Neutronendiffraktometrie, Reichenhainer Straße 70, 09216 Chemnitz

The molar volume and the atomic short range order were measured for liquid Cu-Ni-Fe binary and ternary alloys.

All experiments were performed containerlessly using the technique of electromagnetic levitation. The molar volume was determined by optical dilatometry and the atomic short range order was obtained from x-ray diffraction experiments carried out at ESRF in Grenoble.

The results are discussed in view of the volumetric mixing behaviour of the system. It was found that the excess molar volumes of the ternary alloys and the binary Cu-Fe alloys are similar and strongly positive while it is negative for Cu-Ni.

This was partly confirmed by the x-ray scattering experiments which exhibit similarities in the short range order of Cu-Fe and Cu-Fe-Ni: In these systems, the nearest neighbour distance, R, is almost identical and does not vary with the composition whereas R is significantly smaller and increases monotonically with the Cu-concentration in Cu-Ni. There are also hints that in Cu-Fe and Cu-Fe-Ni the molar volume is mainly determined by the first shell coordination number.

MM 35.15 Wed 16:30 P4

**Investigation of the liquid-liquid miscibility gap in the Cu-Co-Zr-system** — •Björn Schwarz, Norbert Mattern, and Jürgen Eckert — Leibniz Institute for Solid State and Materials Research, Dresden, Germany

For a variety of compositions Cu-Co-Zr prealloys were rapidly quenched by splat-quenching and melt-spinning technique. Concerning the chemical homogeneity, phase constitution as well as amorphicity, that are all essentially influenced by a liquid-liquid miscibilty gap found for this system, the samples were investigated by DSC, SEM, HAADF STEM/HRTEM and XRD. Especially those samples partially exhibitng the (Co/Cu)Zr-phase (B2) with martensitic transformation at low temperature show interesting physical properties that were characterized by measurements of the magnetization and electric conductivity.

MM 35.16 Wed 16:30 P4

**First-principles study of the structure and composition of $Si_3N_4$ surfaces and $Si_3N_4$/TiN interfaces** — •Pawel Rodziewicz and Bernd Meyer — Interdisziplinaeres Zentrum fuer Molekulare Materialien (ICMM) und Computer-Chemie-Centrum (CCC), Department Chemie und Pharmazie Friedrich-Alexander-Universitaet Erlangen-Nuernberg

Due to its hardness as well as thermal and chemical stability, silicon nitride is frequently used as substrate and protective coating. Recently, superhard silicon nitride/titanium nitride-based nanocomposite materials have been synthesized which show a hardness similar to that of diamond. In order to obtain a better understanding of the surface and interface properties of these materials, density functional theory calculations have been applied to study the (0001), $(10\bar{1}0)$, $(1\bar{2}10)$, $(10\bar{1}1)$, and $(1\bar{2}11)$ surfaces of $\beta$-$Si_3N_4$. Surface reconstructions and saturation of the broken surface bonds with H, N, NH, and $NH_2$ have been taken into account. The relative stability of the different surface compositions is analyzed in terms of surface phase diagrams, and Wulff constructions of the equilibrium shape of $\beta$-$Si_3N_4$ crystallites depending on the chemical environment have been obtained. Additionally, first results on the atomic structure and mechanical strength of coherent $Si_3N_4(10\bar{1}0)$/TiN(001) interfaces with different composition will be presented.

MM 35.17 Wed 16:30 P4

**Surface topography evolution during ion beam sputtering of Cu** — •Maria Lenius[1], Reiner Mönig[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen — [2]Institut für Materialforschung II, Forschungszentrum Karlsruhe

Ion beam sputtered surfaces develop complex patterns that are controlled by the interplay of various mechanisms such as surface diffusion, surface energy minimization, and shadowing effects. The pattern evolution is not fully understood, particularly in crystalline materials where literature investigations on low index Cu surfaces have revealed the importance of crystal orientation in addition to temperature, ion flux and dose.

In this study, the sputter erosion profiles of Cu grains with different crystal orientations have been investigated as a function of 30 keV Ga ion beam incidence and dose in a focused ion beam microscope. The resulting patterns (ripples, 'leaf' structure, or craters with length scales from 10 nm to 1 um) were characterized using SEM, AFM, and EBSD and depend on both crystal orientation and ion beam incidence. A comparison with the faceted structures of thermally annealed Cu surfaces will be performed to understand the role of surface energy on pattern formation. The final goal is to understand which mechanisms control pattern evolution at sputtered crystal surfaces.

MM 35.18 Wed 16:30 P4

**Influence of Ga on the melting behaviour of Pb nanoparticles** — •Anna Moros, Harald Rösner, and Gerhald Wilde — WWU Münster, Institute of material physics

In recent years there have been many analyses of the melting of Pb nanoparticles embedded in Al, but the corresponding mechanism of melting is still not completely understood. The current research project analyzes Al-1at%Pb samples, which are prepared by melt-spinning. The melting behaviour of Pb nanoparticles was determined by differential scanning calorimetry. In contrast to findings for free particles and in contradiction to many models of size-dependent melting, it was found that the particles melted at 10-30 K above the melting point of the bulk material. Analyses of TEM-images yielded a bimodal size distribution with most of the small particles in the size range between 2-20 nm. The resolved lattice mismatch between the faceted Pb nanoparticles and the matrix is suggested to be the key to understanding the melting behaviour. What happens if the matrix lattice changes due to alloying of other components? For our project we chose Gallium since it is miscible with Al, but immiscible with Pb. First results were obtained on 6at% Ga and 1at%Pb samples. The results by DSC and TEM are discussed with respect to the impact of the lattice mismatch between particles and matrix on the melting point variation.

MM 35.19 Wed 16:30 P4

**Electrical characteristics of metal-Nb:STO interfaces** —