MM 35: Poster Session II

Time: Wednesday 16:30–18:30 Location: P4

MM 35.1 Wed 16:30 P4

Theoretical study of geometry dependent I-V characteristics of copper and gold quantum point contacts — •Saeideh Mohammadzadeh[1], Reinhard Streiter[1,2], and Thomas Gessner[1,2] — [1]Center of Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Research Institution for Electronic Nano Systems, ENAS, Chemnitz, Germany

Quantum point contacts have attracted significant attention with continuing miniaturization of nanoscale electronic components for the two past decades. In present work, we study the electronic transport properties of copper and gold quantum point contacts using the non-equilibrium Green's function technique on the density functional tight binding method for modelling the geometry dependent I-V characteristics. The copper and gold quantum point contacts are sandwiched between cognate (001) electrodes and the electronic current is deduced according to the Landauer formulation to study the effect of the quantum point contact length scales and geometry defects on the electronic transport properties. The transmission coefficients, conductance and the voltage drop characteristics are calculated as well.

MM 35.2 Wed 16:30 P4

Conductivity measurements on FeSi and the influence of the stoichiometry on the susceptibility — •Miriam Friedemann, Dirk Menzel, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

Conductivity measurements on FeSi single crystals grown via the Czochralski method were performed and interpreted within a model containing two rectangular bands as well as two parabolic bands. The two gaps which are observed in Raman [1] and Fourier-spectroscopy [2] respectively, have been confirmed. We found evidence for an additional small gap of the size 6 meV which most likely stems from the existence of a small amount of impurity atoms acting as acceptors. The susceptibility of $Fe_{1-x}Si_x$ single crystals with light variance of the ratio Fe/Si = 1 was measured. It shows that the lowest residual susceptibility at low temperatures is achieved with a light Si excess. As evidenced by measurements on samples before and after annealing, the residual susceptibility is also affected by crystal defects.

[1] A.-M. Racu et al., Phys. Rev. B **76**, 115103 (2007).

[2] D. Menzel et al., submitted to Phys. Rev. B.

MM 35.3 Wed 16:30 P4

Raman study of FeSi under high pressures up to 35 GPa — •Ivan Jursic[1], Dirk Menzel[1], Joachim Schoenes[1], and Klaus Doll[2] — [1]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie, 38106 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Single crystals of FeSi were grown by tri-arc Czochralski technique. These crystals were investigated by Raman spectroscopy in a diamond anvil cell at pressures up to 35 GPa. The experiment was performed at room temperature.

FeSi crystallizes in the B20 structure, i.e. space group $P2_13$. Factor group analysis predicts 9 Raman active phonon modes for this structure. Measurements outside of the DAC allowed the assignment of the vibrations and showed electron-phonon coupling [1]. Only the strong modes could be observed inside the DAC, i.e. two E-mode vibrations at 180 cm^{-1} and 313 cm^{-1} as well as two T-mode vibrations at 195 cm^{-1} and 310 cm^{-1}.

With increasing pressure the frequencies of the vibrations shift to higher values. The observed shift was compared to density functional theory calculations made within a single particle model. The experiment and theory agree reasonable well. There is a small kink observed in the experiment around 15 GPa which can't be attributed to a structural phase transition and is discussed as electron-phonon coupling.

[1] A.-M. Racu et. al. Phys. Rev. B **76**, 115103(2007)

MM 35.4 Wed 16:30 P4

Semiconductor-to-metal transition in FeSi observed using high-resolution photoemission spectroscopy — •Dirk Menzel[1], Markus Klein[2], Klaus Doll[3], Matthias Neef[4], Damian Zur[1], Ivan Jursic[1], Joachim Schoenes[1], and Friedrich Reinert[2,5] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Experimentalphysik II, Universität Würzburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]Institut für Mathematische Physik, TU Braunschweig, Germany — [5]FZ Karlsruhe, Gemeinschaftslabor für Nanoanalytik, Germany

High-resolution angle-resolved photoemission spectroscopy was performed on Czochralski-grown FeSi single crystals. Special care was taken during the in-situ preparation of the crystal surface, since the quality and the cleanness of the surface is crucial for the reliability of the obtained photoemission spectra. The experimental data compared to single-particle band structure calculations based on the local density approximation show a strong renormalization of the bands in the vicinity of the Fermi energy due to the self-energy resulting from electronic correlation effects [1]. Temperature dependent photoemission measurements show that the self-energy is strongly $\vec{k}$-dependent at elevated temperatures which is due to scattering of thermally excited charge carriers only at particular crystal momenta. The results obtained by the photoemission investigations evidence that FeSi is not determined by a Kondo scenario but has to be described as a narrow-band semiconductor in which electronic correlations are involved.

[1] M. Klein et al., Phys. Rev. Lett. **101**, 046406 (2008).

