

MM 34: Poster Session

Time: Tuesday 18:00–20:00

Location: P4

MM 34.1 Tue 18:00 P4

Simulation of abnormal grain growth in nanocrystalline materials — ●MINGYAN WANG¹, JULES DAKE¹, RAINER BIRRINGER², and CARL KRILL¹ — ¹Institute of Micro and Nanomaterials, Ulm University, Germany — ²FR 7.3 Technical Physics, University of the Saarland, Germany

Despite the rarity suggested by its name, abnormal grain growth (AGG) appears to be a common mode of coarsening in nanocrystalline specimens, observed in a wide variety of materials prepared by a range of synthesis routes. During AGG, a subpopulation of grains manifests rapid growth, leading to grain volumes that are not only much larger than those of their neighbors, but also sometimes highly irregular in shape. The latter observation suggests that, in certain cases, AGG might proceed by a kind of percolation phenomenon occurring on a “grid” defined by the initial ensemble of grains. We have investigated this possibility by extending a conventional phase field algorithm for simulating grain growth to include selection rules for percolation. The resulting simulated abnormal grains are strikingly similar in shape to their experimental counterparts. By quantifying the comparison between simulation and experiment, we hope to shed light on at least one of the underlying physical mechanisms for AGG in nanocrystalline materials.

MM 34.2 Tue 18:00 P4

Grain boundary enthalpy changes by mechanical deformation of nanocrystalline alloys — ●MICHAEL DECKARM¹, JONATHAN SCHÄFER², PATRIC GRUBER³, KARSTEN ALBE², and RAINER BIRRINGER¹ — ¹Universität des Saarlandes, FR 7.2 Experimentalphysik, 66123 Saarbrücken — ²Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, 64281 Darmstadt — ³Karlsruher Institut für Technologie, Institut für Angewandte Materialien, 76344 Eggenstein-Leopoldshafen

In as-prepared nanocrystalline (nc) alloys, grain boundaries (gb) are usually in unknown local non-equilibrium configurations, reflecting the preparation history. However, a thermally activated recovery process below the onset temperature of grain growth permits a local equilibration of the gb and thus providing a well defined reference state. Starting from this reference state we deformed nc (alloy) samples by uni-axial compression and investigated the change of gb enthalpy as a function of plastic strain by calorimetry. The experimental findings are in large parts in excellent agreement with the results of a hybrid MD/MC simulation method for the same material. Surprisingly, annealing leads to significantly increased yield stresses and narrowing of the microplastic regime in uniaxial compression tests. Obviously, the configurational state of the gb seems to significantly influence the overall mechanical behaviour of nc metals at the low end of the nanoscale.

MM 34.3 Tue 18:00 P4

Optimization of a Nanocalorimeter inside an SEM — ●EMANUEL FRANKE¹, CYNTHIA A. VOLKERT¹, FENG YI², and DAVID A. LAVAN² — ¹Institut für Materialphysik, Georg-August-University, Göttingen, 37077 Göttingen — ²Materials Measurement Science Division, Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, USA 20899

As sample length scales reach down to nanometers and the surface to volume ratio becomes large, the thermal properties of materials are changed. The involved energy in such size induced changes is often only a few nano-Joules and cannot be measured by conventional calorimetry which has too low sensitivity. MEMS-based nanocalorimeters with sufficient resolution to measure with nJ resolution have been developed in the last two decades. We present several proof-of-concept experiments using a MEMS based differential calorimeter which has been installed in a field emission SEM. The SEM allows careful observation of the experimental conditions and of any changes in the sample microstructure due to thermal cycling. Enthalpy change can be measured from room temperature up to 1000 K by applying heating rates from 10⁴ K/s to 10⁵ K/s. Sensitivity better than 1 nJ/K for reversible and 10 nJ/K for irreversible processes can be achieved. The limits of the measurement method are explored by studying dewetting and oxidation of copper films and melting of bismuth nanoparticles.

MM 34.4 Tue 18:00 P4

Spatial and orientational tracking of Ostwald ripening in semisolid Al-Cu by 3DXRD microscopy — ●JAMES C. SHATTO¹, JULES DAKE¹, THOMAS WERZ¹, JETTE ODDERSHEDE², HENNING SØRENSEN³, SØREN SCHMIDT², and CARL KRILL¹ — ¹Inst. of Micro and Nanomaterials, Ulm University, Germany — ²Dept. of Physics, Technical University of Denmark — ³Dept. of Chemistry, University of Copenhagen, Denmark

Coarsening, a phenomenon that occurs whenever a polycrystalline material is subjected to thermal processing, has long been a favorite topic of materials scientists. Examples include grain growth (in single-phase samples) and Ostwald ripening (in multiphase materials). Using the relatively new technique of Three-Dimensional X-Ray Diffraction (3DXRD) microscopy, we have investigated the coarsening-induced growth/shrinkage of solid, Al-rich particles embedded in a liquid matrix (of higher Cu content). The measurement technique reveals not only the spatial extent of each crystalline particle but also its lattice orientation at discrete time steps. From this information we can study the migration rates of individual particle boundaries as a function of relative lattice misorientation across the boundary. Such data may yield the first experimental differentiation between the conventional mechanism for Ostwald ripening (atomic diffusion through the second phase) and particle growth via coalescence or diffusion of atoms across single-phase interfaces.

MM 34.5 Tue 18:00 P4

Cooling rate dependent short and medium range order of a CuZrAl glass analyzed by comparing XRD data and MD simulations — ●HELMUT HERMANN¹, VALENTIN KOKOTIN², UTA KÜHN¹, BJÖRN SCHWARZ³, IVAN KABAN⁴, and HORST WENDROCK¹ — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden — ²ThyssenKrupp Steel Europe AG, Kaiser-Wilhelm-Str. 100, 47166 Duisburg — ³Karlsruhe Inst. of Technology, IAM-ESS, Hermann-von Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen — ⁴TU Dresden, Inst. für Werkstoffwissenschaft, 01062 Dresden

The preparation of a CuZrAl glass is simulated at different cooling rates by means of molecular dynamics (MD). The atomic order is studied using generalized Voronoi tessellation. It appears that the fraction of icosahedral Voronoi cells increases with decreasing cooling rate. These differences are visible in changes of the X-ray scattering intensities of the simulated samples. Parallel to the simulations, samples with the same composition are prepared experimentally under different cooling rates which are realized by means of rapid quenching and mould casting techniques, respectively. Synchrotron radiation is used to measure the diffraction curves of the samples. The experimental X-ray scattering curves for the samples obtained at different cooling rates show the same features as the curves calculated from the samples generated by MD simulation at different cooling rates. This confirms the simulation results.

