MM 20: Poster session

Time: Tuesday 14:45–18:00 Location: Poster C

MM 20.1 Tue 14:45 Poster C

Quantitative Characterization of Thin Film Mechanical Properties using the Bulge-Test-Technique — •Peter Leibenguth and Frank Mücklich — Department for Materials Science, Functional Materials, Saarland University, Saarbrücken, Germany

Because of the limited, if not impossible, applicability of macroscopic characterization methods in the thin film regime, several methods coping with this issue have been developed, e.g. nanoindentation, microtensile-test or substrate-curvature-technique. In contrast to the latter examples, the bulge-test-technique is able to circumvent certain experimental and analytical problems. The underlying principle is quite simple: a geometrically well defined (cirular or rectangular) thin film specimen with simply supported edges is being deflected by a differential pressure acting on one side. By means of exact measurement of the pressure and the resulting displacement, the elastic modulus and the residual stresses of the thin film can be quantitatively investigated in only one experiment. We present the results of our investigations using our new bulge-test-setup, which combines several optimizations to the general technique. Those concern the specimen preparation method, and mainly the exact determination of the deflection, which has been performed using a white-light interferometer allowing a height resolution of approximately 1 nm and a full-field imaging of the specimen geometry. Using nanoindentation, x-ray residual stress analysis and an inverse approach via FEM, the efficiency of this setup was demonstrated inverstigating singlelayered SixNy- and multilayered Al-SixNy- and Cu-SixNy-composite membranes.

MM 20.2 Tue 14:45 Poster C

Enthalpy of Mixing in the Binary System Bi-In — •Andriy Yakymovych[1], Stepan Mudry[1], Christoph Luef[2], and Herbert Ipser[2] — [1]Department of Metal Physics, Ivan Franko National University Lviv, UA-79005 Lviv, Ukraine — [2]Department of Inorganic Chemistry/Materials Chemistry, University of Vienna, A-1090 Vienna, Austria

Bi-In alloys are widely used in manufacturing, for example to make fuel tank safety plugs, or in solders. From the scientific point of view this system is very interesting because of the existence of the intermetallic compounds BiIn, Bi_3In_5 and $BiIn_2$. Transport properties in the liquid state show a deviation of the typical temperature dependence in low temperature regions and knowledge of the thermodynamic properties in the liquid state is very important for deeper understanding of the structure and bonding nature of the system. Most of the investigations of the enthalpy of mixing were made at higher temperatures, the measurement results at lower temperatures, in turn, show some disagreement.

Calorimetric studies of the enthalpy of mixing in the system Bi-In have been carried out at 483, 875 and 1023 K. The enthalpy of mixing is negative and shows a minimum at approximately 45 at.% Bi, what indicates a mutual interaction of both components in the alloys. The curve of enthalpy of mixing is asymmetric.

MM 20.3 Tue 14:45 Poster C

Relaxations in metallic glasses investigated by a broad frequency and temperature range — •Dennis Bedorf[1], Thomas Koeppe[1], Jörg Hachenberg[1], Konrad Samwer[1], Annelen Kahl[2], and Ranko Richert[3] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Keck Laboratories MS 138-78 Caltech, Pasadena CA 91125, USA — [3]Department of Chemistry and Biochemistry, Arizona State University, Tempe AZ 85287-1604, USA

We are interested in glassy dynamics and the atomistic processes leading to different relaxations in amorphous materials. To measure the complex elastic constants, two mechanical spectroscopy techniques were employed. The use of a double-paddle-oscillator (DPO) provides sufficient sensitivity to investigate the loss of even thin films. A DPO is driven in eigenfrequency mode at 5.4 kHz and an amorphous metallic film (PdCuSi) is evaporated onto it and measured under UHV conditions. Cooling and heating enables measurements in a broad temperature range with different heating rates.

To survey the elastic constants at higher frequencies, an ultrasonic spectroscopy technique in the MHz regime is used. The pulse-echo method is applied to a bulk metallic glass in order to obtain the shear modulus and attenuation by monitoring shear wave propagation. The results are discussed in the framework of the Cooperative Shear Model.

This work was supported financially by DFG, SFB 602 and Leibniz Programm.

MM 20.4 Tue 14:45 Poster C

Dynamics in glass forming $Pd_{40}Cu_{40}P_{20}$ melts — •Suresh Mavila Chathoth[1], Bernd Damaschke[1], Michael Marek Koza[2], Ranko Richert[3], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Universitaet Göttingen, 37077 Göttingen, Germany — [2]Institut Laue-Langevin,BP 156 - 38042 Grenoble, France — [3]Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287-1604, U.S.A.

The Cu relaxational dynamics and temperature dependence of self-diffusion in the glass forming $Pd_{40}Cu_{40}P_{20}$ melts has been investigated with inelastic neutron scattering. Unlike in $Pd_{40}Ni_{40}P_{20}$ or $Pd_{43}Ni_{10}Cu_{27}P_{20}$ [1] melts self-diffusion in $Pd_{40}Cu_{40}P_{20}$ melt approaches similar values at high temperature but anomalously faster on approaching its liquidus temperature. The intermediate scattering function, $\Phi(q,t)$ of $Pd_{40}Cu_{40}P_{20}$ melts decay to zero rather non-exponentially. A fitting with Kohlrausch-Williams-Watts function in the α-relaxation regime exhibits structural relaxation that shows stretching in time. Moreover $\Phi(q,t)$ shows temperature and q dependent stretching and is more pronounced at lower temperatures. This indicates that in the $Pd_{40}Cu_{40}P_{20}$ melts the increase in heterogeneities on cooling towards its liquidus temperature is responsible for the anomalous behavior in the self-diffusivity. We gratefully acknowledge financial support from the Leibniz program.

[1] S. M. Chathoth, A. Meyer, M.M. Koza, F. Juranyi, Appl. Phys. Lett. **85**, 4881 (2004).

MM 20.5 Tue 14:45 Poster C

Dendritic and eutectic solidification of undercooled Ni-Zr alloys — •Helena Hartmann[1,2], Sven Reutzel[1,2], Peter Galenko[2], and Dieter Herlach[2] — [1]Institut für Experimentalphysik IV, Ruhr-Universität, 44780 Bochum, Germany — [2]Institut für Materialphysik im Weltraum, DLR, 51170 Köln, Germany

New measurements of dendritic and eutectic growth velocity in levitated undercooled Ni-Zr samples are performed as a function of undercooling ΔT. The new data reveal high accuracy and low scattering. The growth velocity is measured by using a high-speed camera and subsequently, the morphology of the microstructure of the solidified samples is investigated. The data for eutectic growth of Ni - 8.8 at.% Zr alloy are compared with the previously measured growth velocity data set of dendritic growth of Ni - 1 at.% Zr alloy. Experimental results on kinetics of dendritic and eutectic growth in Ni-Zr alloy samples are discussed and analysed within the current models of non-equilibrium solidification.

MM 20.6 Tue 14:45 Poster C

Interaction of ceramic particles with an advancing dendritic solidification front — •Matthias Kolbe[1], Thomas Lierfeld[1,2], Thomas Schenk[3], Gunther Eggeler[2], and Dieter Herlach[1] — [1]DLR, Institut für Materialphysik im Weltraum, Linder Höhe, 51170 Köln — [2]Ruhr-University Bochum, Institute of Materials IA1, 44780 Bochum — [3]Lab. de Physique des Matériaux, ÉdM de Nancy, France

The interaction of ceramic particles with a dendritic solid/liquid interface has been investigated by undercooling experiments with different levels of convection: (i) in a terrestrial electromagnetic levitation facility (EML) and (ii) in TEMPUS, a facility for containerless processing, under low gravity conditions during parabolic flights. Entrapment of particles in ground experiments and engulfment of a significant fraction of submicron particles under low gravity conditions are attributed to the lower level of convection in the latter experiments and to morphological features of dendritic solidification. X-ray radiography at ESRF has been used for in-situ observations of directional solidification in Al90Cu10 with alumina particles.

MM 20.7 Tue 14:45 Poster C

Depth-resolution measurement of CDB of layered Al-Sn-Sample — •Philip Pikart[1,2], Christoph Hugenschmidt[1,2], Jakob Mayer[1,2], Martin Stadlbauer[1,2], and Klaus Schreckenbach[1,2]

— [1]Physikdepartment E21, James-Frank-Straße, 85748 Garching — [2]ZWE FRM-II, Lichtenbergstr. 1, 85748 Garching

At the new positron source NEPOMUC at the FRM-II in Munich a moderated positron beam with an intensity of $\geq 10^8$ positrons per second is available. After linear acceleration up to 30 keV at the entrance of the analysis chamber, coincident doppler broadening (CDB) measurements can be performed.