MM 35.5 Wed 16:30 P4

Hybridization Phenomena in the Nearly Half-Filled f Shell Electron System $EuNi_2P_2$ — •Steffen Danzenbächer[1], Denis Vyalikh[1], Yuri Kucherenko[2], Cornelius Krellner[3], Christoph Geibel[3], Serguei Molodtsov[1], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Strasse 40, D-01187 Dresden, Germany

In this contribution we present high resolution angle-resolved photoemission data of the mixed-valent compound $EuNi_2P_2$ that are complimented with band-structure calculations. The study focuses on the behavior of the $4f^6$ final state close to the Fermi energy. Apart from the ^7F_J multiplet splitting as expected for an atomic-like state, this state exhibits additional splittings and dispersions like a valence state. The data are properly reproduced within a calculation that describes the interaction between the $4f$ and valence-band states in the framework of a simplified periodic Anderson model (PAM). The model starts from atomic-like multiplets and considers hopping-interaction to valence-band states. The strength of the interaction of the valence band with $4f$ states depends on band energy, symmetry and partial f character of the valence band states that vary across the Brillouin zone (BZ). Particulary strong interactions between individual terms of the f multiplets and parabolic bands were experimentally found in good agreement with our theory at different points of the surface BZ.

MM 35.6 Wed 16:30 P4

Electron-phonon interaction and spectral weight transfer in $Fe_{1-x}Co_xSi$ — •Paul Popovich[1], Dirk Menzel[2], Natalia Kovaleva[1], Joachim Schoenes[2], Klaus Doll[1], and Alexander Boris[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

The unusual properties of the narrow-gap semiconductor FeSi continue to attract attention of many theoreticians and experimentalists due to its similarities with some rare-earth compounds known as Kondo insulators. We present a comprehensive ellipsometric study on $Fe_{1-x}Co_xSi$ single crystals (x=0-0.2) in the spectral range from 0.01 to 6.2 eV. Direct and indirect band gaps of 73 meV and 10 meV, respectively, are observed in FeSi at 7 K. Four infrared active modes are assigned at 206, 329, 352, and 458 cm^{-1} for FeSi. Two of them are asymmetric at low temperatures, reflecting the phonon-phonon and electron-phonon coupling in the system. As temperature increases, the indirect gap changes sign manifesting semiconductor to semimetal crossover. The corresponding spectral weight gain at low energies is recovered within an energy range of several eV. The present findings imply that the electron-phonon interaction and semimetallic character of FeSi play the dominant role in the broad-band spectral weight transfer and strongly support the model that $Fe_{1-x}Co_xSi$ can be well described in an itinerant picture taking into account self-energy corrections.

MM 35.7 Wed 16:30 P4

A theory for electrical resistivity for amorphous metals — •golam Mohammed bhuiyan[1], md. abdur rashid[2], and a. z. ziauddin ahmed[3] — [1]department of theoretical physics, university of dhaka, dhaka-1000, bangladesh — [2]department of physics, university of dhaka, dhaka-1000, bangladesh — [3]department of physics, university of dhaka, dhaka-1000, bangladesh

An attempt has been made to develop a theory for the electrical resistivity for amorphous metals beyond the Ziman's formalism. The starting point of the proposed theory is the Baym's general formula for electrical resistivity. The Baym's theory is then extended within the quasi-crystalline approximation to have two important terms describing the normal and Umklapp scattering. The present theory thus gives a better picture to understand basic scattering processes which are very much involved in the real electronic transport mechanism. The proposed theory will also give better insight to understand resistivity of disordered systems like liquid metals in particular in the supercooled state.

MM 35.8 Wed 16:30 P4

Primary Crystallisation in Al-rich Metallic Glasses at unusually low Temperatures — •Joachim Bokeloh[1], Nancy Boucharat[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe

The initial stage of the primary crystallisation reaction and the glass transition of the marginal metallic glass Al-Y-Fe has been investigated in conventional and modulated DSC, microcalorimetry, XRD and TEM.

A sharp onset of the primary crystallisation was found in microcalorimetry and XRD studies at temperatures 120 K below the primary crystallisation peak observed in conventional DSC.

A systematic MDSC study of annealed samples revealed a wide spectrum of glass transition onsets which show a strong dependence on the annealing temperature and duration. In addition, the glass transition onsets can be linked to the initial stage primary crystallisation.

The observed spectrum of glass transition onsets may be interpreted as experimental evidence for a phase separation that precedes the nucleation and growth of aluminium nanocrystals in the respective al-rich metallic glasses.

MM 35.9 Wed 16:30 P4

New detectors improve the performance of ASAXS beamline B1 at HASYLAB, DESY — •Ulla Vainio, Tom Schubert, Michael Lohmann, Stephan Botta, Thorsten Kracht, and Rainer Gehrke — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

B1 at the DORIS synchrotron at DESY is one of the first anomalous small-angle x-ray scattering (ASAXS) beamlines. Several upgrades will make the beamline again competitive. During 2008 many improvements have been made to the beamline: A new, thicker Si (311) monochromator crystal is now used. A cooling system for the first monochromator crystal was designed and applied. Better alignment of the whole beamline was made, so a smaller beamstop for the primary beam can be used. Automated sample heating programs were implemented to the measurement program, allowing in situ measurements. A PILATUS 100k detector was tested at the beamline. It was shown that PILATUS has at 11 000 eV about ten times better efficiency and much better resolution than the old 2D gas detector. ASAXS measurements showed very good quality. In 2009 the PILATUS detector and a new system allowing for simultaneous SAXS and wide-angle x-ray scattering (WAXS) measurements will be available. A 1D MYTHEN detector can be used as a WAXS detector. All the improvements combined with new Matlab based data processing tools developed 2007 and 2008 allows for speedy and easy SAXS, WAXS and ASAXS measurements that can be analysed on site right after the measurement of the sample.