MM 34.6 Tue 18:00 P4

Visualization of scattering properties by Neutron Grating Interferometry — ●BENEDIKT BETZ¹, EBERHARD LEHMAN¹, RUDOLF SCHAEFER^{2,3}, PETER RAUSCHER³, and CHRISTIAN GRUENZWEIG¹ — ¹SINQ, Paul Scherrer Institut, Villigen, Switzerland — ²IFW, Dresden, Germany — ³Technische Universität Dresden, Dresden, Germany

The neutron Grating Interferometer (nGI) is a standard user instrument at the ICON beamline at SINQ at PSI. The setup is able to deliver simultaneously information about the attenuation, phase shift [1] and scattering properties in the so called dark-field image (DFI) [2] of a sample. Due to the interaction of neutrons with the nucleus only, they are able to penetrate deeper into matter, in particular heavier materials, than X-rays do. A further advantage of neutrons compared to X-rays is the interaction of the neutrons* magnetic moment with magnetic structures, that allows for the investigation of magnetic domain structures using the nGI technique [3]. In the forseen talk, the nGI-setup and its technique for imaging with cold neutrons will be explained. In the forseen talk, the nGI-setup and its technique for imaging with cold neutrons will be explained. Furthermore examples for the investigation of magnetic structures in Grain-oriented and non-oriented steel laminations (FeSi) will be presented. [1]:F. Pfeiffer et al. Neutron phase imaging and tomography, Phys. Rev. Lett. 96, 215505,

(2006)[2]:C.Grünzweig et al. Neutron Decoherence Imaging for Visualizing Bulk Magnetic Domain Structures. Phys. Rev. Lett. 101, 025504 (2008) [3]:C.Grünzweig et al. Bulk magnetic domain structures visualized by neutron dark-field imaging. Appl. Phys. Lett. 93, 112504(2008)

MM 34.7 Tue 18:00 P4

Influence of different loading stresses to duplex steel in the VHCF regime — ●ANNE HÜSECKEN¹, MARCUS SÖKER², KONSTANTIN ISTOMIN¹, BENJAMIN DÖNGES¹, and ULLRICH PIETSCH¹ — ¹Universität Siegen — ²Hochschule Osnabrück

Damage mechanisms in the VHCF regime are still not sufficiently understood. Experiments on austenitic-ferritic duplex steels up to 10⁹ cycles have revealed that elastic anisotropy causes stress concentrations at grain and phase boundaries leading to slip band emanation preferentially in the fcc austenite phase [1]. Slip bands raise locally the residual stress level in the neighbouring bcc ferrite grains. So, crack initiation along pronounced slip bands and grain/phase boundaries were observed [1,2]. There is a need to analyse the development of dislocations and their formation to slip bands within the grains in order to correlate the observed microstructure with relevant damage mechanisms. We present a new way of fatigue analysis measuring the change of shape of selected austenite and ferrite X-ray Bragg reflections for single grains as function of the number of VHCF cycles and different loading stresses in-situ. It was explored that selected austenite reflections show an increasing peak splitting as function of load cycles whereas ferrite reflection kept nearly unchanged. This finding can be attributed to the formation of stress induced dislocations bunches in austenite grains which may acts as nuclei for crack formation in neighbored ferrite grains [3]. [1] U. Krupp: Fatigue Crack Propagation in Metals and Alloys (Wiley, 2007). [2] H. Knobbe et al, J. Phys.: Conf. Ser. 240 (2010) 012061 [3] K.Istomin et .al. Fatigue, submitted 2013

MM 34.8 Tue 18:00 P4

Simulation of Grazing-Incidence Small-Angle Scattering on Cu nano-size clusters — CELINE DURNIK¹, ●MARINA GANEVA¹, CHRISTIANE A. HELM², RAINER HIPPLER², OXANA IVANOVA¹, GENNADY POSPELOV¹, WALTER VAN HERCK¹, and JOACHIM WUTTKE¹ — ¹Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — ²Institut für Physik, Universität Greifswald, Greifswald, Germany

Grazing-incidence small-angle scattering (GISAS) is increasingly used to investigate the structural properties of thin films, layered materials, deposited nanoparticles and many others. To prepare a successful experiment and to analyze the measured data, appropriate simulations are required.

BornAgain [1] is a multi-platform open-source project that aims at supporting scientists in the analysis and fitting of their GISAS data, both for synchrotron (GISAXS) and neutron (GISANS) facilities. It is provided with a sample model and an instrument model accounting for the resolution effects, and simulates the scattering process using the distorted-wave Born approximation (DWBA).

Here we show GISAXS and GISANS images simulated using BornAgain. The influence of the sample properties and experimental parameters on the scattering pattern is discussed. Cu clusters, produced using a DC magnetron-based gas aggregation source and deposited to a Si substrate, are taken as a case study.

[1] <http://apps.jcms.fz-juelich.de/doku/sc/bornagain:start>

MM 34.9 Tue 18:00 P4

Heterogeneous shear elasticity of glasses: Instability, anharmonicity and fractional-power scaling — ●WALTER SCHIRMACHER^{1,2}, ALESSIA MARRUZZO^{2,3}, ANDREA FRATALOCCHI³, GIANCARLO RUOCCO², and TULLIO SCOPIGNO² — ¹Institut für Physik, Universität Mainz, Germany — ²Dipt. of Fisica, Universit'a "La Sapienza", Italy — ³Faculty of Electr. Eng., Applied Mathematics and Computational Science, King Abdullah University of Science and Technology, Saudi Arabia

Dynamical heterogeneity is the hallmark of glassy dynamics both on the liquid and on the solid side of the glass transition. On the solid side elastic heterogeneity causes a wealth of anomalous vibrational phenomena such as an enhancement of the vibrational spectrum over the Debye expectation ("boson peak") and anomalous sound dispersion and attenuation. Above the boson peak frequency region the anomalies are entirely due to harmonic degrees of freedom and are caused by the disorder-induced breakdown of translational invariance. Below this region - as we report here by comparing experimental sound atten-

uation data with simulations on a soft-sphere glass and an appropriate theory - there develops a dynamical scaling scenario caused by the combined action of disorder, local instability and anharmonicity.