The implantation depth of the positrons can be varied using different beam energies, and scanning of the positron beam enables lateral resolved analysis of the sample. In this experiment, the minimal visible thickness of the tin-layer is determined by DB measurements and by CDB with improved elemental sensitivity.

For this reason, samples were prepared, which are containing a wedge-shaped layer of tin with a thickness in the range of 1-200nm, on an aluminum substrate and covered by an aluminum layer of constant thickness of $\geq$ 100 nm. The samples were grown out of high purity materials in a MBE-chamber.

The results of the DB-measurements were then compared to CDB-measurements on the same sample with same conditions in order to determine a sensitivity threshold for DB and CDB respectively.

MM 20.8 Tue 14:45 Poster C

Interface Design for adhesion between NiTi shape memory alloy and Polyamide 6 — Stephane Youcheu Kemtchou[1], Guido Grundmeier[2], •Klaus Neuking[1], and Gunther Eggeler[1] — [1]Lehrstuhl Werkstoffwissenschaft, Ruhr-Universität Bochum — [2]Lehrstuhl Technische und Makromolekulare Chemie, Universität Paderborn

Composite Materials consisting of NiTi shape memory alloys as fiber and polymer as matrix have been studied in previous years due to their interesting properties for various applications like vibration control or as actuator. Because of their beneficial properties, especially better adherence to NiTi than thermoplastic polymers, elastomer and thermoset polymers such as epoxy were mostly used as polymer matrix. The aim of the present work was to study different interface systems including organo-functional silane to promote adhesion between NiTi and thermoplastic polymers. A pseudo elastic NiTi alloy and Polyamide 6 as thermoplastic matrix were used for this purpose. The sample was manufactured by injection moulding using in-mould assembly method. Pull- out tests were performed to study the change in adhesion relating to the interface used. The obtained results show significant increase in adhesion related to the interface system used.

MM 20.9 Tue 14:45 Poster C

Formation of rare earth zirconia pyrochlores on yttria-stabilized ZrO_2 single crystals by solid state reactions — •Andreas Schubert, Stephan Senz, and Dietrich Hesse — Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

$RE_2Zr_2O_7$ (RE=La, Pr, Nd, Sm, Gd, Ho)-based pyrochlore islands were grown on Y_2O_3-stabilized ZrO_2 (YSZ) single-crystals by reaction between RE_2O_3 and YSZ. After a vapour-solid reaction at 1200 °C at a rate of 0.6 nm/min for 6.5 min between La_2O_3 vapour and YSZ(001), islands with eight domains were formed. Four domains were tilted by 2.1° around <110> and the other four were tilted by 0.9° around <100>. To understand this effect, other experiments were performed with different substrate orientations and other rare earth oxides, to study the influence of the misfit. $La_2Zr_2O_7$ (LZO) has a relatively large misfit to YSZ of 5 % but other rare earth-based pyrochlores have lower misfits of 4.0 % ($Pr_2Zr_2O_7$) to 1.2 % ($Ho_2Zr_2O_7$). The reaction products were investigated by AFM, XRD and TEM. On YSZ(110), four domains were found by XRD pole figure measurements, two were tilted around $[1\bar{1}0]$ with a maximum at a tilt angle of 0.6° and the other two were tilted by 0.9° around [001]. AFM and TEM plan-view images show stripe-shaped islands with the long edge along $[1\bar{1}0]$ and the short edge along [001]. In addition to these vapour-solid reactions some experiments with solid-solid reactions were performed. For the solid-solid reaction of La_2O_3 and YSZ(001) it was determined by XRD-measurements that the relation (001)LZO ∥ (001)YSZ is valid without any systematic tilt (FWHM=0.5°).

MM 20.10 Tue 14:45 Poster C

Removing relativistic effects for the determination of optical properties using EELS — •Michael Stöger-Pollach, Anita Laister, and Peter Schattschneider — Institute for Solid State Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/138, A-1040 Vienna, Austria

Since the energy resolution of modern energy loss (EELS) experiments in a transmission electron microscope (TEM) has improved to less than 0.2 eV full width at half maximum in the elastic peak, valence EELS has attracted interest again. However, due to the fact that the acceleration voltages of conventional TEMs are in the range of 100-300 kV retardation effects become important. The condition for Cerenkov radiation is fulfilled if $v > c/n$, with c as the speed of light, v as the speed of the probe electron and n as the refractive index of the material.

For determination of optical properties Kramers-Kronig Analysis (KKA) is applied after an iterative removal of relativistic effects and surfce plasmons. Conventinal software does not take relativistic effects into account. Our method therefore gives more precise information on the optical properties of materials. Moreover faint differences of the response function between similar layers can be probed with very high accuracy.

We present the result on two similar SiN:H layers with different H concentration. The difference in the optical refractive index is 2% and can be identified with an accuracy of less than 1%.

MM 20.11 Tue 14:45 Poster C

ELNES at Internal Copper-Silicon Dioxide Interfaces — •Oliver Heckl[1], Ferdinand Haider[1], and Jürgen Gegner[2] — [1]Universität Augsburg, Institut für Physik, Lehrstuhl für Experimentalphysik I, Physik Geb. Nord, Ebene 3, Universitätsstr. 1, D-86159 Augsburg — [2]SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany, E-mail: juergen.gegner@skf.com

Metal-silicon dioxide interfaces are of special importance in semiconductor technologies (e.g. MOS structures). A Cu-Si alloy containing 1.5 at.% Si is produced by arc melting. Samples of 200μm in thickness are completely internally oxidized in a Rhines pack powder mixture at 1000°C. Spherical amorphous SiO_2 precipitations are formed homogeneously dispersed within the copper matrix.

The heterophase boundary between the base metal and the embedded oxide particles is examined with high spatial resolution using a scanning transmission electron microscope (STEM) that is equipped with an electron energy loss (EEL) spectrometer. Typical features of the electron energy loss near-edge fine structure (ELNES) of the oxygen O-K ionization edge allow to determine the bonding state of oxygen and thus to detect interlayers at the phase boundary. The validity of the Kirchheim structural vacancy model of oxygen segregation at metal-oxide interfaces shall be verified this way: for amorphous precipitations, it predicts that no interfacial accumulation of excess oxygen atoms should occur.

MM 20.12 Tue 14:45 Poster C

SIMS and XRD Measurements for the Critical Review of Carbon Diffusivity Derivation from Hardness Profiles — •Jürgen Gegner — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Microhardness decarburization profiles are often used in the industry to estimate the carbon distribution in steels. For quantitative evaluation, an analysis based on diffusion theory must be performed, the fundamentals and mathematical basics of which are presented. If the relationship between hardness and carbon content is known, microhardness-distance curves of steels can be analyzed in this way. For martensitic grades, for instance, a linearized expression holds in the concentration range from 0.15 to 0.6 m.% C. Microhardness depth profiles of higher carbon steels and other microstructures, however, are also evaluated in the literature. The applicability of quantitative diffusion modeling is discussed in detail. Through hardenable rolling bearing steel 100Cr6 (1.3505, SAE 52100) serves as model material: carbon concentration-distance curves are measured with high accuracy by secondary ion mass spectrometry (SIMS) and compared with microhardness decarburization profiles for tempered and untempered martensitic and near-equilibrium microstructures, which are further characterized by metallographic micrographs. Also, the correlation to X-ray diffraction (XRD) characteristics is considered.

MM 20.13 Tue 14:45 Poster C

Experimental and Theoretical Analysis of Fatigue Phenomena in Rolling Contact — •Jürgen Gegner and Wolfgang Nierlich — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Material mechanics theories of rolling contact loading can be reassessed by recording the alteration of X-ray diffraction (XRD) characteristics measured from the edge to the core. Exceeding metallographic investi-

gations, the developments of residual stresses and XRD line width represent the relevant information carrier. Material changing permits a specific correlation to failure probability distributions. These relationships differ significantly for sub- and near-surface fatigue. Recent findings from demanding bearing applications point to different equivalent stresses for describing the material response in both loading types: for classical sub-surface rolling contact fatigue (RCF) that is characterized by strengthening and softening processes below the Hertzian contact area, shear stress-based hypotheses are indicated, whereas for the surface failure mode that is accompanied by embrittlement, the main normal stress-based hypothesis should additionally be considered. Cyclic tensile stresses caused by friction can act on material-inherent crack sources. In both cases, line width changes, which mainly stem from plastic deformation with rearrangement of the dislocation configuration and martensite decay with carbon diffusion, serve as powerful sensor for material aging. Rig tests under controlled mixed friction conditions give an example of near-surface RCF.