MM 35.10 Wed 16:30 P4

Preparation and characterisation of graphite particle reinforced $Zr_{48}Cu_{36}Ag_8Al_8$ BMG composites — •Enrico Mund[1], Jayamani Jayaraj[2], Annett Gebert[2], and Ludwig Schultz[1,2] — [1]TU Dresden, Helmholtzstr. 10, 01069 Dresden — [2]IFW , Helmholtzstr. 20, 01069 Dresden

Bulk metallic glasses exhibit good mechanical properties such as high strength and high hardness. The deformation and fracture properties of BMGs are controlled by the initiation and propagation of shear bands. In order to improve further the mechanical properties, manipulation of the shear band propagation is eminent. By creating ex-situ particle reinforced BMG composites the fracture strength and plasticity can be increased. The particles can act as crack-stopper for the shear bands and become barriers for the shear band propagation.
In this work we use graphite particles due to their easy availability and designated properties. A way to fabricate graphite particle reinforced BMG is demonstrated for a selected ZrCuAgAl alloy with a high glass forming ability. Samples are characterised by various analyses methods in comparison to the monolithic BMG. XRD, SEM and DSC examinations show the influence of the graphite particles to the phase evolution upon casting and the thermal alloy behaviour. Compression tests are carried out to clarify the effect of different graphite particle volume fractions on the mechanical properties. Furthermore the influence of different particle size distributions on the mechanical properties is examined. An optimal relation between particle size and volume fraction for a reinforced BMG with increased plasticity will be proposed.

MM 35.11 Wed 16:30 P4

Relaxation behavior and rheologie of amorphous solids in the cooperative shear zone-model — •Moritz Schwabe, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In the model of the potential energy landscape (PEL) from Stillinger and Weber, it is important to distinguish two different (beta and alpha) relaxations. In the PEL this is described in the change-over to a new local configuration (intrabasin hopping) or to a configuration with a convert potential energy (interbasing hopping). [1] To describe the response of the system in the cooperative shear zone - model to an external stress, a Frenkal-approach is chosen, which shows the decrease of the barrier height in the PEL. [2]

With this background we study the transition from the elastic to the anelastic response of a metallic glass (PdCuSi) via the change of the temperature and the force. To describe this transition from the linear to the nonlinear behavior we will present on the one hand stress-strain curves in the range from ambient temperature to above Tg and on the other hand creep tests with different forces and temperatures. We thank the SFB 602 and the GRK 782 for financial supporting.

[1] John S. Harmon, Marios D. Demetriou, William L. Johnson and Konrad Samwer, Phys. Rev. Lett., 99, p.135502 (2007) [2] William L. Johnson, K. Samwer, Phys. Rev. Lett., 95, p.195501 (2005)

MM 35.12 Wed 16:30 P4

Study of local and global elastic properties by atomic force acoustic microscopy and ultrasonic spectroscopy of a metallic glass — •Hannes Wagner[1], Stefan Küchemann[1], Christian Vree[1], Walter Arnold[2], and Konrad Samwer[1] — [1]I.Physikalisches Institut, Universität Göttingen — [2]Permanent address: Department of Materials and Technology, Saarland University, Saarbrücken

We are looking for local variations of the indentation modulus of a metallic glass. To visualize this effect we use an atomic force acoustic microscope, where the cantilever of an atomic force microscope is excited by a transducer at ultrasonic frequencies while the sensor tip is contacting the sample surface. From various resonance frequencies of this contact we obtain information about the local stiffness. By using the mechanical model of a vibrating cantilever [1] we are able to derive the indentation modulus of the metallic glass.

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.

We would like to thank the SFB 602 for financial support.

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

MM 35.13 Wed 16:30 P4

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 Nanotechnol-

ogy, 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 β-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 β-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 — •Gesine Saucke, Jörg Hoffmann, and Christian Jooss — Georg-August-Universität Göttingen, Göttingen, Germany

Because of the chemical stability and the small lattice mismatch, strontium titanate (STO) is a widely used substrate material for many perovskite oxides. In addition the conductivity can be tuned by doping with Nb from insulting to a low-resistance behaviour. Therefore Nb:STO is not only of particular importance for deposition of perovskites, but also for the fabrication of novel devices like heterostructures, tunnel- or pn-junctions. In order to examine devices like this, it is important to understand the electrical contact to Nb:STO.

In the vicinity of metallic contacts Schottky barriers are formed, which give rise to a highly non-linear current-voltage relation in two-point configuration. However, the interface resistance not only depends on the work function of the involved materials, but also on the detailed defect structure, e.g. related to the deposition method. In this contribution we summarise our results concerning the fabrication of metallic

contacts like Ti, Au, Ag on Nb:STO prepared by sputter deposition techniques with respect to pre-treatment of the substrates, choice of electrode materials and additional post annealing steps.