MM 34.10 Tue 18:00 P4

Showdown! Comparing phase field simulations to time-resolved x-ray tomography measurements of Ostwald ripening in 3D — THOMAS WERZ¹, NAN WANG², MICHAEL HEINZE³, STEFAN ODENBACH³, LONG-QING CHEN², and ●CARL KRILL¹ — ¹Inst. of Micro and Nanomaterials, Ulm University, Germany — ²Dept. of Materials Science and Engineering, The Pennsylvania State University, USA — ³Inst. of Fluid Mechanics, TU Dresden, Germany

It's not only moviegoers whose imagination has been captured by the 3D revolution in imaging technology—even materials scientists have been swept up in the hype. Their excitement is understandable, given the power of techniques like x-ray microtomography to map out microstructural evolution with high spatial and temporal resolution. However, not everyone believes that the resulting 3D "movies" are worthy of Oscar consideration: after all, computational materials scientists have generated thousands of 3D simulations without winning a single Academy Award! Perhaps voters are still waiting for the computational algorithms to be validated against experiment. We have addressed the latter issue by investigating Ostwald ripening in the model system Al-5 wt% Cu, using x-ray microtomography to obtain real-time 3D image sequences of particle growth and shrinkage. We then employed a phase-field model to simulate coarsening in the same sample region, starting from the measured initial configuration. The stage is now set for a showdown in 4D (3 spatial dimensions + time) between experiment and computer simulation. The results could decide once and for all whether theorists can lay claim to simulating reality!

MM 34.11 Tue 18:00 P4

The Grain Mapper at the High Energy Beamline HEMS — ●TORBEN FISCHER, LARS LOTTERMOSER, SVEN KLEEBAND, NORBERT SCHELL, MARTIN MÜLLER, and ANDREAS SCHREYER — Helmholtz-Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht, Germany

The 3D investigation of polycrystalline materials allows the study of the relationship between macroscopic and micro structural properties at the level of single grains. A main objective is the measurement of the 3D strain state between single grains. The High Energy Materials Science Beamline (HEMS), operated by the Helmholtz-Zentrum Geesthacht (HZG), has a dedicated hutch for such 3D techniques. HEMS is situated at the high brilliance synchrotron storage ring PETRA III at DESY in Hamburg and has a tuneable energy range between 30 and 200 keV. Fast detector systems and high photon flux allow for highly dynamic investigations, e.g. of phase transformation or catalysis. The X-ray beam can be focused down to micrometre size with compound refractive lenses (CRLs). The grain mapper is an optimized endstation for the 3D-XRD technique. The grain mapper consists of a solid granite substructure, a high precision rotation stage and portals for far- and near-field detectors. The instrument has finished commissioning phase and first results will be presented. The main scientific topics addressed are the investigation of new joining and machining processes, metallurgy, chemistry and material physics.

MM 34.12 Tue 18:00 P4

Ordered Mesoporous Thin Films; Elastic Modulus Determination by Humidity Driven Pore Lattice Deformation — ●PARVIN SHARIFI¹, BENEDETTA MARMIROLI², BARBARA SARTORI², FERNANDO CACHO-NERIN^{2,3}, HIENZ AMENITSCH², CHRISTIAN GANSER¹, CHRISTIAN TEICHERT¹, and OSKAR PARIS¹ — ¹Institut für Physik, Montanuniversität Leoben (Franz-Josef Strasse 18, 8700 Leoben, Austria) — ²Institute of Inorganic Chemistry, TU Graz (Stremayrgasse 9/IV, 8042 Graz, Austria) — ³Current address: Beamline I14, Diamond Light Source, Harwell Science and Innovation Campus, OX11 0DE Didcot (Oxfordshire), UK

Adsorption induced deformation of mesoporous powders and thin films can provide valuable information about their mechanical properties. Two types of mesoporous thin films were prepared by dip- and spin-coating on silicon substrates using a sol made of TEOS and triblock copolymer (P123) in acidic solution followed by calcination at 400°C. GISAXS measurements revealed ordered mesoporous films with 2D hexagonal structure with a macroscopic alignment of the pore axis within the plane of the substrate. The pore-lattice deformation due to adsorption of water was determined by in-situ GISAXS in a relative humidity range of RH=5% to RH=95%. Both films showed a

reversible out-of-plane contraction due to the condensation of water in the pores. Pore lattice strain vs RH, called strain isotherms, were used to determine the *pore load modulus* of the films. The results showed clear differences between the two types of samples.

MM 34.13 Tue 18:00 P4

In-situ tomography on the magnetostructural transition of La(Fe,Si)13 — ●ANJA WASKE¹, BRUNO WEISE^{1,6}, KONSTANTIN SKOKOV², STEFAN SCHMIEDERER^{3,4}, ALEXANDER RACK³, WOLFGANG LUDWIG⁵, OLIVER GUTFLEISCH², and JÜRGEN ECKERT^{1,6} — ¹IFW Dresden, Institute for Complex Materials, Dresden, Germany, — ²TU Darmstadt, Department of Materials Science, Darmstadt, Germany, — ³European Synchrotron Radiation Facility, Grenoble, France, — ⁴University of Manchester, X-ray Imaging Facility, School of Materials, UK, — ⁵GEMPPM-MATEIS, INSA de Lyon, Lyon, France, — ⁶Institute of Materials Science, Dresden University of Technology, 01062 Dresden, Germany

Magnetocaloric material of the composition La(Fe,Si)13 shows a magnetostructural transition connected to a volume expansion of up to 1.5%, which can be induced either by applying a magnetic field or by lowering the temperature below the material's Curie temperature. We conducted a temperature dependent study of this magnetostructural transition to study how the nucleation of the low-temperature state proceeds in the sample as the temperature is lowered. Powderized and bulk samples were compared to study the influence of the neighbouring particles and the constraints those present for other particles (or grains) to transform.

MM 34.14 Tue 18:00 P4

Combined X-ray/Neutron reflectometer NREX - advanced tool for studying surfaces films and heterostructures — ●OLAF SOLTWEDEL, YURY KHAYDUKOV, THOMAS KELLER, FRANZ TRALMER, MANFRED OHL, and BERNHARD KEIMER — MPI für Festkörperforschung, Heisenbergstraße 1, 70569, Stuttgart

This presentation will introduce neutron reflectometry, a unique tool to investigate properties of thin films like chemical composition, interdiffusion, magnetic depth profiling etc. in buried films and dedicated sample environments on nanometre scale. Besides few theoretical aspects scientific applications ranging from polymer films at the solid/liquid interfaces over chemical depth profiling in amorphous hydrogenated carbon to magnetic thin films are presented. Finally, the realisation of a combined x-ray and neutron reflectometer will be shown in details. Here at the NREX reflectometer (FRM2, Garching, Germany) a conventional X-ray (Cu-K α : $\lambda = 1.541\text{\AA}$) add on offers the unique possibility to combine X-ray and neutron reflectometry in-situ.