MM 20.14 Tue 14:45 Poster C

Miniaturisation of the shear compression specimen — •Markus Ames, Jürgen Markmann, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

The shear compression specimen has been developed for large strain testing of materials. It consists of a short cylinder or cuboid with two slots oriented at 45° relatively to the longitudinal axis (gauge section). As a result of this geometry, uniaxial compression leads to a predominant shear deformation localized across/along the gauge section. The obtained data has been evaluated by comparing the experimental data with finite element simulations of the deformation process, using material properties like young modulus and yield stress as input parameters.

The purpose of the present study was to explore the potential for miniaturising this specimen geometry in order to become applicable for mechanical testing of small-sized nanostructured materials. Therefore, the geometry of the conventional shear compression specimen (a cylinder of 20mm height and 12.65mm in diameter) has been stepwise affinely shrunk to cuboids of 7 x 3.6 x 0.5mm in size. We used the spark erosion technique to prepare specimen of OFHC copper, and we will discuss, based on yield stress and modulus, under which conditions the mechanical behaviour of such miniaturised specimen appears shape and size invariant.

MM 20.15 Tue 14:45 Poster C

Calculation of the *Peierls stress* from atomistic simulations for bcc tungsten: screw vs. edge dislocations — •Bernd Eberhard[1,2], Juergen Almanstoetter[2], and Ferdinand Haider[1] — [1]Universität Augsburg, Institut für Physik — [2]OSRAM GmbH, Mittelstetter Weg 2, 86830 Schwabmünchen

For bcc metals, it is commonly assumed, that the mobility of screw dislocations is significantly lower than that of edge dislocations and, therefore, should control the low temperature plastic deformation behaviour. The mobility of dislocations depends on their *Peierls energy barrier*, defined as the activation energy required to move a dislocation in an otherwise perfect crystal. This connection between atomistic features and the overall mechanical behaviour makes a more detailed investigation of the atomistic system necessary. Also, the violation of *Schmid's Law*, stating that the critical resolved shear stress is constant and independent of the slip system and the external stress, is an important ingredient for the construction of macroscopic flow rules of the material, suitable e.g. for *finite element* calculations.
In present work, these effects are studied for $1/2a\,\langle 111\rangle$ *screw* and *edge* dislocations in tungsten.
To this end, we constructed dislocation dipoles using elasticity theory in a periodic simulation cell. After relaxation within a NPT MD-simulation, we applied an external shear stress to the system in order to force the dislocations to move at low simulation temperatures. The *Peierls energy barriers* and the corresponding *Peierls stresses* are derived.

MM 20.16 Tue 14:45 Poster C

Analytical and numerical evaluation of the critical tensile stress for failure event in single-crystal sapphire detected by the combined application of normal and lateral forces — •Maksim Karniychuk[1], Vladimir Kolchuzhin[2], and Frank Richter[1] — [1]Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz — [2]Technische Universität Chemnitz, Fakultät für Elektrotechnik und Informationstechnik, 09107 Chemnitz

The new possibilities for mechanical characterization of bulk and coated materials by the combined application of normal (UMIS 2000, CSIRO) and lateral (LFU, ASMEC) forces were recently developed [1,2]. Among others, the possibility for experimental detection of crack formation was offered. As an example, the crack formation was detected in single-crystal sapphire from the shape of the lateral force-displacement curves at a given normal force. Thus, the value of critical tensile stress for crack formation in material can be evaluated by both analytical and numerical approaches at the known critical normal and lateral forces.

The presented work reports results of comparison of critical tensile stress evaluations performed by both mentioned approaches. The analytical approach uses the Hanson model for bulk materials realized by the software Elastica (ASMEC). Finite Element Method is used for numerical evaluation by means of the commercial software ANSYS.

[1] V. Linss, T. Chudoba, M. Karniychuk, F. Richter, Thin Solid Films 494 (2006) 179

[2] M. Karniychuk, Ph.D. thesis, TU Chemnitz, 2006

MM 20.17 Tue 14:45 Poster C

Martensite formation in a ductile Cu47.5Zr47.5Al5 bulk metallic glass composite — •Simon Pauly, Jayanta Das, Cécilie Duhamel, and Jürgen Eckert — IFW Dresden, Postfach 27 01 16, D-01171 Dresden

A Cu47.5Zr47.5Al5 alloy was solidified into rods of 2, 3 and 5 mm diameter and the microstructures as well as the elastic and plastic properties were investigated along the length of each rod. It was found that neither the microstructure nor the mechanical properties vary significantly along the length of the specimens, except for the 5 mm diameter rod where the top part was proved to be fully crystalline containing cubic B2 CuZr (austenite) and monoclinic CuZr (martensite) phases. A composite microstructure consisting of B2 CuZr embedded in an amorphous phase was revealed in the other parts of the 5 mm diameter and along the 2 mm and 3 mm diameter rods. The differently solidified alloys show high strength (σy up to 1721 MPa) and a distinct deformability (ϵp up to 10.1 %) under uniaxial compression and a work hardening-like behavior.

MM 20.18 Tue 14:45 Poster C

In-situ Observation of Phase Formation in Undercooled Nd-Fe-B-melts with Synchrotron Radiation and High-Speed Video Analysis — •Jörn Strohmenger[1,2], Thomas Volkmann[2], Jianrong Gao[3], Sven Reutzel[1,2], Dirk Holland-Moritz[1], Oliver Heinen[1], and Dieter Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum f. Luft u. Raumfahrt, 51170 Köln — [2]Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum — [3]Key Lab of Electromagnetic Processing of Materials, Northeastern University Shenyang, 110004, P.R. China

Competitive crystallisation of stable and metastable phases in undercooled Nd-Fe-B melts was investigated using electromagnetic levitation technique combined with in-situ X-ray diffraction experiments at the ESRF. It is shown that the primary crystallizing phase is influenced by undercooling, e.g a metastable phase can be directly observed which initiates the formation of the intermetallic Phi-phase. It can be identified as a ternary extension of the rhombohedral Nd2Fe17 phase being stable in binary Nd-Fe alloys. The growth velocity of Phi-phase is determined with a high-speed camera sytem.It is shown that growth velocity is affected by induced melt convection. A phase selection diagram showing the different solidification pathways as a function of undercooling and alloy composition will be analyzed within theories of nucleation and crystal growth. This work was supported by DFG under contract No. HE1601/14.

MM 20.19 Tue 14:45 Poster C

USAXS measurements of short- range ordering in mesoscopic systems — •Ina Klassen[1], Patrick Wette[1], Dieter Herlach[1], Dirk Holland-Moritz[1], and Stephan Roth[2] — [1]Institute of Materials Physics in Space, 51147 Cologne, Germany — [2]Hasylab at Desy, 22603 Hamburg, Germany

High resolution ultra- small x- ray scattering techniques at Hasylab are used to determine the fluide and crystalline structure factor of charged colloidal suspensions. We analyse charged stabilised silica particles of 200nm radius with different volume fractions and salt concentrations. By varying the salt concentration we tune the electrical potential which influences the structural behavior of colloidal crystals. In addition to x-ray scattering we show light scattering experiments and compare the experimental results of both techniques with respect to structural information.