MM 35.20 Wed 16:30 P4

Transmission electron microscopy study of the interface $Pr_{1-x}Ca_xMnO_3$ / $YBa_2Cu_3O_{7-d}$ — •Jonas Norpoth[1], Thilo Kramer[1], Christian Jooss[1], Hiromi Inada[2], and Yimei Zhu[2] — [1]Institut für Materialphysik, Universität Göttingen — [2]Institute for Advanced Electron Microscopy, Brookhaven National Laboratory

Interfaces between highly correlated electron systems may exhibit novel electronic properties that are absent in the isolated materials. Especially, complex oxide interfaces often feature nontrivial electronic behaviour, the understanding of which needs a careful analysis of the relation between interface structure and electronic properties at the atomic scale. In this work we study the interface between the high-T_c superconductor $YBa_2Cu_3O_{7-d}$ and the hole-doped perovskite $Pr_{1-x}Ca_xMnO_3$. Thin film multilayers fabricated with pulsed laser deposition on epitaxial substrates exhibit atomically sharp interfaces as was demonstrated by high-resolution transmission electron microscopy. Electron energy loss spectroscopy indicates electron transfer across the interface from PCMO to YBCO according to a band bending scenario from the difference in the materials‘ workfunctions. Furthermore, short-range interdiffusion of Ca and Y cations is observed. These charge transfer processes establish doping gradients in the interfacial region capable of affecting both the polaronic transport in the manganite and the characteristics of the superconductivity.

MM 35.21 Wed 16:30 P4

Line stress from step edges and its impact on cantilever bending — •Weina Li[1,2], Huiling Duan[2], Maxim Smetanin[1], and Jörg Weissmüller[1,3] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Peking University,Beijing,P.R.China — [3]Universität Des Saarlandes, Saarbrucken

It is well known that the surface of a solid exerts a mechanical force on the underlying volume phase. This force has important ramifications for the behaviour of nanoscale objects. It is quantified by the surface stress, the derivative of a suitably defined surface excess free energy function with respect to the projection of the bulk strain tensor onto the local tangent plane. By analogy, the line elements at solid surfaces, such as triple lines, edges, or steps may also interact mechanically with the bulk. The relevant forces may be derived by taking the derivative of the line tension - an excess in energy per line length - with respect to the strain. Dimensional considerations might suggest that the line stress will emerge as a vector directed along the local line orientation. Yet, it is well known that parallel step edges interact by lateral dipole forces, so that a more general state of stress may be associated with line elements on a surface. Cantilever bending experiments provide sensitive probes for changes in the elastic interaction of the matter at the surface of a solid with the bulk. We discuss how the presence of step edges impacts the bending of cantilevers. Of particular interest are changes in the bending, either due to the creation of steps or due to the change in line stress during electrochemical cycles or reversible adsorption.

MM 35.22 Wed 16:30 P4

In-situ TEM and STM studies of dislocations in nano-scale metal samples — Burkhard Roos[1], •Sönke Schmidt[1], Daniel S. Gianola[2], Gunther Richter[3], Astrid Pundt[1], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Insitut für Materialforschung II, Forschungszentrum Karlsruhe — [3]Max-Planck-Institut für Metallforschung, Stuttgart

Metals at the nano-scale exhibit mechanical properties that are different from those at the macro-scale. The best known effect is the increase in strength with decreasing crystal size. However, present dislocation-based models fail to explain this effect. It is the goal of the studies described here to directly observe dislocations in small volumes in order to understand how they contribute to size dependent mechanical response. Two different experimental approaches are being taken. In the first approach, in-situ TEM is used to observe dislocation nucleation and storage during tensile testing of metal nano-wires. Initial results from ˜100 nm diameter, single crystal Cu whiskers will be presented. In the second approach, in-situ STM will be used to observe the dislocation traces left at the surface of freshly deposited metal films. Results from deformed Cu films will be presented to show the feasibility of this method for providing quantitative information on dislocations during deformation.

MM 35.23 Wed 16:30 P4

Effect of Surface Roughness on the Deformation of Micron-Sized Specimens of Cu — •Matthias Büchsenschütz-Göbeler and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

A variety of studies on deformed small scale metal specimens (100 nm to 10 μm) have shown that dislocation storage becomes rarer as the crystal size is decreased. This implies that plastic deformation, which is usually controlled by dislocation interactions, changes to a dislocation nucleation limited mechanism in sub-micron samples. In the study presented here, the effect of surface roughness on the mechanical behavior of single crystal Cu pillars is investigated. It is expected that surface roughness at the 10-100 nm length scale will influence the ease of dislocation nucleation and thus the mechanical behavior in sub-micron specimens. One and 4 μm diameter Cu pillars with varying degrees of surface roughness have been fabricated using a focused ion beam and then compressed using a flat punch tip in a nanoindenter. No effect of the ripples on the stress-strain behavior of the columns was observed, suggesting that deformation is not limited by dislocation nucleation at this length scale. Further tests on even smaller pillars are underway.

MM 35.24 Wed 16:30 P4

Zerstörungsfreie Beobachtung der räumlichen Verteilung von elastischen Konstanten in weicher Materie — •Jessica Mende, Marcus Radicke, Ole Oehms und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany

Mit Ultraschall (US), der während einer Spin-Echo-Sequenz in einem medizinischen Tomographen eingestrahlt wird, können verschiedene elastische Konstanten in weicher Materie dreidimensional und zerstörungsfrei dargestellt werden. In Proben mit unterschiedlichen Festigkeiten werden Kugeln aus einer Öl-in-Gelatine-Mischung eingebracht. Die Proben bestehen aus Agar-Agar und Kieselerde. Agar ist ein biologisches Geliermittel. Die Kieselerde dient zur Absorption des US. Die Kugeln besitzen ein höheres Elastizitäts- und Schubmodul als die Umgebung aus Agar-Agar und Kieselerde.