MM 34.15 Tue 18:00 P4

In-situ high energy x-ray diffraction studies on the phase evolution during decomposition of arc evaporated (Ti,-Cr,-Al)N coatings — ●DANIEL M. OSTACH¹, NORBERT SCHELL¹, ANDREAS SCHREYER¹, JENS BIRCH², JEREMY SCHROEDER², LINA ROGSTRÖM³, MATTS P. JOHANSSON-JÖEASAR⁴, and RACHID M'SAOUBI⁴ — ¹Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Max-Planck-Straße 1, 21502 Geesthacht — ²Thin film physics, IFM, Linköping University, 581 83 Linköping, Sweden — ³Nanostructured materials, IFM, Linköping University, 581 83 Linköping, Sweden — ⁴SECO Tools AB, Fagersta, Sweden

Hard and wear resistant cubic (c)-(Ti,Al)N based coatings are widely used in industrial applications, as in the case of coated metal cutting tools. During cutting, the coated tool is exposed to high temperatures and large forces. c-(Ti,Al)N decompose in two stages under such conditions; first a spinodal decomposition into coherent c-TiN and c-AlN rich domains followed by a second stage where c-AlN transforms to hexagonal (h)-AlN. Alloying of Cr in (Ti,Al)N coatings provide an additional decomposition route through the formation of intermediate c-(Al,Cr)N and c-(Ti,Cr)N ternary phases prior to the final stage when h-AlN and c-(Ti,Cr)N are formed. In effect, Cr in (Ti,Al)N has shown to delay the detrimental effect of h-AlN on the coating's hardness. In this study, in-situ high-energy synchrotron x-ray diffraction studies during annealing have been performed to study the phase evolution during decomposition of (Ti,Al,Cr)N coatings.

MM 34.16 Tue 18:00 P4

Development and integration of an intelligent detector for grating based phase-contrast tomography — ●PAVEL LYTAEV¹, FELIX BECKMANN¹, JULIA HERZEN¹, ALEXANDER HIPPI¹, STEPHAN MEYER-LOGES¹, JOERN PLEWKA¹, ANDREAS KOPMANN²,

MICHELE CASELLE², and ANDREAS SCHREYER¹ — ¹Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Karlsruhe Institute of Technology, Karlsruhe, Germany

Helmholtz-Zentrum Geesthacht (HZG) is operating the microtomography stations using synchrotron radiation at DESY, Hamburg. Absorption contrast and phase contrast techniques were developed and applied to samples in the fields of medicine, biology, and materials science. The present work is devoted to the development of an intelligent detector with high-speed data capturing for experiments for grating based phase-contrast imaging. The detector is based on the Ultrafast streaming camera platform developed at the Karlsruhe Institute of Technology (KIT). Characterization (in terms of photon transfer curve) of some different cameras, such as CMOS and CCD, is presented. These characteristics are required to optimize the operation of the detector according to the one or to the other requirements of processing speed and image quality in the course of phase-contrast imaging process. The detector will be optimized to its implementation at the microtomography setups installed at the beamlines IBL and HEMS of the high brilliant third-generation synchrotron light source PETRA III.

MM 34.17 Tue 18:00 P4

Band gap measurement of SiC nanowires by Valence EELS — ●ANJA BONATTO MINELLA^{1,2}, DARIUS POHL¹, CHRISTINE TÄSCHNER¹, ROLF ERNI³, LUDWIG SCHULTZ^{1,2}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Dresden, Germany — ²TU Dresden, Dresden, Germany — ³Electron Microscopy Center, Empa, Dübendorf, Switzerland

Silicon carbide (SiC) nanowires (NW) of different polytypes have been prepared by Plasma-Enhanced Chemical Vapour Deposition. Their formation proceeds simultaneously with the growth of carbon nanofibres (CNF) leading to a heterostructure of SiC-filled CNF. In order to study the band gap of the SiC the graphitic layers of the CNF have to be removed by a heat treatment in oxygen atmosphere.

The (direct) band gap measurement is carried out using Valence Electron Energy Loss Spectroscopy (VEELS). SiC NW are found to exhibit a large direct band gap of 5.5 eV irrespectively of their polytype. Simulations using the optical properties of cubic SiC and DFT calculations show a similarly large value.

Another feature of the deconvoluted spectrum (after the removal of the zero loss peak) is the occurrence of energy losses that precede the onset of the band gap. This is probably caused by retardation losses or surface states. Possible ways of describing these residual features will be discussed, and the value of the band gap will be compared to reference data.

MM 34.18 Tue 18:00 P4

one-dimensional metal nanowire arrays prepared by hard-template synthetic method for SERS — ●YONG-TAE KIM¹, STEFAN L. SCHWEIZER¹, and RALF B. WEHRSPHORN^{1,2} — ¹Martin-Luther-University Halle-Wittenberg, Halle, Germany — ²Fraunhofer Institute for Mechanics of Materials, Halle, Germany

One-dimensional nanostructures such as nanowire and nanotube arrays have been intensively investigated due to its novel magnetic and optical properties depending on dimensional and size reduction. Especially in case of one-dimensional nanowire arrays with periodic structure, their applications will be extended to many devices for example biosensors, photonic crystals, and electro chemical devices. Therefore the fabrication of one-dimensional nanowire arrays with controlled morphologies and compositions becomes more important on a large scale.

Metal nanowire arrays with high aspect ratio have been prepared using a number of techniques including electron beam or focused ion beam (FIB) lithography, vapor-solid-liquid (VLS) growth process, and template synthetic method. Among these methods, template synthetic method is one of most promising one as increasing emphasis is placed on low cost, high throughput, and ease of production.

In this study, one-dimensional metal nanowire arrays composed of nickel, silver, and gold with single- or multi-segmented structures have been fabricated by electrochemical deposition method using AAO hard template. And these one-dimensional metal nanowire arrays will be estimated as highly active surface-enhanced Raman scattering (SERS) substrates.

MM 34.19 Tue 18:00 P4

Impact of hydrodynamic parameters on the regularity of self-assembling nanostructures — ●DENNIS LANGENKÄMPER, STEFAN OSTENDORP, NINA WINKLER, JÖRN LEUTHOLD, MARTIN PETERLECHNER, and GERHARD WILDE — Institut für Materialphysik, WWU

Münster, Germany

One promising technique for fabricating large nanostructure arrays is based on Anodic Aluminium Oxide (AAO) membranes as fabrication masks or templates. With these structures it is possible to fabricate large-scale arrays of highly regular surface nano-structures including nano-particles as well as wires and tubular structures. Thereby AAO based surface nano-structuring provides an exceptional high throughput at low fabrication costs. Additionally structural parameters such as the size, shape and spacing of resulting nano-structures can be tuned by adjusting the masks' fabrication parameters. It has been shown that especially the anodization temperature and the used electrolyte and its concentration at given anodization voltage determine the properties and regularity of the AAO membrane. Our work now focuses on the impact of hydrodynamic fabrication parameters on the structures' regularity. Membranes fabricated under different hydrodynamic conditions varying in laminar and turbulent flow and flux of the respective electrolyte used during anodization have been analyzed by a computational/graphical method based on Delauney Triangulations and Voronoi Diagrams applied to high resolution SEM micrographs of the respective structures.