MM 20.20 Tue 14:45 Poster C

Primary crystallization of the hypoeutectic Ni-17at% P alloy by ASAXS and SANS — Dragomir Tatchev[1], •Rainer Kranold[2], Armin Hoell[3], Günter Goerigk[4], and Stephan Armyanov[1] — [1]Institute of Physical Chemistry, BAS, Sofia 1113 — [2]Institute of Physics, Rostock University, Rostock — [3]Hahn Meitner Institute, Glienicker Str. 100, Berlin — [4]Institute of Solid State Research, Jülich Research Centre, P.O. Box 1913, Jülich

We investigated the primary crystallization of Ni(P) particles in the amorphous hypoeutectic Ni-17 at.% P alloy with anomalous small-angle X-ray scattering (ASAXS) [1] and small-angle scattering of polarized neutrons (SANS) [2]. Using the maximum entropy method, the particle size distribution, the size dependence of the particle composition and the amorphous matrix composition were determined simultaneously. The size distribution shows a peak at particle radius of 1 nm and a tail spanning from 2 to 15 nm. The composition of the particles of the peak changes from 14 to 2 at.% P as their radius grows from 0.7 to about 3 nm. The particles in the tail of the size distribution (2-15 nm) have nearly constant P content in the range of 0-2 at.%. The matrix composition tends to the eutectic composition with 19 at.% P at the end of the primary crystallization process. It should be mentioned that our experimental results completely confirm the predictions made in a generalized Gibbs' approach to nucleation theory [3] developed recently. [1]D. Tatchev et al., J. Appl. Cryst. 38 (2005) 787. [2]D. Tatchev et al., Physica B 369 (2005) 8. [3]J.W.P. Schmelzer et al., J. Colloid Interface Sci. 272 (2004) 109.

MM 20.21 Tue 14:45 Poster C

Modeling of dendritic solidification *in undercooled dilute Ni-Zr melts — Denis Danilov[1], Peter Galenko[2], •Britta Nestler[1], and Dieter Herlach[2] — [1]Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany — [2]Institut für Raumsimulation, DLR, Köln

The dendritic and eutectic solidification in undercooled Ni-Zr samples is analyzed using new experimental results, theoretical studies based on a sharp-interface model and phase-field simulations. Predictions of a sharp interface model and of a diffuse interface model describing the phase transition under the consideration of both, thermal and solutal diffusion are compared with the experimental results evaluating the dendritic tip velocity in electromagnetically levitated Ni-Zr samples.

MM 20.22 Tue 14:45 Poster C

Phase-field modelling of solute trapping during rapid solidification of a Si–As alloy — Denis Danilov and •Britta Nestler — Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany

The effect of nonequilibrium solute trapping by a growing solid under rapid solidification conditions is studied using a phase-field model. Considering a continuous steady-state concentration profile across the diffuse solid-liquid interface, a new definition of the nonequilibrium partition coefficient in the phase-field context is introduced. This definition leads, in particular for high growth velocities, to a better description of the available experimental data in comparison with other diffuse interface and sharp-interface predictions.

MM 20.23 Tue 14:45 Poster C

Monte Carlo Simulation of Phase Separation Including Elastic Relaxations — •Rolf Anders and Ferdinand Haider — Universität Augsburg, Institut für Physik

We developped a real space technique which includes local atomic relaxation after each MC step, allowing thus to study phase transformations with strong elastic contributions. The MC step consists of a vacancy jump, exchange of nearest neighbours or atom type change. The activation energy is computed using phenomenological interaction potentials (Lennard-Jones or EAM). After an accepted MC step the atomic coordinates in the vicinity of the modification are relaxed in order to minimise the total energy.

This method was used to study segregation to an edge dislocation. The pinning force was calculated by shifting the concentration profile and subsequent relaxation of the lattice. Furthermore the method was applied to calculate the phase diagram using an EAM potential. This was done using grand canonical simulations at different temperatures and chemical potentials.

MM 20.24 Tue 14:45 Poster C

Nucleation kinetics in deionized charged colloidal model systems: a quantitative study by means of classical nucleation theory — •Patrick Wette[1] and Hans Joachim Schöpe[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln — [2]Institut für Physik, Johannes Gutenberg Universität , Staudinger Weg 7, 55128 Mainz

We have studied the nucleation kinetics of charged colloidal model systems under salt free conditions covering a wide range of particle number densities $18\mu m^{-3} \leq n \leq 66\mu m^{-3}$.We employed direct video-microscopic observation of individual nucleation events to obtain time resolved nucleation rate densities. Polarization microscopy and static light scattering on the resulting solids in combination with Avrami-theory is used to determine the steady state nucleation rate at high undercoolings. The final nucleation rate densities J from different methods are observed to be consistent with each other. By increasing the difference in the chemical potential between melt and crystal $\Delta\mu$ about one order of magnitude J increases over eight orders of magnitude. The data can be well analyzed and interpreted using classical nucleation theory (CNT) leading to a linearly increasing melt/crystal surface tension. Surprisingly the reduced surface tension is about one order of magnitude larger compared to other system (metals, hard sphere colloids). The critical radius of the crystal nuclei is decreasing down to a very small value of 1.5 coordination shells. The determined kinetic prefactors are up to 15 orders of magnitude smaller than the prefactor calculated by CNT.

MM 20.25 Tue 14:45 Poster C

Analytical bond order potential for bcc and fcc iron - comparison with established EAM potentials — •Michael Müller, Paul Erhart, and Karsten Albe — TU Darmstadt. Institut für Materialwissenschaft, FG Materialmodellierung, Petersenstr. 23, D-64287 Darmstadt

A new analytic bond-order potential for iron is presented that has been fitted to experimental data and results from first-principles calculations. The angular dependent functional form allows a proper description of a large variety of bulk, surface and defect properties, including the Bain-path, phonon dispersions, defect diffusivities and defect formation energies. By calculating Gibbs free energies of bcc and fcc iron as a function of temperature, we show that this potential is able to reproduce the transitions from alpha-iron to gamma- and delta-iron before the melting point. The results are compared to four widely used embedded atom method potentials for iron.

MM 20.26 Tue 14:45 Poster C

Sample preparation from mechanically alloyed CuFe powders by means of focussed ion beam — •Malte Schmidt, Talaat Al-Kassab, Catharina Wille, and Reiner Kirchheim — Georg-August-Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

The focussed ion beam (FIB) has been utilised to shape tip samples for field ion micrsocopy (FIM) and tomographic atom probe (TAP). These tips were prepared from powder particles of $Cu_{97.5}Fe_{2.5}$, $Cu_{95}Fe_5$ and $Cu_{90}Fe_{10}$. Such powder particles are first produced using a high-energy planetary ball mill under protective Ar atmosphere, using elemental powders of high purity and milling tools made of hardened steel. Subsequently the milled powder was dusted onto a double-stick carbon tape adhered to a FIB-specimen holder.

A modified lift-out method, which is usually used to fabricate transmission electron microscope lamellae, is applied as a first step of the procedure. After cutting out the lamella of a single particle of the powder, a longish cuboid with an approximate $2\mu m$ x $2\mu m$ base area is lifted out of the particle and immediately welded onto a modified tungsten tip by means of platinum ion assisted deposition. Subsequently the actual FIM - tip can be shaped out of this cuboid. In this contribution the different steps of the novel procedure are explained and discussed in detail emphasising the sharpening techniques. In addition first results of measurements of such prepared samples will be presented.

Financial support from the Deutsche Forschungsgesellschaft under contract KI-230/33-1 is gratefully acknowledged.

MM 20.27 Tue 14:45 Poster C

Sintering without grain growth? A strategy for compacting nanostructured powders to high density without loss of nanocrystallinity — •Lionel Kroner and Carl Krill — Institute of Micro and Nanomaterials, Ulm University, D-89081 Ulm

Most synthesis routes for nanocrystalline materials result in thin films

or powders, which can in principle be formed into bulk specimens via compaction. However, achieving near-100% density generally requires the simultaneous application of high temperature, which in turn induces grain growth, and the final product is no longer nanocrystalline! A potential strategy for sintering without significant grain growth would be to suppress the driving force for coarsening through the deliberate addition of an atomic species that segregates to the grain boundaries. Such *thermodynamic stabilization* of nanocrystallinity has already been demonstrated for ball-milled Pd doped with Zr [1]; however, no attempt was made to compact the resulting powders into bulk specimens. In this work, we examine the grain size and porosity of nanocrystalline $Ni_{1-x}Zr_x$ powders as a function of Zr concentration and temperature, both under atmospheric pressure and after compaction. The microstructural evolution during pressureless annealing is followed nondestructively using high-temperature wide-angle x-ray diffraction, and the density of compacted powders is determined by Archimedes' method. The influence of Zr addition on the sinterability of the powders is assessed.

[1] C. E. Krill III, H. Ehrhardt and R. Birringer, *Z. Metallkd.* **96** (2005) 1134–1141.