Von den Proben werden Phasenbilder gemacht, die die Phase der Spins in Grauwerten kodiert darstellen. Die Verschiebung innerhalb der Probe durch den Schallstrahlungsdruck ist abhängig von den elastischen Eigenschaften innerhalb der Probe. Die Darstellung der Verschiebung im Bild erfolgt durch ein Paar von magnetischen Feldgradienten. Während einem dieser Gradienten wird der US mit einer Frequenz von ca. 2,5 MHz und einer Länge von 20 ms eingestrahlt. In den Bildern wird eine Phasenverschiebung durch eine Verschiebung auf der Grauskala sichtbar. In Differenzbildern mit und ohne US können Rückschlüsse auf die räumliche Verteilung der elastischen Eigenschaften der Probe und der darin befindlichen Fremdkörper gezogen werden.

MM 35.25 Wed 16:30 P4

Deformations of auxetic periodic strut frameworks — •Holger Mitschke, Klaus Mecke, and Gerd E. Schröder-Turk — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

We study the deformation behaviour, in particular Poisson ratios, of planar periodic strut frameworks with rigid struts connected at flexible joints. We systematically search for yet unknown auxetic frameworks (i.e. with negative Poisson ratio) and to understand the relationship between structure morphology (quantified by integral geometric Minkowski measures) and deformation behaviour.

These frameworks are defined by their symmetry group with two lattice vectors $\vec{a}$ and $\vec{b}$, the position of joints $\vec{p}_i$ and strut vectors of length l_{ij}. A deformation of an initially rigid network is obtained, if possible, by changing the lattice vector $\vec{a} \to (1+\delta)\vec{a}$ with $\delta \in \mathbb{R}, |\delta| \ll 1$ but maintaining all initial strut lengths l_{ij} and translational periodicity. The Poisson ratio is extracted from the relative change in the resulting new $\vec{b}$. The deformed network is numerically obtained by a multi-dimensional Newton-Raphson method. Here we present an analysis of strut frameworks based on Archimedean tilings and tilings of star polygons [1].

[1] B. Grünbaum and G.C. Shephard, : *Tilings and patterns*, W.H. Freeman, 1987.

MM 35.26 Wed 16:30 P4

High Temperature deformation of Tungsten — •Armin Huber[1], Bernd Eberhard[2], Andreas Spörhase[1], and Ferdinand

Haider[1] — [1]Univ. Augsburg — [2]Osram GmbH, Schwabmünchen

To study the high temperature deformation behaviour of tungsten wires at temperatures up to or beyond 2000°C, we constructed a high temperature deformation chamber. The wire is heated by direct current flow, temperature is controlled pyrometrically and the local elongation is measured optically. We present the construction, validation and first results for tensile deformation experiments of tungsten wires as a function of deformation temperature, wire thickness and material composition. These results are compared to results of conventional experiments at lower temperature.

MM 35.27 Wed 16:30 P4

Mechanical properties of LiB_3O_3 at nanoscale — •Irina P. Shakhverdova[1], Peter Paufler[1], Rimma S. Bubnova2[2], Stanislav K. Filatov[3], and Dirk C. Meyer[1] — [1]Institut für Strukturphysik, TU Dresden, 01062 Dresden, Germany — [2]Institute of Silicate Chem., Russian Academy of Sciences, Ul. Odoevvskogo, 24/2, St.Petersburg 199155, Russia — [3]Dept. of Crystallography, St.Petersburg State University, Univ.Emb.7/9, St.Petersburg 199034, Russia

Indentation hardness (H), scratch hardness (H_S) and reduced Young's modulus (E_r) of LiB3O5 single crystal plates with different orientation as well as of glass with the same composition have been investigated using nanoprobes. Microhardness (H_M) tests were done for comparison. Both hardness and Young's modulus of glass appeared smaller compared to corresponding single crystal data ($H \sim 7$–8 GPa, $H_M \sim 6$ GPa, $E_r \sim 70$–80 GPa for glass and $H \sim 10$–15 GPa, $H_M \sim 6$–11 GPa, $E_r \sim 93$–155 GPa for single crystal). H, H_S, E_r and the plane of crack propagation proved orientation-dependent. Cracks in the glass sample were not observed up to 0.49 N microindentation load, whereas for the single crystal the cracks appeared already at 0.098 N. In single crystals the observed cleavage planes {211} and/or {412} are oriented nearly parallel to planes of B-O rings. The dependence of scratch morphology on the direction of scratching is demonstrated quantitatively. The coefficient of friction depends on normal load and varies between 0.25 and 0.37. The oscillating friction reflects elementary processes of plastic deformation at nanoscale. Dislocations created during scratching have been detected by etching.

MM 35.28 Wed 16:30 P4

Simulation of phase diagrams of nanoscale particles — •Michael Gährken, Harald Rösner, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149

The phase diagram of nano-sized binary particles changes compared to macroscopic particles. A theoretical model, based solely on the thermodynamic contribution of the inner phase boundery, was already developed for a simple eutectic system and has been modified for systems with limited solid solubility.

The simple eutectic system's thermodynamic properties follow basically an ideal solution behavior in both the liquid and the solid phase, whereas the solid solubility was introduced by a regular solution behavior in the solid phase.

