MM 15: Poster session I

Posters should be displayed by 4 pm. The MM poster price will be awarded during the annual general assembly on Wednesday evening.

Posters submitted to: Integrated computational materials engineering for design of new materials, Methods in Computational Materials Modelling, Structural Materials, Frontiers of Electronic Structure Theory, Transport, Microstructure and Phase Transformations, Mechanical Properties, Liquid and Amorphous Metals

Time: Monday 18:00–20:00 Location: Poster B3

MM 15.1 Mon 18:00 Poster B3

Forces in the KKR method — •Roman Kováčik, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

An accurate calculation of the ionic forces in the Korringa-Kohn-Rostoker Green function (KKR-GF) method is crucial for its applicability to large scale material science simulations. In turn, the calculation of forces relies on an accurate evaluation of the electrostatic potential, especially in the interstitial regions where the intersite terms exhibit very poor convergence with the angular momentum expansion. We explore and analyze an alternative method for the numerical solution of Poisson's equation, based on a direct integration within space-filling Voronoi polyhedra [1]. An accurate and efficient isoparametric integration scheme without the use of shape functions is employed [2]. Furthermore, an alternative summation form is applied to the expressions in the Ewald procedure [3]. This approach is implemented and tested within the KKR-GF framework in the KKR*nano* computational code [4].

[1] A. Alam *et al.*, Phys. Rev. B 84, 205106 (2011).
[2] A. Alam *et al.*, Phys. Rev. B 84, 045105 (2011).
[3] R. Zeller, J. Phys.: Condens. Matter 27, 306301 (2015).
[4] A. Thiess *et al.*, Phys. Rev. B 85, 235103 (2012).

MM 15.2 Mon 18:00 Poster B3

Statics and dynamics of point defects in TiC — •Hossein Ehteshami[1], Weiwei Sun[2], and Pavel A. Korzhavyi[1] — [1]Materials Technology, Deptartment of Materials Science and Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — [2]Materials Theory, Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

In this study, we present the results of a systematic ab initio study of point defects in titanium carbide. The electronic spectra and atomic structures for the metal and non-metal vacancies, interstitials, and antisite defects (including the split interstitial and split antisite conformations) are calculated within the generalized gradient approximation of density functional theory, using the projector augmented wave method as implemented in the Vienna Ab-initio Simulation Package VASP. In many cases the symmetric point defect configuration is found to be unstable agains a symmetry-breaking distortion via the Jahn-Teller mechanism. An enhanced stability of titanium dumbbells is obtained for sub-stoichiometric TiC where the dumbbels form clusters with the carbon vacancies. Possible migration pathways for point defects and their clusters are explored in order to create a database of possible mechanisms of self-diffusion in TiC. The obtained information about the electronic of point defects, as well as about their formation and migration energies, can be useful in experimental (spectroscopic) and theoretical (atomistic modeling) studies of TiC and related materials.

MM 15.3 Mon 18:00 Poster B3

Analysis of electronic and structural properties of surfaces and interfaces involving $LaAlO_3$ and $SrTiO_3$ — •Irina Piyanzina[1,2], Thilo Kopp[2], and Volker Eyert[3] — [1]Institute of Physics, Kazan Federal University, Kremlyovskaya St. 18, 420008 Kazan, Russia — [2]EP VI and Center for Electronic Correlations and Magnetism, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany — [3]Materials Design SARL, 18 rue de Saisset, 92120 Montrouge, France

Recently, it was established that a two-dimensional electron system can arise at the interface between the two oxide insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) [A. Ohtomo and H. Hwang, Nature **427**, 423 (2004); S. Thiel et al., Science **313**, 1942 (2006)]. This paradigmatic example furthermore exhibits magnetism between the non-magnetic oxides. Despite the huge amount of both theoretical and experimental work a thorough understanding has yet to be achieved.

The aim of the present study is to investigate the electronic properties and structural distortions of surfaces and interfaces based on LAO and STO by means of density functional theory. We analyzed the structural deformations of the $LaAlO_3$ (001) slab induced by hydrogen adatoms and oxygen vacancies at its surface. Moreover, we investigated the influence of surface reconstruction on the density of states and determined the spatial dependence of the density of state at the Fermi level for bare $LaAlO_3$ surfaces and $LaAlO_3/SrTiO_3$ interfaces. In addition, the Al-atom displacements and distortions of the TiO_6-octahedra were estimated.