MM 20.28 Tue 14:45 Poster C

Reactive interdiffusion in sandwich type Al/Cu thin-films — •Constantin Buzau Ene[1], Carsten Nowak[1], Guido Schmitz[2], Talaat Al-Kassab[1], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Friedrich-Hund Platz 1, D-37077, Göttingen, Germany — [2]Institut für Materialphysik, Wilhelm-Klemm-Str.10, D-48149 Münster, Germany

Al/Cu/Al and Cu/Al/Cu triple layers with approximately 10nm single layer thickness deposited on tungsten substrates and planar (100) Si were analyzed in the early stages of reactive interdiffusion by atom probe tomography and TEM. The first reaction product is found after 5 min at 110°C and identified with a composition around the Al_2Cu. Surprisingly, we found a significant asymmetry in the reaction rate with the stacking sequence as a particularity of the tip-shaped tungsten tips: The thickness of the product grown at the interfaces Cu grown on Al layer, is approximately 1.5 to 2 times thicker than at the other interfaces at which Al grows on a Cu layer. Compared to the recently proven delayed nucleation of the first product phase in the case of Al/Co thin-films, which has been explained by the concept of a critical gradient, the reaction in Al/Cu develops quite differently. Applying the critical gradient concept to the Al/Cu system leads to the prediction of a critical nucleation thickness of 6.8 nm. This is in obvious contrast to the experiment, which reveal parabolic growth from the very beginning with no precursory interdiffusion and no distinct nucleation process. Thus,in the case of Al/Cu the first reaction product might be a metastable one. Pasichnyy et al, Phys. Rev. B 72 (2005).

MM 20.29 Tue 14:45 Poster C

Nanolayered and nanoparticle-dispersed WC/C coatings: frictional and wear behavior — Maik Gubisch[1], •Yonghe Liu[2], Sven-Erik Wulf[1], Thomas Haensel[2], Mikhail Kosinskiy[2], Lothar Spiess[1], and Juergen A. Schaefer[2] — [1]Institut für Werkstofftechnik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany — [2]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

The control of friction plays a critical role in the developing of wide scanning-range nanopositioning technology, which usually employs bearings to cover the wide distance. A series of WC/C coatings have been developed for the application on the bearings. They are processed in two kinds of microstructures: nanoscale multilayer of WC and amorphous carbon, and nanoscale crystalline WC particles in an amorphous carbon matrix. In this work, we compared their frictional and wear behaviour measured by a microtribometer, and correlated with the microstructure of the worn tracks and transfer films characterized by SEM, EDS, FIB and TEM. Though the frictional behaviour seems quite similar, the wear resistance of the coatings is quite different. These findings are discussed with the formation and redistribution of the transfer films.

MM 20.30 Tue 14:45 Poster C

Boron Sheets and Boron Nanotubes — •Jens Kunstmann[1] and Alexander Quandt[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Institut für Physik der Universität Greifswald, Domstraße 10a, 17489 Greifswald

Based on a numerical ab initio study, we discuss a structure model for a broad boron sheet, which is the analog of a single graphite sheet, and the precursor of boron nanotubes. The sheet has linear chains of sp hybridized sigma bonds lying only along its armchair direction, a high stiffness, and anisotropic bonds properties. The puckering of the sheet is explained as a mechanism to stabilize the sp sigma bonds. The anisotropic bond properties of the boron sheet lead to a two-dimensional reference lattice structure, which is rectangular rather than triangular. As a consequence the chiral angles of related boron nanotubes range from 0 to 90 degrees. Given the electronic properties of the boron sheets, we demonstrate that all of the related boron nanotubes are metallic, irrespective of their radius and chiral angle, and we also postulate the existence of helical currents in ideal chiral nanotubes. Furthermore, we show that the strain energy of boron nanotubes will depend on their radii, as well as on their chiral angles. This is a rather unique property among nanotubular systems, and it could be the basis of a different type of structure control within nanotechnology.

MM 20.31 Tue 14:45 Poster C

Influence of bonding on the I-V-characteristics of Si29H24 and organic molecules on Si surfaces — •Samuel Baltazar-Rojas[1,4], Daungruthai Jarukanont[1], Mario De Menech[1,2], Ulf Saalmann[2], Aldo Romero[3], and Martin Garcia[1] — [1]Theoretische Physik, FB 18, Universität Kassel, Kassel, Germany — [2]Max–Planck–Institut für Physik komplexer Systeme, Dresden, Germany — [3]CINVESTAV, Queretaro, Mexico — [4]Advanced Materials Department, IPICYT, San Luis Potosi, Mexico

In the last years, much attention has been given to the study of transport properties through supported clusters and molecules, and it has become more intensive in the last years due to the different potential applications of these systems to electronic devices. We present a theoretical study of charge transport through clusters and molecules supported on silicon surfaces. The method simulates the measurement of the I-V characteristics with the help of a STM tip. The electronic properties of the cluster (molecule) coupled to the surface and the STM are calculated using non-equilibrium Green's functions based on effective single-particle Hamiltonians. In particular, we have computed conductance spectra of H-passivated silicon cluster $Si_{29}H_{24}$ on an ideal Si surface, showing the importance of the surface to modulate and control the I-V curve. Also, we have considered organic molecules such as styrene and show that negative differential resistance can appear due to the shifting of the electronic levels near bulk of the Si substrate with the external bias. We analyze the effect for different configurations of the supported organic molecule.

MM 20.32 Tue 14:45 Poster C

Microstructure in Damascus Sabres — •Marianne Reibold[1], Peter Paufler[1], Dirk Meyer[1], Alexander Levin[1], and Werner Kochmann[2] — [1]Institut für Strukturphysik, TU Dresden, D-01062 Dresden, Germany — [2]Krüllsstrasse 4b, D-06766 Wolfen

Damascus steel is famous for its beauty and excellent mechanical properties. Damascus blades - originating in India - were manufactured from so-called "wootz" steel.

For a better understanding of the ancient technology by analysis of the microstructure of damascene steel, high-resolution electron microscopy (TEM) and X-ray diffraction are eligible tools. The specimens investigated were taken from a genuine Damascus sabre produced by the blacksmith Assad Ullah in the seventeenth century.

The main results are as follows: Besides ferrite and perlitic cementite, we observed a third form of cementite forming so-called nanowires. These nanowires often arrange in colonies. Preferably, the {010}-lattice planes of the nanowires are oriented along the longitudinal direction. The surrounding of the nanowires often could be idendified as alpha-ferrite.

After dissolution of the sample in hydrochloric acid, carbon-nanotubes became visible. Some remnants showed evidence of incompletely dissolved cementite nanowires, indicating that these wires could have been encapsulated and protected by the carbon nanotubes. [1]

[1] Reibold et al., Nature 444,(2006) 286.

MM 20.33 Tue 14:45 Poster C

Development of an EAM potential for ruthenium — •Frank Römer and Thomas Kraska — Physical Chemistry, University Cologne, Luxemburger Str. 116, D-50939 Köln

The embedded atom method (EAM) is an effective potential model for metals that consists of a functional of the local electron density, being a multibody interaction, and a pairwise additive repulsion po-

tential for the atomic cores. In the context of the development of an EAM potential for the hcp metal ruthenium different concepts are investigated in detail. The ability to reproduce mechanical and caloric properties are analysed for various methods generating the different terms of the potential. Instead of fitting to experimental data, a new analytical expression for the screening function or the effective core charge, based on the electron distribution, is proposed. Because of the lack of knowledge about the effective electron configuration of ruthenium, which is also the case for several other transition metals, the influence of given electron configurations and the resulting electron distribution function on the physical properties is investigated. The properties included here are the stable structure, the lattice constants, and the cohesive energy. In this way the electron configuration can be determined from the associated preferred bulk structure. Vice versa the correlation between the devolution of the electron density and the difference in energetic stability of the two close-packing of spheres, hcp and fcc, are investigated.