MM 34.20 Tue 18:00 P4

Core-shell nanoparticles from the gas phase — ●JÖRG PRIBBENOW^{1,2}, ALEXANDER SURREY^{1,3}, DARIUS POHL¹, LUDWIG SCHULTZ^{1,3}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, D-01069 Dresden, Germany — ²TU Dresden, IFWW, D-01062 Dresden, Germany — ³TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

Core-shell nanoparticles allow for the combination of different materials for the creation of systems with a wide range of functionalities. The gas-phase based preparation of such heterogeneous particles is reported here. The cores of the nanoparticles are generated by inert gas condensation in a high-pressure magnetron sputter source. While the latter is already well established, the subsequent in-flight coating of such particles with a second material by linear magnetron sputtering is a rather novel approach. Series of electrostatic lenses provide for collimation and deceleration of unipolarly charged nanoparticles in the coating chamber. The present work is focused on the preparation of particles with a molybdenum or silver core and a copper shell. Aberration-corrected high-resolution transmission electron microscopy (HRTEM) is used to investigate the local structure and chemical composition. The influence of the electrical field profile on the resulting core-shell particles will be discussed.

MM 34.21 Tue 18:00 P4

Investigation of Nanoparticle Growth in a Dusty Acetylene Plasma — ●ALEXANDER HINZ¹, ERIK VON WAHL², MAIK FRÖHLICH², THOMAS STRUNSKUS¹, and HOLGER KERSTEN² — ¹CAU zu Kiel, Technische Fakultät, LS Materialverbunde, Kaiserstraße 2, 24143 Kiel — ²CAU zu Kiel, IEAP, AG Plasmatechnologie, Leibnizstraße 11-19, 24098 Kiel

Dusty plasmas are not only of fundamental interest but also of practical importance. Formation in plasmas is seen as a new route to prepare nanoparticles of well defined size and composition. While the particle formation in silane plasmas is well investigated it is less understood in acetylene plasmas. In particular the early stages of the particle growth are not well investigated since they are experimentally inaccessible by standard methods like Mie-Scattering. In order to get a better insight into the early stages of the particle growth a novel collection method based on neutral drag was tested. Size-distributions of the nanoparticles at different points of the growth cycle were determined ex-situ and correlated with in-situ measurement of the bias voltage of the capacitively-coupled discharge plasma. Additionally, preliminary experiments employing grazing-incidence small angle X-ray scattering (GISAXS) were performed ex-situ on the collected carbonaceous nanoparticles.

MM 34.22 Tue 18:00 P4

Crystalline structure of silver nanowires within a soft template — ●EGON STEEG, FRANK POLZER, HOLM KIRMSE, YAN QIAO, JÜRGEN P. RABE, and STEFAN KIRSTEIN — Institut für Physik, Humboldt-Universität zu Berlin

The reduction of AgNO₃ in the presence of tubular J-aggregates was used to prepare silver nanowires [1]. These wires are about 7 nm in diameter and have lengths exceeding micrometers. Within the wires single crystalline domains with length exceeding 100 nm are found by

means of high resolution transmission electron microscopy (HRTEM). The structure of these domains is analyzed further by selected area electron diffraction (SAED) on single nanowires. The resulting diffraction pattern cannot be explained by the simple silver fcc lattice, although energy-dispersive X-ray spectroscopy on the wires confirms the chemical composition of silver. Different structure models are discussed taking into account stacking faults [2], internal strain, and the formation of silver complexes with organic components.

[1] D.M. Eisele et al., J. Am. Chem. Soc. 132 (2010) 2104.

[2] V. Germain et al., J. Phys. Chem. B, Vol. 107, No. 34, 2003

MM 34.23 Tue 18:00 P4

TEM investigation of segregation phenomena in Nd-Fe-B nanoparticles — ●FRANK SCHMIDT^{1,2}, DARIUS POHL¹, LUDWIG SCHULTZ¹, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — ²TU Dresden, IFWW, D-01062 Dresden, Germany

Nd₂Fe₁₄B is a comparably hard magnetic phase as L₁₀-ordered FePt, however, with a smaller Curie temperature. Therefore, Nd₂Fe₁₄B nanomagnets could be an interesting materials alternative the widely discussed L₁₀-FePt in HAMR media. There are different methods to synthesize Nd₂Fe₁₄B nanoparticles, such as chemical methods or surfactant-assisted ball milling.

The purpose of this study is to investigate free Nd-Fe-B nanoparticles prepared by inert gas condensation and how different thermodynamic conditions affect them. In-flight optical annealing of the nanoparticles allows to compare unheated particles with heated particles, which are assumed to be closer to the thermally equilibrated state. Transmission electron microscopy was used to determine the atomic structure and chemical composition of the particles. Unheated particles are found to be mainly amorphous, while rapidly optically annealed particles are crystalline. We observe both a Nd enrichment in the shell and a Fe enrichment in the core of the differently treated particles. This segregation is more pronounced for heated particles, where a clear core-shell structure is formed that can be explained by a reduction of the surface energy.

MM 34.24 Tue 18:00 P4

Transport Properties of Single TiO₂ Nanotubes — ●MARKUS STILLER¹, JOSE BARZOLA-QUIQUIA¹, ISRAEL LORITE¹, PABLO ESQUINAZI¹, ROBIN KIRCHGEORG², SERGIU P. ALBU², and PATRIK SCHMUKI^{2,3} — ¹Division of Superconductivity and Magnetism, Institute for Experimental Physics II, University of Leipzig, D-04103 Leipzig, Germany — ²Chair for Surface Science and Corrosion Department Material Science and Engineering, University of Erlangen, D-91058 Erlangen, Germany — ³Department of Chemistry, King Abdulaziz University, Jeddah, Saudi Arabia

We have investigated the electric transport properties of single TiO₂ nanotubes separated from an anodic titania nanotube array. The nanotubes have been contacted using electron beam lithography and several transport properties have been measured. The temperature dependence of the resistance, measured with the conventional four point method, of all investigated samples, show a Mott variable range hopping behavior. The results obtained with two contacts indicate the existence of a potential barrier between the Cr/Au contacts and samples surfaces, which influence is clearly observable for temperatures less than 150 K. Impedance spectroscopy in the frequency range of 40 Hz to 1 MHz carried out at room temperature, indicates that the electronic transport of these polycrystalline tubes is dominated by the grain cores.