In addition to theoretical analyses, experimental investigations were conducted on binary Sn-Bi nanoparticles that were embedded in an Al matrix. The obtained results from calorimetry measurements are critically discussed in view of the comparison between experiments and idealized model behavior.

MM 35.29 Wed 16:30 P4

Ultra-fast diffusion in severely deformed NiTi and Ti — •Jochen Fiebig[1], Sergiy Divinski[1], Ruslan Valiev[2], Yuri Estrin[3], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische-Wilhelms Universität Wilhelm-Klem Str. 10 48149 Münster, Deutschland — [2]Institue of Physics of Advance Materials, Ufa State Aviation University, 12K. Marx Street 450000 Ufa, Russian Federation — [3]Monash University, Claytoon, Victoria, Australia

Severely deformed materials attain nowadays a growing technological interest due to their advanced properties and property combinations. In the present study, were focus on the diffusion properties of nanocrystaline NiTi produced by high pressure torsion(HPT) and of ultra-fine grained titanium deformed by equal channel angular pressing (ECAP). The radiotracer method was used with the radioactive isotopes ^{44}Ni and ^{44}Ti in combination with the parallel sectioning technique. Our results discover the existence of ultra-fast diffusion pathways in HPT-processed NiTi, especially after certain heat treatments. The diffusion data are analysed in relation to the existence of 'non-equilibrium' grain boundaries in severely deformed materials, but also with respect of the possible presence of a percolating network of nanocracks and nanovoids in severely deformed materials.

MM 35.30 Wed 16:30 P4

Experimental determination of excess energy contributions in nanocrystalline Pd — •Matthias Wegner[1], Markus Ames[2], Jürgen Markmann[2], Jörg Schmauch[2], Gerhard Wilde[1], and Rainer Birringer[2] — [1]Universität Münster, Institut für Materialphysik, 48149 Münster, Germany — [2]Universität des Saarlandes, Technische Physik, 66041 Saarbrücken, Germany

Nanocrystalline materials with grain sizes considerably below 100nm are characterized by significant contributions of grain boundaries and triple lines to the overall energetics. Until today, the magnitude of triple line energies is unknown and even the sign of their excess energy contribution is discussed. In this contribution, a method is indicated that investigates the excess contributions of grain boundaries and triple junctions for inert gas condensed (IGC) Palladium (Pd) with an average grain size of about 10 nm by micro calorimetric and micro structural investigations. Measurements were done simultaneously at room temperature (23 °C) on two identical halves of the same sample in order to correlate both experiments. A reduction of microstrain and grain coarsening accompanied by annihilation of grain interfaces are observed, which lead to a reduction of free energy. The results and the influence of different geometric grain models underlying the analysis are also discussed in the presented work.

MM 35.31 Wed 16:30 P4

Patterning graphene by electron-assisted local oxidation nano-lithography — •Danny Haberer, Thomas Mühl, Mark H. Rümmeli, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research (IFW) Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The research interest in graphene, a single layer of graphite, is mainly driven by its remarkable electronic properties as well as its recent experimental success. Of the various routes for graphene device fabrication, oxygen plasma etching is a successful technique to apply arbitrary designs to this material. We have recently developed a route through which carbon-based materials can be patterned on the nm-scale by electro-oxidation using a scanning electron microscope with the assistance of water vapor (10 to 100 Pa). We show this method can pattern graphene without the need for an additional lithography step as is necessary with plasma etching. Further, we show the patterning of free-standing graphene membranes, which is far more challenging using conventional etching techniques.

MM 35.32 Wed 16:30 P4

Creep measurements on high pressure torsion treated materials — •Jörn Leuthold, Harald Rösner, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, 48149 Münster, Germany

In ultrafine grained and in nanocrystalline materials the small grain size and the presence of defects with high specific excess energy densities lead to modifications of the basic mechanisms that can accommodate externally applied mechanical stresses. Additionally, for plasic deformation, grain boundary controlled mechanisms, such as grain boundary (GB) emitted dislocations and partial dislocations, twinning, GB diffusion and sliding can be more important or even dominant. To study the modified deformation behaviour several copper samples were prepared by high pressure torsion (HPT), a technique to induce high shear stresses on a specimen to produce fine grained or even nanocrystalline material. A device for creep measurements was built to perform tensile stress-strain-rate tests at room temperature for the measurement of strain-rate sensitivity of the HPT samples. The results are discussed with respect to the modified plasticity mechanisms in ultrafine and in nanocrystalline metals.

MM 35.33 Wed 16:30 P4

Simulating structural and thermodynamical properties of iron nanoclusters — •Denis Comtesse, Alfred Hucht, and Peter Entel — Universität Duisburg-Essen D-47048 Duisburg

Based on molecular dynamics (MD) simulations using EAM potentials we obtain structural and thermodynamical properties of iron nanoclusters and their sintering. The simulations are performed for magic number cluster sizes up to a number of 12431 atoms per cluster. These special sizes are leading to e.g. icosahedral (ICO) clusters with closed

atomic shells. In particular we focuss on the shellwise Mackay transformed (SMT) morphology described in Phys. Rev. Lett **99** 083402 (2007). Our EAM potential perfectly reproduces this morphology for clusters with more than 5 closed atomic shells. Because of the MD simulations allowing us to expand the investigation of this morphology to finite temperatures we find a structulral phase transformation from SMT to ICO structure. The transition temperatures are found to grow monotonic with the cluster sizes taken into account. The sintering of SMT and ICO particles is found to induce a transition in the fcc dominated ICO structure to more bcc dominated structure.