MM 20.34 Tue 14:45 Poster C

Spatiotemporal stroboscopic interferometry on nanomechanical resonators — •Fabian Giesen[1,2], Miroslav Belov[3], Joseph Losby[1], Jennifer Moroz[1], Alastair Frasier[1], Graham McKinnon[3], Yuebin Ning[3], and Mark R. Freeman[3,4] — [1]Department of Physics, University of Alberta, Edmonton, Canada T6G 2G7 — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Str. 2A, 12489 Berlin — [3]Norcada Inc., 4465 - 99 street, Edmonton, Canada T6E 5B6 — [4]National Institute for Nanotechnology, Edmonton, Canada T6G 2M9

Despite the fundamental and application oriented interest of nanomechanical structures, the detection of their motion remains a challenge. We present spatiotemporal interferometric detection of the motion of microstructured cantilevers and doubly-clamped beams. This technique is capable of broadband detection with picosecond time resolution and micrometre spatial resolution. The actuation is achieved through fast voltage pulses triggered by a pump laser pulse. The subsequent motion is detected through the interferometric contrast of a probe laser spot reflected from the vibrating structure and the sustrate. We discuss the calibration of the interferometric contrast to obtain absolute values of the vibration of our silicon based nanostructures. We also demonstrate the capability of imaging the out-of-plane flexural modes of our cantilevers. Our work was supported by iCore, CIAR, and NSERC

MM 20.35 Tue 14:45 Poster C

Aspects of the electrical resistance of hydrogen loaded Pd thin films — •Stefan Wagner and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37073 Göttingen

While the knowledge on the electrical resistance response of bulk Pd due to hydrogen loading is well established in literature, little is known on the response of Pd thin films. In the present contribution first results of systematic studies on sputtered Pd films in the thickness range from 10 to 200 nm will be presented. Hysteretic effects and hydrogen-content dependent response times of the resistance propagation have been observed, that will be discussed in terms of kinetic and structural aspects of the Pd-H system. The electrical resistance turns out to be an easily operated measure for the determination of the phase boundaries of the Pd-H system.

MM 20.36 Tue 14:45 Poster C

Hydrogen in epitaxial V-8at%Fe films on Al2O3 substrate — •Ryota Gemma, Talaat Al-Kassab, Reiner Kirchheim, and Astrid Pudnt — Institut fuer Materialphysik, Goettingen, Germany

In this study, P-C-T properties and hydrogen-induced stresses of V-8at%Fe 100nm thick films with different microstructures and different initial strain conditions were investigated by measuring electromotive force (EMF) and in-plane stress simultaneously. The phase boundaries for the solid solution cH,α and the hydride cH,β were determined. The local chemistry of the hydride (deuteride) was investigated by performing tomographic atom probe analysis (TAP). The phase boundaries were found to be microstructure dependent: The α-phase solubility limit cH,α=0.1 H/V and cH,β= 0.45 H/V for films with small domain size, and cH, α=0.1 H/V and cH,β= 0.6 H/V for films with large domain size. The total in-plane compressive stress was smaller in small-domain samples compared to larger-domain samples. It was shown that the measured slope of P-C isotherm depends on initial stress condition and the microstructure. TAP analysis at 22K detected a plate-like deuteride VD0.65 at Pd/V interface. The concentration of this precipitate was in accordance with the expectations.

MM 20.37 Tue 14:45 Poster C

Preparation and optical characterisation of rare earth hydride films — •Helge Schröter, Stefan Weber, and Joachim Schoenes — Inst. für Physik der Kondensierten Materie, Medelssohnstraße 3 38106 Braunschweig, Germany

It is well known that rare earth metals like yttrium or europium show a metal insulator transition, if they are exposed to a hydrogen atmosphere. Yttrium changes from a reflective metal to a very weakly transparent metal (YH2) and finally to a transparent insulator (YH3). Europium also undergoes a metal to insulator transition, in contrast to yttrium-hydride it additionally undergoes a transition from antiferromagnetism to ferromagnetism. For an understanding of the mechanism driving this metal-insulator transition, the precise measurement of the optical properties is mandatory. Therefore the change of the optical properties of the samples connected with the metal insulator transition, was examined by spectroscopic ellipsometry which allows a direct measurement of the dielectric function. Because of the reactivity of the pure rare earth metals it is difficult to grow stable films. We have used two methods to prepare hydride-films: (I) growth of in-situ hydrogenated films by pulsed laser deposition in a hydrogen atmosphere. By variation of the hydrogen pressure thereby, it is possible to grow layers with different hydrogen concentrations. (II) growth of pure rare earth metal films by molecular beam epitaxy and subsequent evaporation of a protective Pd cap-layer . These films have been hydrogenated ex-situ in an hydrogen-cell which is directly inserted into the ellipsometer.

MM 20.38 Tue 14:45 Poster C

Optical properties of neodymiumhydride from FIR to VUV — •Stefan Weber and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig

Many rare-earth metals show a metal to insulator transition when they are loaded with hydrogen. The dramatic changes in the optical and electronical properties are accompanied by a transition from an antiferromagnetic metal to a ferromagnetic semiconductor in the particular material system of neodymium.

Thin films of Nd have been grown onto different substrates by molecular beam epitaxy. They need a functional cap layer of Nb and Pd on top in order to allow hydrogen loading and to prevent the samples from corrosion in ambient air.

Temperature dependent transmission and reflection measurements have been performed with a FT-IR-spectrometer in the energy range of 5meV to 1eV. The structures in the spectra can unambiguously be assigned to hydrogen vibrations using the isotope effect which is a shift of the phonon frequencies by a factor of $\sqrt{2}$ by loading the samples with hydrogen or deuterium, respectively. The measurement of the optical properties of NdH_x is supplemented by UV/Vis-spectrometry which determines the optical band gap of the semiconductor. VUV ellipsometry in the energy range up to 10eV has been performed using synchrotron radiation at BESSY II which yields the pseudodielectric function. Simulating the thin film spectra with a multilayer model reveals the optical properties of NdH_x.

MM 20.39 Tue 14:45 Poster C

Electric field gradient and chemical bonding in intermetallic gallides — •Katrin Koch[1], Frank Haarmann[1], Klaus Koepernik[1,2], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW, Dresden, Germany

The understanding of the metallic bond is still a challenging task. Here, we investigate experimentally and theoretically two series of compounds: the hexagonal MGa_2 with M=Ca,Sr,Ba and the tetragonal MGa_4 with M=Na,Sr,Ba. Ga forms a planar network of 3-fold coordinated atoms in MGa_2. In MGa_4 a 3-dimensional network of 4- and 5-fold coordinated Ga atoms is formed. The different bonding situations in these compounds indicate a flexibility of Ga with respect to the chemical bonding. We present a study of the electrical field gradient (EFG) for the different Ga sites in these materials. The quadrupolar coupling constants were measured by NMR, and the EFG was calculated using a DFT band structure code (WIEN2k). In comparison, the results of our calculation allow a unique assignment of the different signals to specific Ga sites. In addition, the calculations reveal that the EFG is very sensitive to internal structural parameters. For the optimized Ga positions (with respect to the total energy) we find excellent agreement of the measured and calculated EFG values. The

large quadrupole coupling constants indicate clearly the covalent nature of the Ga bonds. Studying in detail the influence of the cations using the virtual crystal approximation we show that a simple point charge model can not be applied for this family of covalent metals.
The DFG SPP 1178 is acknowledged for financial support.

MM 20.40 Tue 14:45 Poster C

Paarkorrelationsspektroskopie an Festkörperoberflächen — •Robert Wallauer, Stefan Voss, Inka Lauter, Till Jahnke, Horst Schmidt-Böcking und Reinhard Dörner — Institut für Kernphysik, Frankfurt

Der Aufbau eines neuen Experimentes zum koinzidenten Nachweis zweier Elektronen emittiert durch ein Photon aus einer Festkörperoberfläche (Dopppelphotoemission DPE) soll hier präsentiert werden. Mit Hilfe dieser Technik gelang es der Gruppe Kirschner (Halle) mit grossen Erfolg die ersten Messungen an NaCl(100) und C60 durchzuführen und erstmals direkt die Elektron-Elektron Abstoßung sowie das Korrelationsloch sichtbar zu machen.

In unserer Gruppe wurde ein Paarkorrelationsspektrometer durch Mirko Hattass aufgebaut mit dem es erste erfolgreiche Messungen an Cu(100) gab. Ziel ist es nun die Technik auf Materialien mit stärkeren Korrelationseffekten, wie z.B. Supraleiter, zu übertragen und dabei hohe Impulsauflösung bei beiden Elektronen zu erreichen.

MM 20.41 Tue 14:45 Poster C

Optical investigations on $Fe_{1-x}Co_xSi$ single crystals using Raman spectroscopy under high pressure and far-infrared ellipsometry — •Ivan Jursic[1], Dirk Menzel[1], Pavlo Popovich[2], Alexander Boris[2], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelsohnstrasse 3, 38106 Braunschweig — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Single crystals of $Fe_{1-x}Co_xSi$ grown by the tri-arc Czochralski technique have been investigated using far-infrared spectroscopic ellipsometry. The band gap of the semiconductor FeSi, which is 33 meV at low temperatures, is filled with electrons when the temperature is increased. In the far-infrared range four infrared phonons can be identified. The full width of half maximum (FWHM) of these oscillators show different behaviour for the varying Co concentration. While for low Co content the FWHM of all phonons increases with rising temperature, for intermediate Co concentrations some of the peaks show a maxmimum in width as function of temperature. Also the oscillator strength has an unusual temperature dependence for certain phonons and concentrations. This striking behaviour is interpreted in terms of an electron–phonon interaction. The infrared data are compared to additional Raman investigations which have been performed with a diamond anvil pressure cell under high pressure.