MM 34.25 Tue 18:00 P4

Molecular dynamics simulations of morphology transitions during growth of copper nanoclusters — ●ALEXEY TAL¹, E. PETER MÜNGER¹, NILS BRENNING², IRIS PILCH¹, ULF HELMERSSON¹, and IGOR ABRIKOSOV¹ — ¹Linköping University, Linköping, Sweden — ²The Royal Institute of Technology, Stockholm, Sweden

The study of metal nanoclusters has been a subject of intense research activities in recent years. This is due to their great importance in a variety of applications. Properties of nanoclusters crucially depend on growth methods and conditions during the growth. An understanding of the growth process during the early stages is of particular interest since the morphology of the seeds may determine the structure of the final large clusters. Morphology transition of the seed should be treated as a dynamical process, a requirement is met by classical MD simulations. In principle morphology transition is determined by both, thermodynamics and kinetics. Thermodynamics tends to min-

imize surface energy and internal stresses. But observations of large clusters with thermodynamically unfavorable structures suggest that kinetics also plays an important role. In this study the morphology transition of clusters at an early stage is considered. The influence of the angular distributions of incoming particles is determined for Cu clusters growth from a seed with 147 atoms. It is shown that growth kinetics crucially affects the morphology transition for small clusters and forbids transition to a most favorable structure for large clusters. The temperature distribution inside the cluster during the growth is calculated and the role of temperature fluctuations is discussed.

MM 34.26 Tue 18:00 P4

Grain Refinement in Ball-Milled Nanocrystalline Iron in Dependence of its Oxygen Content — ●MARIE TRYNOGGA, CHRISTINE BORCHERS, and REINER KIRCHHEIM — Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Nanocrystalline iron-oxygen alloys with different oxygen contents were prepared by ball milling of iron and hematite (Fe_2O_3) powder for 50 hours. The composition was identified using synchrotron diffraction and atom probe tomography (APT). The samples consist mainly of α -iron, segregated oxygen and magnetite (Fe_3O_4). The microstructure was investigated by X-ray diffraction (XRD), transmission electron microscopy (TEM) and APT. We observe that the grain size decreases with increasing oxygen concentration. This is interpreted as a decrease of the grain boundary energy of iron. To examine thermal stability, differential scanning calorimetry (DSC) and synchrotron diffraction measurements were performed in-situ during heating, revealing the formation of magnetite and grain growth. The nanocrystalline structure persists at higher temperatures indicating the formation of a grain boundary phase consisting of magnetite. Above 570°C the magnetite partly transforms into wüstite (FeO). We relate our findings to the results of a previous work studying nanocrystalline iron-carbon alloys after 100 hours of ball milling [1].

[1] Y.Z. Chen, A. Herz, Y.J. Li, C. Borchers, P. Choi, D. Raabe, R. Kirchheim, Nanocrystalline Fe-C alloys produced by ball milling of iron and graphite, *Acta Materialia* 61:3172-3185, 2013.

MM 34.27 Tue 18:00 P4

Analysis of the pressure dependence of plasticity in nanocrystalline Pd90Au10 — ●ANJA STEINBACH, NICOLE FÈVRE, CHRISTIAN BRAUN, and RAINER BIRRINGER — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

We examine the pressure or normal stress dependence of the mechanical behavior of nanocrystalline Pd90Au10 by utilizing the miniaturized shear compression specimen (m-SCS) [1]. In this specific testing geometry, the plastic deformation caused by dominant shear stress is confined to the gauge section which is inclined at an angle α ($\alpha = 45^\circ$ for standard geometry) relative to the loading direction. Variations of the inclination angle allow varying the superimposed hydrostatic pressure in the gauge section. Based on the experimentally determined force-displacement diagram, the stress-strain-curve and further parameters like the hydrostatic pressure are calculated using FEM-simulations. On this poster we present inclination angle-dependent stress-strain-curves obtained from inert gas condensed Pd90Au10 samples with a mean grain size of 10 nm. In agreement with theory [2], we find that nanocrystalline Pd90Au10 is stronger under pressure.

[1] M. Ames, J. Markmann, R. Birringer, *Mater. Sci. Eng. A* 528, 526 (2010) [2] A.C. Lund, C.A. Schuh, *Acta Mater.* 53, 3193 (2005)

MM 34.28 Tue 18:00 P4

Solute content and structural configuration dependent mechanical properties of nanocrystalline PdAu alloys — ●NICOLE FÈVRE, CHRISTIAN BRAUN, MICHAEL DECKARM, JONAS HEPPE, ANDREAS LEIBNER, and RAINER BIRRINGER — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

We investigate elasticity and plasticity of nanocrystalline PdAu by systematically varying the Au concentration. From calorimetry we find that grain boundaries in as-prepared specimens manifest non-equilibrium configurations. Thermal annealing leads to grain boundary relaxation and so local equilibrium configurations are generated. In particular, we determine high frequency elastic moduli and Vickers hardness for as-prepared and relaxed specimens and discuss the composition-dependent evolution of strength.

MM 34.29 Tue 18:00 P4

Microstructure, Texture and Properties of severely

twinned copper wires — ●ALEXANDER KAUFFMANN^{1,2}, JENS FREUDENBERGER^{1,3}, HANSJÖRG KLAUSS¹, VOLKER KLEMM³, WOLFRAM SCHILLINGER⁴, V. SUBRAMANYA SARMA⁵, and LUDWIG SCHULTZ^{1,2} — ¹IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — ²TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — ³TU Bergakademie Freiberg, Institute of Materials Science, Gustav-Zeuner-Str. 5, 09599 Freiberg, Germany — ⁴Wieland-Werke AG, Graf-Arco-Strasse 36, 89079 Ulm, Germany — ⁵Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai 600036, India

Due to the a drawing process in liquid nitrogen a drastic refinement of the microstructure of pure copper can be achieved by the activation of severe deformation twinning. In order to facilitate and enhance the refinement process an additional reduction of stacking fault energy by alloying can be applied. We are presenting the influences of severe deformation twinning on the microstructure and texture of copper and single-phase copper-aluminium alloys on the one hand and the mechanical and electrical properties on the other hand.