MM 15.4 Mon 18:00 Poster B3

Machine Learning of Structural and Electronic Properties of Semiconductors — Benedikt Hoock[1,2], Ute Werner[1], Karsten Hannewald[1,2], Luca Ghiringhelli[2], Matthias Scheffler[2], and •Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin, DE

High-level solid-state computational methods enable very precise calculations of material properties such as lattice parameters and band structures. However, they usually also require a considerable computational effort. In order to circumvent such time-consuming calculations, recently machine learning techniques have emerged as an alternative predictive tool with potentially high accuracy. For example, Ghiringhelli et al. [*] could predict the crystal structure of binary octet semiconductors with the LASSO regression technique applied on an extended feature space. Using a similar methodology, we demonstrate that the lattice parameter can be learned from purely atomic and dimer data. Further, we explore the viability of learning ab initio band gaps from atomic and dimer data and/or low cost tight-binding calculations.

[*]: L.M. Ghiringhelli et al., Phys. Rev. Lett. 114, 105503 (2015)

MM 15.5 Mon 18:00 Poster B3

Anharmonically stabilized temperature-dependent cluster-expansions applied to β-NiTi — •Sascha B. Maisel, Dominique Korbmacher, Blazej Grabowski, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, 40239 Düsseldorf, Germany

The high temperature state β-NiTi is unstable with respect to transformation to a low-symmetry state at lower temperatures and to different phases at off-stoichiometric compositions. This poses several methodological challenges when developing effective models for the Ni-Ti system, which are integral in order to understand its intrinsic shape memory effect. Using recently improved methods for the temperature-dependent cluster-expansion (CE) approach, we derive and compare a hierarchy of descriptions of varying sophistication for the β-Ni-Ti high-temperature state. These descriptions are all based exclusively on ab-initio data or an ab-initio-based thermodynamic upscaling method known as the TU-TILD method [1], but yield surprisingly different results. This high sensitivity to the DFT input parameters is a consequence of the strong relaxations and dynamical instabilities that are ultimately responsible for the material's shape-memory properties. The various approaches are critically discussed regarding both their computational efficiency and their ability to reproduce CALPHAD free energies.

[1] A. I. Duff et al.: PRB **91**, 214311 (2015)

MM 15.6 Mon 18:00 Poster B3

Accelerating path integral molecular dynamics — •Venkat Kapil[1] and Michele Ceriotti[2] — [1]Laboratory of Computational Science and Modelling, Institute of Materials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Laboratory of Com-

putational Science and Modelling, Institute of Materials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

The cost of modelling quantum nature of light nuclei in an ab initio setup is still prohibitive, despite many recent developments that reduce the computational overhead. We illustrate how multiple time step integrators, used simultaneously with ring polymer contraction and appropriate thermostatting schemes, can reduce the overhead of modelling nuclear quantum effects, while describing inter-atomic forces at high levels of electronic structure theory, virtually to zero. This approach can be used together with other accelerated path integral techniques, such as generalized Langevin equation thermostats or high-order factorizations of the Boltzmann operator.

MM 15.7 Mon 18:00 Poster B3

Probing texture-induced abnormal grain growth in polycrystalline materials in 4D — •Mingyan Wang, Jules Dake, Anton Manin, and Carl Krill — Institute of Micro and Nanomaterials, Ulm University, Germany

Although abnormal grain growth (AGG) has been investigated in polycrystalline materials for more than 70 years, our understanding of the underlying mechanisms remains incomplete. Conventional studies based on micrographs cannot capture the real physical processes that take place in 3D. Instead, a non-destructive 3D characterization method is needed to probe these phenomena. Employing three-dimensional x-ray diffraction (3DXRD) microscopy, we were able to collect a sequence of microstructural snapshots, which could then be combined into a full 4D (3D + time) dataset. Analysis of particle trajectories show that a subpopulation of grains grows much faster than expected, indicating the occurrence of AGG. Comparing the microstructural evolution in our sample to a simulation of normal grain growth, we find large discrepancies in coarsening behavior. By extending a 3D phase field simulation to include texture-dependent grain boundary properties, we achieve much better agreement with the measured changes in grain size and morphology.

MM 15.8 Mon 18:00 Poster B3

Temperature dependent fracture of defected graphene sheets: a Molecular Dynamics study — •Samaneh Nasiri and Michael Zaiser — Institute of Materials Simulation, Friedrich-Alexander University Erlangen-Nürnberg , 90762 Fürth, Germany

Pristine graphene is known as the strongest material in terms of its in-plane tensile strength- a property which makes it a candidate for novel structural applications on the nano scale. However defects are unavoidable during the synthesis and fabrication of graphene-based devices. In this Paper we investigate the effect of defects on the temperature-dependent rupture strength of graphene sheets, for two different types of defects, namely randomly distributed point defects (vacancies) and single extended defects (cracks). We first study the effect of different vacancy concentrations and crack sizes on the fracture strength of graphene sheets at various temperatures and interpret our results with reference to continuum fracture mechanics concepts which we generalize to account for discreteness of the atomic and defect structure.