MM 20.42 Tue 14:45 Poster C

Raman study of the semiconductor to metal phase transition in $Fe_{1-x}Co_xSi$ ($0 \leq x \leq 1$) — •Dirk Menzel[1], Ana Maria Racu[1], Thorsten Donig[1], Klaus Doll[2], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

A complete Raman spectroscopy study of $Fe_{1-x}Co_xSi$ with x between 0 and 1 is presented. All the 9 Raman active modes predicted by the factor group analysis are observed and assigned to the A, E and T symmetry species. A density functional calculation of the phonons in FeSi and in CoSi is consistent with the experimentally obtained frequencies of the Raman modes. When Co substitutes Fe in FeSi the most striking effect is a strong shift of the A-type mode of the transition element to a lower frequency. This shift is attributed to the different electronic surroundings of the vibrating atoms as follows: the interaction between the Co atoms is screened by the free electrons in the metallic compound CoSi in contrast to the semiconducting FeSi, leading to a decrease of the Raman mode frequency.

MM 20.43 Tue 14:45 Poster C

Post annealing effect on electrical transport properties and defect annealing of La 0.67 Ca 0.33 MnO 3 films grown on vicinal substrate — •Lan Yu[1,2], Hanns-Urich Habermeier[1], Pengxiang Zhang[1,2], and Jialin Shun[2] — [1]Max-Planck Institute for Solid State Research. Heisenberg str.1, 70569, Stuttgart,Germany — [2]Kunming University of Science and Technology,

La 0.67 Ca 0.33 MnO 3 thin films have been grown on 10°,15 *,20* vicinal cut LaAlO3 (100) substrates by PLD using identical growth conditions. The films have been subjected after characterization to a high temperature * high oxygen pressure annealing step. The films are characterized by transport measurements as well as dedicated X-ray analysis. As compared to as-grown films they showed drastic changes of the resistance- temperature curve , with enhancements of Tc from 257K to 291K and an obvious decreases of resistance. This effects are especially pronounced in films grown on 20 * miscut LAO. The as grown films show a systematic change of the resistivity and the peak temperature associated to the Curie temperature before annealing. The results are discussed with respect to the defect formation and other subsequent annealing arising from both, oxygen related as well as substrate-induced defects. Especially the role of the miscut angle and its relation to the defect formation will be highlighted and the role of oxygen reordering and strain relaxation upon annealing is discussed.

MM 20.44 Tue 14:45 Poster C

Wavefunction-based ab initio method for metals: applying the method of increments to magnesium — •Elena Voloshina and Beate Paulus — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Calculations based upon the incremental scheme [1], that is an expansion of the total correlation energy in terms of one-body, two-body, and higher contributions, have been performed on a variety of solids [2]. Metals require special treatment because of two distinct features. Since the conduction bands are only partially filled, we cannot construct well localized orbitals from them. Furthermore, we must deal properly with charge screening which obviously is a correlation effect. One would expect that the metallic solid should be well described within DFT. Indeed, it is possible usually to select a DFT-functional that will yield good agreement of experimental and calculated properties. At the same time, it is well known, that the present DFT-based approaches are not amenable to systematic improvements. A starting point for the treatment of the many-body correlation effects in solids is a reliable HF SCF result for the infinite system. For magnesium HF model, ignoring the correlations, gives rather good agreement with experiment of one lattice parameter (c), but incorrect value for c/a ratio because of too high lattice parameter a. Application of the method of increments allow us not only to improve the HF values, but also explain the reason for these changes.

[1] H. Stoll, Phys. Rev. B 46, 6700 (1992).
[2] B. Paulus, Phys. Rep. 428, 1 (2006).

MM 20.45 Tue 14:45 Poster C

Electron correlation in 3*d* metals calculated with FLEX — •Andreas Gierlich[1], Arno Schindlmayr[1], Václav Drchal[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Prague 8, Czech Republic

The standard approach to material calculations, the density-functional theory (DFT) in its local-density or generalized gradient approximation, incorperates electronic correlations only rudimentarily. Our goal was to better understand the effects of electron correlation on the materials' properties of 3*d* transition metals which fall into the regime of intermediate correlation strength. The FLEX (fluctuation exchange) method, a diagrammatic technique that incorporates a range of two-particle scattering processes, allows a more accurate characterization of the correlation effects via the dynamic self-energy. We perform *ab initio* DFT calculations using the full-potential linearized augmented-plane-wave method and subsequently apply FLEX in a perturbative manner to explicitly include two-particle correlation for electrons in the *d* band. The self-energy is determined within the framework of dynamic mean-field theory. We present results for ferromagnetic (Fe, Co, Ni), antiferromagnetic (Cr) as well as non-magnetic 3*d* transition metals and compare the contributions of the different scattering channels for these groups of materials.

MM 20.46 Tue 14:45 Poster C

The Enatom in Simple Metals and Its pressure Evolution — •Jens Kunstmann[1], Lilia Boeri[1], and Warren Pickett[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Department of Physics, University of California Davis, Davis, California, 95616, USA

We present the first realization of the generalized pseudoatom concept introduced by Ball, and adopt the name enatom to minimize confusion. This enatom, which consists of a unique decomposition of the

total charge density (or potential) of any solid into a sum of overlapping atomic-like contributions that move rigidly with the nuclei to first order, is calculated using (numerical) linear response methods, and is analyzed for both fcc Li and Al at pressures of 0, 35, and 50 GPa. These two simple fcc metals (Li is fcc and a good superconductor in the 20-40 GPa range) show different physical behaviors under pressure, which reflects the increasing covalency in Li and the lack of it in Al. The non-rigid (deformation) parts of the enatom charge and potential have opposite signs in Li and Al; it becomes larger under pressure only in Li. These preliminary results show that the enatom construction could be used to obtain a real-space understanding of the vibrational properties and electron-phonon interaction in solids.

MM 20.47 Tue 14:45 Poster C

The *GW* approximation in semi-infinite scattering setups — •Swantje Heers, Arno Schindlmayr, Daniel Wortmann, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

A proper description of electronic transport in nanoscale junctions must consider infinite systems without periodic boundary conditions. In addition, it is often desirable to include explicit electronic correlation, but the geometric setup makes the calculation of the electronic self-energy in the *GW* approximation much more complicated than for finite or periodic systems. We present an application of the *GW* approximation to a non-periodic model system with a simple one-dimensional scattering potential. The initial Green function is calculated with the embedding method in a finite region containing the scattering potential. The semi-infinite leads are taken into account by so-called embedding potentials. This Green function is the starting point for the *GW* approximation which requires solving Hedin's equations for the polarisation function, the dielectric function, the screened Coulomb interaction and the self-energy.

MM 20.48 Tue 14:45 Poster C

DFT-Investigations of Vanadium Silicides — •Mike Thieme and Sibylle Gemming — Forschungszentrum Dresden-Rossendorf, POB 51 01 19, 01314 Dresden, Germany

Vanadium and silicon form several binary compounds; the most well characterized structures have the compositions V:Si= 3:1, 6:5, 5:3, 1:2. Density-functional band-structure calculations with a plane-wave basis for the valence electrons and norm-conserving pseudopotentials for the core-valence interaction have been carried out to investigate the structural properties and the phase stability for the experimentally known binary crystals. As the early transition metal silicides belong to the class of refractory materials, also the elastic properties were determined. It is furthermore shown that the electronic properties of the compounds depend strongly on the composition.