MM 35.34 Wed 16:30 P4

On the quality of electrical contacts between carbon nanofibers in composite-materials — •Michael Konter[1], Pablo Carballera[2], Frank Haupert[2], Bernd Wetzel[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany

We have investigated the electric transport properties of composite materials using temperature dependent dielectric spectroscopy (10 Hz - 2 GHz, 40 K - 290 K). The samples consist of epoxy-resin containing up to 2 vol.% carbon nano-fibers. We observe percolation above a threshold of about 0.05vol.%. The dc-conductivity is associated with a polarization process at high frequencies. The latter one stems from an interfacial polarization process at the contacts between the fibers, which act as barriers. The analysis of the data reveals microscopic information on the quality of these contacts. It is poor close to the percolation threshold and improves with increasing concentration of nano-fibres.

MM 35.35 Wed 16:30 P4

Oxygen diffusion in an reaction rate of cobalt nanoparticles stabilized with different ligands — •Britta Vogel, Axel Dreyer, Nadine Mill, Anna Regtmeier, Inga Ennen, Daniel Ebke, Simone Herth, and Andreas Hütten — Department of Physics, University of Bielefeld, D-33615 Bielefeld, Germany

Cobalt nanoparticles with a diameter of 12nm have initially been prepared with TOPO. Subsequently a ligand exchange was carried out to employ different ligands to the nanoparticles while keeping direct comparability. The decrease of the magnetic moment of the nanoparticles corresponds directly to their oxydation. According to a model of Crank for irreversible reaction in a spherical particle the uptake of oxygen in the particles was analyzed. From the fit of the obtained data to the model, information about the diffusion of oxygen in cobalt and cobalt oxide as well as the oxidationrate is deduced. Additionally the temperature dependence is discussed.

MM 35.36 Wed 16:30 P4

Studies on the Phase Diagram of Boron Employing a Neural Network Potential — •Tobias Morawietz[1], Jörg Behler[1], and Michele Parrinello[2] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780-Bochum, Germany — [2]Department of Chemistry and Applied Biosciences, ETH Zürich, USI-Campus, CH-6900 Lugano, Switzerland

The crystalline phases of elemental boron have a structural complexity unique in the periodic table. The complex connection pattern of the icosahedral building blocks forms a formidable challenge for the construction of accurate but efficient potentials.

We present a high-dimensional Neural Network potential for boron, which is based on first-principles calculations and can be systematically improved. The potential is several orders of magnitude faster to evaluate than the underlying density-functional theory calculations and allows to perform long molecular dynamics and metadynamics simulations of large system. By a stepwise refinement of the potential and an application of the potential in metadynamics simulations we show that starting from random atomic positions the structure of α-boron is predicted in agreement with experiment. Further, pressure-induced phase transitions of α-boron are discussed.

MM 35.37 Wed 16:30 P4

Kinetic and thermodynamic aspects of crystallization in the phase-change material $Ge_{15}Sb_{85}$ — •Peter Zalden[1], Vanessa Coulet[2], Christophe Bichara[3], Michael Klein[1], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen — [2]IM2NP - UMR CNRS 6242, Aix-Marseille Université Campus de Saint Jérôme, case 142, 13397 Marseille — [3]CINaM - UPR CNRS 3118, Campus de Luminy - Case 913, 13288 Marseille

Phase-change materials exhibit a very rare combination of properties as they do not only show crystallization on the nanosecond time scale but also show a pronounced change of the optical reflectivity and the electronic resistivity upon crystallization. This property combination is already exploited in rewritable optical data storage and is explored in Phase-Change Memories (PCM), which are considered to be the most promising candidate for future non-volatile electronic data storage.

In this study, structural modifications in sputtered thin films during the transition from the as-deposited amorphous to the crystalline phase are analysed, employing a combination of Differential Scanning Calorimetry and X-Ray Diffraction. This survey includes a systematic study of heat capacities and transition temperatures for different annealing conditions in the amorphous and partially crystallized state. In addition, diffractograms have been recorded ex-situ during different stages of the thermal treatment. These results indicate a segregation of a Ge-rich phase. A comparison to conventional tellurium based phase-change materials is presented.

MM 35.38 Wed 16:30 P4

Simulations of martensitic phase transitions in FeNi- and NiTi-alloys — •Daniel Mutter and Peter Nielaba — Physics Department, University of Konstanz, 78457 Konstanz, Germany

In order to find out possibilities of a realization of shape-memory systems on the nanometer scale, molecular-dynamics simulations were carried out for iron-nickel- and nickel-titanium-alloys with a maximum of about 5000 particles.
The used potentials arise from the embedded-atom method and can be found in the literature (FeNi [1], NiTi [2]).
The origin of shape-memory behavior are the martensitic and austenitic phase transitions between different crystal structures at certain temperatures or external stresses.
In our simulations, we investigated the temperature-driven phase transformations under the following conditions: free or periodic boundary conditions, surfaces of different structures, on which the simulated systems were placed, vacancies in the systems and various alloy compositions.
An evaluation of bond-orientational order-parameters [3] gives detailed information of the local structure during the phase changes.