MM 34.30 Tue 18:00 P4

Ab-initio study of impurities diffusion in copper — ●ANTON BOCHKAREV and MAXIM POPOV — Materials Center Leoben Forschung GmbH, A-8700 Leoben, Austria

We present results of an ab initio study of impurity diffusion in bulk copper. Two types of impurities are investigated: oxygen and aluminum. The mechanisms we considered are the interstitial diffusion and the vacancy-mediated diffusion. To discover the impurity migration paths describing the elementary diffusion processes we employed the nudged elastic band (NEB) method. Arrhenius pre-factors were estimated in the framework of the transition state theory (TST). We find that oxygen is likely to diffuse through interstitials, whereas aluminum prefers vacancy-driven diffusion. The diffusivities obtained in our work are in reasonable agreement to the available experimental data.

MM 34.31 Tue 18:00 P4

effect of gap-size on phonon tunneling in Au(111)/vacuum/Au(111) — ●SAEIDEH EDALATI BOOSTAN, MICHAEL CZERNER, MICHAEL BACHMANN, and CHRISTIAN HEILIGER — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Recent experimental and theoretical investigations have shown that phonons can transport across vacuum gaps of a few angstroms wide which called "phonon tunneling"[1,2,3]. In this work we perform ab initio calculations by using abinitio software package to get interactions between atoms, which are modeled by spring constants. These interatomic force constants are used within an Atomistic Green's Function (AGF) method to calculate phonon tunneling in Au(111)/Vacuum/Au(111) system for different gap-sizes.

[1] Igor Altfeder et al., *Phys. Rev. Lett.* 105, 166101 (2010)

[2] Mika Prunnila and Johanna Meltaus, *Phys. Rev. Lett.* 105, 125501 (2010)

[3] D. P. Sellan et al., *Phys. Rev. B* 85, 024118 (2012)

MM 34.32 Tue 18:00 P4

Calculations of Thermal Conductivity across an Interface using Beam Matching — DEBANJAN BASU¹, ●CYNTHIA VOLKERT², CHRISTIAN JOOSS², and PETER BLOECHL¹ — ¹Institute for Theoretical Physics, Clausthal University of Technology — ²Institute for Material Physics, University of Goettingen

Thermal conductivity is an important factor affecting the efficiency of thermoelectric devices. Our goal is to explore the thermal transmission due to phonons in multilayered structures on a mode-by-mode basis using the Beam Matching Technique. For this purpose, we determine the "complex bandstructure", which describes propagating as well as evanescent phonon modes of the individual materials of this multilayer. We describe how to extract the matching conditions from the classical equations of motion for the atoms.

MM 34.33 Tue 18:00 P4

Accessing the excitation and relaxation pathways in the ultrafast Carrier dynamics of BaSnO₃:La perovskite — ●KESTUTIS BUDZINAUSKAS¹, ROLF VERSTEEG¹, MATTEO MONTAGNESE¹, XUAN LUO², SANG W. CHEONG^{2,3}, and PAUL H.M. VAN LOOSDRECHT¹ — ¹II Physikalisches Institut, University of Cologne, Cologne, Germany — ²Laboratory of Pohang Emergent Materials and Department of Physics, Pohang, Korea — ³Rutgers Center for Emergent Materials

and Department of Physics and Astronomy, New Jersey, USA

The Lanthanum doped Barium tin oxide $\text{BaSnO}_3\text{:La}$ is a transparent conducting oxide (TCO). Unlike other perovskites It shows an extremely high electron mobility, reaching values up to $320 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at room temperature, making it a promising alternative to other more expensive or unstable TCO's for applications.

The microscopic mechanisms leading to such high and uncharacteristic electron mean free paths are not fully understood. We have studied the non-equilibrium carrier dynamics in the material employing ultrafast time-resolved spectroscopy in the visible, near Infrared and THz range of the optical spectrum. In this way we are able to track and elucidate the different carrier excitation and relaxation pathways in this intriguing compound.

MM 34.34 Tue 18:00 P4

Interdiffusion studies of B2 Ni-Al-Si alloys at 1173 K — ●DANDAN LIU^{1,2}, LIJUN ZHANG¹, YONG DU¹, SERGIY DIVINSKI², and GERHARD WILDE² — ¹State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan, 410083, PR China — ²Institute of Materials Physics, Westfälische-Wilhelms University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

The knowledge of diffusion is fundamental for the production of B2 NiAl alloys as well as their use in technological applications. In the present work, Si was added to B2 NiAl alloys, and the interdiffusion of B2 Ni-Al-Si alloys at 1173 K was investigated via the Matano-Kirkaldy method by utilizing five groups of bulk diffusion couples and the electron probe microanalysis technique. The reliability of the obtained interdiffusion coefficients was validated by thermodynamic constraints as well as by Fick's second law applied to a numerical simulation. The results show that the presently obtained diffusivities can satisfactorily simulate the measured concentration profiles. Besides, the addition of Si was found to have different effect on the diffusion of Al in Ni-rich and nearly stoichiometric NiAl alloys. The possible reasons were interpreted in terms of cross diffusivities, site occupations, and different diffusion mechanisms. The present work provides valuable information for understanding diffusion in B2 NiAl-X alloys, where X occupies the Al sublattice.

MM 34.35 Tue 18:00 P4

Scanning Transmission Electron Tomography on three-dimensional defects in semiconductor heterostructures — ●MICHAEL NIEHLE and ACHIM TRAMPERT — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

Shrinking structures incorporated into opto-electronic devices require an understanding of structure-property relations on a scale of only a few nanometers. In this context, the interest in three-dimensional (3D) structures of crystal defects is growing as their detailed influence on device functionality has to be considered. The combination of scanning transmission electron microscopy (STEM) with tomography allows for an investigation of the defects' 3D structure on a respective length scale. We present the application of STEM tomography on 3D objects embedded in GaSb based semiconductor heterostructures grown on Si substrates. The unique possibility to characterize the complex morphology in great detail is demonstrated. Challenges to apply STEM tomography as a routine tool in materials sciences are discussed with respect to materials comprising elements with a rather high atomic number. Strategies to complement investigations by conventional TEM techniques are sketched.