MM 20.49 Tue 14:45 Poster C

^{119}Sn Mössbauer Spectroscopy of tin containing float glass — •Verena Jung[1], Ksenofontov Vadim[1], Claudia Felser[1], Maria Luisa Aigner[2], Thomas Pfeiffer[2], and Dirk Sprenger[2] — [1]Johannes Gutenberg - Universität, 55099 Mainz, Germany — [2]Schott AG, 55122 Mainz, Germany

According to the production process of float glasses tin is used as a common refining agent. Since the surface quality of the glass strongly depends on the local distribution of Sn-redox states, the influence of process parameters on Sn^{2+}/Sn^{4+} ratios and the assignment to their structural role in the glass network is extremely helpful. Therefore, glass compositions based on SiO_2-Al_2O_3-B_2O_3-CaO-SnO_2 were molten with additions of 0,1, 0,3 and 0,5 wt% SnO_2. All samples were tempered for 7 days at 1400^{o}C in N_2 and N_2-air mixtures with controlled p_{O2}-values of 10^{-2} and 10^{-5} bar, respectively. Hyperfine parameters for the tin nucleus in different structural units and their oxidation states were calculated from ^{119}Sn Mössbauer spectra, using theoretical simulations of electron densities and electric field gradients with the Wien2k software. Finally, the thermochemical impact of oxygen on the structure of Sn-bearing glasses is discussed.

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A phase-field model to Investigate heterogeneous nucleation in peritectic materials — •Ricardo S. Siquieri[1] and Heike Emmerich[2] — [1]siquieri@ghi.rwth-aachen.de — [2]emmerich@ghi.rwth-aachen.de

Here we propose a phase-field approach to investigate the influence of convection on peritectic growth as well as the heterogeneous nucleation kinetics of peritectic systems. For this purpose we derive a phase-field model for peritectic growth taking into account fluid flow in the melt, which is convergent to the underlying sharp interface problem in the thin interface limit. Moreover, we employ our new phase-field model to study the heterogeneous nucleation kinetics of peritectic material systems. Our approach is based on a similar approach towards homogeneous nucleation in (Phys. Rev. Let. **88** 20 (2002)). We applied our model successfully to extend the nucleation rate predicted by classical nucleation theory for an additional morphological term relevant for peritectic growth. Further applications to understand the mechanisms and consequences of heterogeneous nucleation kinetics in more detail are discussed.

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Calculation of transport coefficients from ab-initio methods — •Laurent Chaput[1,2], Pierre Pecheur[1], and Hubert Scherrer[1] — [1]Laboratoire de Physique des Matériaux, Nancy, France — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

A module to calculate transport properties of thermoelectric materials has been implemented. The system response is described within the framework of Boltzmann transport theory and the electronic structure of the system is taken as the one of Kohn-Sham electrons. This way we obtain the Onsager coefficients from which the thermoelectric tensor, the Hall tensor and the Lorenz coefficient are calculated. These quantities depend crucially on electron velocities. These are calculated using the spectral differentiation method. Therefore we obtain a very high accuracy while keeping the time-cost of the method relatively low. The other advantage of this method is that it is independent of the basis used for the electronic structure calculation. The module can therefore be used with a variety of methods. In this contribution we consider the peculiar dependence with respect to temperature of the thermoelectric power of the MAX phase Ti_3SiC_2 . It has been reported to be essentially zero. The calculation of the thermoelectric tensor show that this come from a compensation between the components of the thermoelectric tensor. They are positive in the basal plane and negative along the z axis. We also derive a sum rule for the relaxation time. This simplify the calculation of the Hall tensor.

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Tailoring phase change materials: Stoichiometrical trends in the Ge-Sb-Te system — •Michael Klein, Daniel Wamwangi, and Matthias Wuttig — I. Physikalisches Institut 1A, RWTH Aachen, 52056 Aachen, Germany

Phase change materials are widely used as the active layer in rewritable optical media. This layer can be reversibly switched with a laser beam between an amorphous and crystalline state. As there is a pronounced optical contrast between these two phases, this provides the possibility to write, read and erase data. The speed of this method is limited by the speed of crystallization, as crystallization is the slower process. One possibility to make this process faster is to change the composition of this active layer. Thus it is very interesting to investigate how the process of crystallization is affected by a variation of stoichiometry. Although phase change materials technology is already used, there is little knowledge of the phase change process itself. Today the usability of phase change materials is still identified by try and error methods. We will show stoichiometrical trends of different properties relevant for data storage, e.g. the crystallisation temperature, which governs the room temperature stability of the amorphous phase and thus is a measure for the data retention time.

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Photoinduced ultrafast volume changes in intermediate valence solids — •momar diakhate and martin garcia — Theoretishe, physik,Universitat Kassel,D-34132 Kassel, Germany

We present a theoretical model for the description of the ultrafast structural response of intermediate valence solids to femtosecond laser excitation. Based on the promotional Ramirez-Falicov model we consider the femtosecond laser heating of gamma-Cerium and the subsequent ultrafast lattice expansion dynamics.

In particular we determine the thermodynamic and electronic properties of cerium at very high electronic temperatures (simulating the laser excitation). The possibility for a non-equilibrium photoinduced inverse volume collapse transition is discussed. The p-v-T equation of state is obtained from the Helmoltz free energy in the usual way of thermodynamic derivatives by considering an adiabatic expansion of the crystal at high temperature. We take into account both the laser excited and the unexcited parts of the system, in oder to account for

inertial confinement.

By means of the Hugoniot theory the shock velocity variation in the surrounding (unheated) part of the sample was obtained and used to calculate the time dependence of the thermodynamic properties in the heated material.

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Microstructure Characterization of Cu2MnAl Heusler-Type Alloys using SEM-EBSD and TEM — Tien Hung Luu[1,3], Huy Dan Nguyen[2], Vong Vo[2], •Steffen Schulze[3], and Michael Hietschold[3] — [1]Department of Physics, Vinh University, Nghean, Vietnam — [2]Institute of Materials Science, VAST, Hanoi, Vietnam — [3]Institute of Physics, TU Chemnitz, Chemnitz, Germany

Cu2MnAl heusler-type alloys prepared by the melt-spinning show soft magnetic behavior with a coercivity less than 1.6 kA/m and a Curie temperature as high as 600 K and after annealing a large negative magnetoresistance of more than 4%. In this work, we report microstructure investigations of these Cu2MnAl heusler alloys as-quenched and after annealing at 773 K for 24 hours using Electron Backscattered Diffraction (EBSD), Energy Dispersive X-ray Analysis (EDX), Selected Area Electron Diffraction (SAED) and High Resolution Transmission Electron Microscopy (HRTEM). The results show that the as-quenched sample is composed of Cu2MnAl in the fcc structure L21 only. These crystallites are of extremely elongated shape with sizes ranging between 1 to 3um in width and 5 to 15 um in length. After annealing we found two crystalline phases. The predominating one is still of L21 structure with grain sizes from 2 to 7 um but there is a Mn-rich phase too appearing in a wide variety of grain sizes. Some of them range between 10 and 20 nm and others are as big as 1 um in diameter. The appearance of these crystalline phases in the ribbons take essential effect on the magnetic and magnetoresistance properties.

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Towards a combination of an electrical conductor with a thermal insulator — Ana Smontara[1], Igor Smiljanić[1], •Ante Bilušić[1,2], Benjamin Grushko[3], Sergiy Balanetskyy[3], Zvonko Jagličić[4], Stanislav Vrtnik[5], and Janez Dolinšek[5] — [1]Institute of Physics, Zagreb, Croatia — [2]Faculty of Science, Univ. of Split, Croatia — [3]Forschungszentrum Jülich, Germany — [4]Institute J. Stefan, Ljubljana, Slovenia — [5]Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

ϵ-phases in the Al-Pd-(Mn,Fe,Co,Rh, ...) alloys are complex intermetallics characterized by giant unit cells with quasicrystals-like cluster substructure. To see how the coexistence of two competing physical length scales affect their physical properties, we studied the magnetic, electrical, thermal transport and thermoelectric properties of the ϵ-Al-Pd-Fe, ϵ-Al-Pd-Co and ϵ-Al-Pd-Rh. Magnetic measurements reveal that the materials are diamagnetic, containing tiny fractions of magnetic transition-metal atoms (10-100 ppm). Electrical resistivity shows weak temperature dependence for $T = 4 - 300$ K. The thermal conductivity is low, comparable to that of thermal insulators amorphous SiO_2 and Zr/YO_2 ceramics at room temperature. While SiO_2 and Zr/YO_2 are also electrical insulators, ϵ-phases exhibit electrical conductivity typical of metallic alloys, so we deal with a combination of an electrical conductor with a thermal insulator. The thermoelectric power of the investigated ϵ-phase families is small, so that these materials do not appear promising candidates for the thermoelectric application. This work was done within the FP6 EU NoE "Complex Metallic Alloys".