[1] R. Meyer, P. Entel, *Phys. Rev. B* **57**, 5140 (1998).
[2] W. S. Lai, B. X. Liu, *J. Phys. Cond. Mat.* **12**, L53-L60 (2000).
[3] P. J. Steinhardt et al., *Phys. Rev. B* **28**, 784 (1983).

MM 35.39 Wed 16:30 P4

Crater Formation in Metals Induced by Femtosecond Laser Pulses — •Steffen Sonntag, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

We investigate femtosecond laser ablation of metals using a hybrid simulation scheme. Two coupled equations are solved simultaneously: a generalized transport equation for the electronic system which accounts for laser energy absorption and electronic part of the heat conduction, the other for the dynamics of the lattice where the ablation process takes place. For the electron temperature the generalized heat-conduction equation is solved by applying a finite difference scheme. For the lattice properties, e.g. pressure, density or temperature, we use common molecular dynamics. Energy transfer between the subsystems is allowed by introducing an electron-phonon coupling term. This combined treatment of the electronic and atomic systems is an extension of the well known two-temperature model [1].

Atomic scale images of the ablation process are shown. We discuss the crater formation induced by Gaussian beam profiles, i.e. by TEM00 modes. Ablation and melting thresholds for different metals will be presented.
[1] S.I. Anisimov, B.L. Kapeliovich and T.L. Perel'man: Sov. Phys. JETP 39, 375(1974)

MM 35.40 Wed 16:30 P4

Salt Precipitation in Complexes of Polyethylene Oxide and Alkali Metal Iodides — •Manuel Reschke, Jens Bastek, Nicolaas Stolwijk, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, 48149 Münster

Thermodynamic properties of polymer electrolytes have been the subject of many scientific reports. DSC measurements were performed on $PEO_{20}RbI$ over the temperature range from 0°C to 170°C for different heating rates. The calorimetric curves show an endothermic peak

at about 110°C which can be assigned to the precipitation process of the RbI salt out of the polymer matrix. With lower heating rates, the endothermic peak monotonically shifts to a lower temperature. By extrapolation to zero heating rate, the critical precipitation temperature T_C was determined. These T_C values can be compared with earlier data from conductivity measurements and NMR analyses [1]. Salt precipitation in $PEO_{30}CsI$ was observed by X-ray diffraction after quenching of the complex from Temperatures larger than T_C. Current experiments should provide information about the size of the RbI precipitates by detailed analysis of the diffraction peaks.

[1] J. Bastek, Th. Köster, L. van Wüllen, N.A. Stolwijk, Electrochem. Acta. submitted

MM 35.41 Wed 16:30 P4

Aging dynamics at the martensitic phase transition of Au-Cd quantified by XPCS — •L. Müller[1], M. Waldorf[1], C. Gutt[2], A. Madsen[3], G. Grübel[2], T.R. Finlayson[4], and U. Klemradt[1] — [1]II. Physik. Inst., RWTH Aachen Univ. — [2]HASYLAB at DESY, Hamburg — [3]ESRF, Grenoble — [4]School of Physics, Univ. of Melbourne

Aging phenomena of martensites have been discussed controversially for decades. Although they were successfully associated with defect-related diffusion processes in the low temperature phase (Ren and Otsuka, Nature **389**, 579 (1997)), so far no experiments have directly addressed the characteristic time scales associated with nanoscopic structural changes. Using a $Au_{50.5}Cd_{49.5}$ single crystal X-ray photon correlation spectroscopy (XPCS) measurements in diffraction geometry were carried out at ESRF beamline ID10A. High temperature resolution (0.1 K) and stability (±4 mK) were employed to resolve potential slow dynamics in the vicinity of the phase transition, 2D scattering data close to the (001) Bragg reflection were recorded with a sampling time into the detector of 0.2 s at 1.4 s intervals.

For each temperature one-time correlation functions show significant dynamics only near T_c, being fastest at the transition in disagreement with any critical slowing down scenario. Two-time correlation functions reveal a generally non-stationary behavior and also avalanches in the sample. Characteristic timescales were determined as a function of the aging-time by calculating one-time-correlation functions at a specific age. Fits of Kohlrausch-Williams-Watts functions reveal time constants ranging from ≈ 400 s to over 6000 s at largest aging-times.

MM 35.42 Wed 16:30 P4

Physical significance of the flexibility window in zeolites — •Asel Sartbaeva[1] and Stephen Wells[2] — [1]Inorganic Chemistry laboratory, South Parks Road, Oxford OX1 3QR, UK — [2]Department of Physics and Center for Scientific Computing, University of Warwick, Coventry CV4 7AL, UK

We have recently noted that aluminosilicate zeolite frameworks, modelled as a periodic system of corner-linked polyhedra, display a range of densities within which the polyhedra can in principle be made geometrically ideal. Outside this range, distortions are inevitable due to either stretching of bonds or collisions between oxygen atoms on adjacent tetrahedra. The densities of high-silica zeolites at room conditions is found to lie at the low-density edge of the window, indicating that zeolites are maximally expanded structures. We present new evidence, from a theoretical/experimental study of zeolites with ANA topology, that the flexibility window is a valuable guide in explaining the structures and structural phase transitions of zeolites.