MM 34.36 Tue 18:00 P4

Lateral Resolved EELS on organic bulk heterojunctions - a low-dose approach to optimized spatial and energy resolution in the TEM — ●ANNE K. KAST^{1,2,3}, MARTIN PFANNMÖLLER¹, MARCO OSTER¹, PHILIPP WACHSMUTH⁴, RALF HAMBACH⁴, GERD BENNER⁵, DIANA NANOVA^{2,3}, ROBERT LOVRINCIC^{2,3}, WOLFGANG KOWALSKY^{2,3}, UTE KAISER⁴, and RASMUS R. SCHRÖDER^{1,3} — ¹Cryo-EM, Universitätsklinikum Heidelberg — ²IHF, TU Braunschweig — ³innovationLab GmbH, Heidelberg — ⁴Materialwissenschaftliche EM, Uni Ulm — ⁵Carl Zeiss GmbH, Oberkochen

We implement a novel analytical method using EFTEM which allows visualizing donor and acceptor materials in organic solar cell thin films by analyzing electronic excitations features in the optical and plasmonic energy region. Segmentation by EELS reveals that these carbon based materials show characteristic optical excitations in energy-loss spectra. However, the blend materials are very sensitive to radiation damage, which impedes spatial spectral mapping using EELS in con-

ventional scanning beam mode. We introduce an automated scheme that exploits the inherent spatial resolution in the EEL spectrum as it is obtainable from aberration corrected imaging energy filters. It involves automatic scanning of the image of a slit aperture in the illumination beam path. To eliminate residual image distortion in the EEL spectrum we apply correction algorithms for quantitative spectrum interpretation. Application of such automated laterally resolved EEL spectroscopy allows spatial mapping of high-resolution spectra in two dimensions at low-dose conditions.

MM 34.37 Tue 18:00 P4

STEM with focused vortex beams - a route towards local EMCD measurements? — ●DARIUS POHL¹, SEBASTIAN SCHNEIDER^{1,2}, LUDWIG SCHULTZ^{1,2}, and BERND RELLINGHAUS¹ — ¹IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — ²TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany

X-ray magnetic circular dichroism is a well established method to study element specific magnetic properties of a material, while electron magnetic circular dichroism (EMCD), which is the electron wave analogue to XMCD, is scarcely used today. Recently discovered electron vortex beams, which carry a discrete orbital angular momentum (OAM) L , are predicted to also reveal dichroic signals. Since electron beams can be easily focused down to sub-nanometer diameters, this novel technique provides the possibility to quantitatively determine local magnetic properties with unrivalled lateral resolution. As the spiralling wave front of the electron vortex beam has an azimuthally growing phase shift of up to 2π and a phase singularity in its axial center, specially designed apertures are needed to generate such non-planar electron waves. We report on the preparation and successful implementation of spiral apertures into the condenser lens system of an aberration-corrected FEI Titan³ 80-300 transmission electron microscope (TEM). This setup allows to perform scanning TEM (STEM) with vortex beams carrying user-selected OAM. First experiments and simulations on the interaction of the vortex beam with a crystalline sample will be presented.

MM 34.38 Tue 18:00 P4

Combined experimental and theoretical study showing D1_a-type local order in Ni-Re — ●SASCHA B. MAISEL¹, NILS SCHINDZIELORZ¹, ALESSANDRO MOTTURA², ROGER REED³, and STEFAN MÜLLER¹ — ¹Institute of Advanced Ceramics, TUHH, 21073 Hamburg, Deutschland — ²School of Metallurgy and Materials, University of Birmingham, B15 2TT Edgbaston, United Kingdom — ³Department of Engineering Science, University of Oxford, OX1 3PJ Oxford, United Kingdom

Since the 1980s rhenium has been used as an addition to nickel-based high-temperature superalloys, since even small amounts of rhenium have a dramatic effect on creep resistance. However, the mechanisms behind this so-called *rhenium-effect* are still ill-understood. Using both experimental and theoretical methods, we show that the currently known phase diagram is inaccurate, and neglects a stoichiometric compound at 20 at.% Re Ni₄Re. This is expected to affect the microstructure of Ni-Re alloys, with important ramifications for Ni-based superalloys. The Ni₄Re compound is shown to be stable by means of quantum mechanical high-throughput calculations at 0K, aided by the cluster-expansion methods. Monte Carlo simulations show that it is thermally persistent up to 1100 K when considering configurational entropy. The existence of this compound was experimentally confirmed using extended x-ray absorption fine spectroscopy on a Ni_{0.97}Re_{0.03} alloy.

MM 34.39 Tue 18:00 P4

A synchrotron analysis of deformation-induced martensitic transformation in the as-cast Cu₄₀Co₁₀Zr₅₀ — ●FATEMEH A. JAVID^{1,2}, NORBERT MATTERN¹, JOZEF BEDNARCIK³, MOHAMMAD SIAHATGAR⁴, MIHAI STOICA¹, SIMON PAULY¹, and JÜRGEN ECKERT^{1,2} — ¹Leibniz Institute for Solid State and Materials Research, Dresden, Germany — ²Technische Universität, Dresden, Germany — ³DESY, Forschungsbereich FS, Hamburg, Germany — ⁴Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

The deformation-induced martensitic transformation in Cu₄₀Co₁₀Zr₅₀ alloy under mechanical load was investigated using a synchrotron X-ray diffraction. The *in-situ* compression tests were performed in both track control and load control modes. The X-ray diffraction results show that the position of the diffraction peaks shifted to higher q values (reciprocal space) and peaks broaden due to increasing of strain. Considering

the phase transformation fractions, the kinetics of phase transformation was studied in the longitudinal and transversal directions. In the case of track control test, the measured $B2$ (Cu,Co)Zr \rightarrow M(Cu,Co)Zr transformation fractions indicates a 100% of martensitic transformation under compression loading and the microstructure consists of a fully martensitic (Cu,Co)Zr. Whilst upon load control test, the martensitic transformation occurred $> 90\%$. The changes in the strain tensor and subsequently the shear components versus applied stress were studied.

MM 34.40 Tue 18:00 P4

Dependence of accessible undercooling on prior liquid overheating by differential fast scanning calorimeter — •BIN YANG¹, JOHN H. PEREPEZKO², JÜRGEN W. P. SCHMELZER¹, YULAI GAO³, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Department of Materials Science and Engineering, University of

Wisconsin-Madison, 1509 University Avenue, Madison, WI 53706, USA — ³School of Materials Science and Engineering, Shanghai University, Shanghai 200072, P.R. China

The dependence of accessible undercooling on prior overheating of a pure tin single micron-sized droplet was studied by differential fast scanning calorimetry (DFSC) with cooling rates from 500 to 10,000 K/s. It is observed experimentally that (i) the degree of undercooling increases first gradually with increasing of prior overheating and reaches then an undercooling plateau; (ii) the accessible undercooling increases initially with increasing cooling rate. However, above a certain cooling rate the accessible undercooling decreases strongly with increasing cooling rate. For overheating levels above that for the onset of the undercooling plateau the undercooling increases with increasing cooling rate. These observed unusual behavior is successfully explained by heterogeneous nucleation in cavities. This mechanism can possibly also describe nucleation in other similar rapid solidification processes.