Keywords: Graphene, Vacancies, Cracks, Temperature, Molecular Dynamics, Fracture Mechanics.

MM 15.9 Mon 18:00 Poster B3

A Compressed Sensing Approach to Select Accurate Atom-Centered Basis Functions for Advanced Density Functional and Quantum Chemistry — •Niklas Menzel[1], Chenchen Wang[1,2], Luca Ghiringhelli[1], Gitta Kutyniok[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]University of California, Santa Barbara, USA — [3]Technische Universität, Berlin, DE

The choice of basis sets is one of the most important factors in quantum chemical calculations. Commonly used basis sets for advanced exchange-correlation functionals are not sufficiently accurate to represent Kohn-Sham Hamiltonian and its eigenfunctions. This leads to basis set extensions, such as the most famous correlation-consistent basis sets by Dunning. Due to computational costs, such basis sets have been so far used mainly for light atoms and their molecules. We have developed a basis-set selection approach that makes use of compressed sensing (CS), a recently developed signal processing technique, based on l1-norm regularization. As introductory example, we select via our CS-based approach Gaussian basis functions (GTO) from a large pool of various GTOs. The number of chosen GTOs can be tuned. We calculate the total energy for atoms from H to O, and then extend to molecules, e.g. H2, and O2. For H, He, and Li, our total-energy results are within 0.05 % compared with STO-6G energies. Starting from Be, CS selected basis set provide significantly better results than STO-6G, even when only 5 GTOs are considered. Our new approach enables us to determine accurate basis sets for heavier atoms and molecules.

MM 15.10 Mon 18:00 Poster B3

Rapid theory-guided prototyping of ductile Mg alloys — Zongrui Pei[1,2], •Martin Friák[3,1,2], Stefanie Sandlöbes[4,1], Bob Svendsen[1,2,5], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschun, GmbH, Düsseldorf, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — [3]Institute of Physics of Materials, Brno, Czech Republic — [4]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, Aachen, Germany — [5]Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen, Aachen, Germany

Magnesium alloys are promising structural materials with high specific strength. However, their broader use is limited by their low formability at ambient temperatures. It is known that Mg alloys containing small amounts of yttrium or rare-earth (RE) elements exhibit up to 5 times higher room temperature ductility but finding other solutes with the same effect is highly desirable. In order to identify a method allowing for a corresponding rapid alloy and solute assessment, we analyze relations between the I_1 stacking fault energies, which were shown to be related to the macroscopic ductility in Mg alloys (Acta Mater. 60 (2012) 3011), and the atomic volume V of pure solutes, their electronegativity ν and bulk modulus B. Comparing the impact of solutes with that of yttrium we propose a single numerical quantity (called yttrium similarity index, YSI) that is based on these interrelations. We evaluate YSI for 2850 Mg-ternaries and identify 133 promising solute pairs not including any RE elements (New J. Phys. 17 (2015) 093009).

MM 15.11 Mon 18:00 Poster B3

An *ab initio* high throughput approach to identify Mg-alloys with exceptionally high yield strength — Zongrui Pei[1,2], Duancheng Ma[1], •Martin Friák[3,1,2], Bob Svendsen[1,2,4], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschun, GmbH, Düsseldorf, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen, Aachen, Germany — [3]Institute of Physics of Materials, Brno, Czech Republic — [4]Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen, Aachen, Germany

Using *ab initio* calculations and symmetrized plane waves, we analyze the basal-plane generalized stacking fault energies in pure Mg and Mg-Y alloys and show that the knowledge of energies of only five specific points is sufficient to accurately predict the core structures and Peierls stresses of ⟨a⟩-type edge dislocations in these alloys. Our five-point approach substantially reduces the computational cost related to the Peierls-Nabarro (PN) model and allows for a high-throughput application of the PN model to study Peierls stress changes in Mg upon alloying. We employ our approach to study Mg binary alloys containing nine rare-earth (RE) and 11 other solutes. Based on the Peierls stresses of these 20 Mg alloys calculated from the Peierls-Nabarro model, the solutes are divided into three groups according to the dislocation core structure, the magnitude of Peierls stress, and their either strengthening or softening effect (Phys. Rev. B 92 (2015) 064107).

MM 15.12 Mon 18:00 Poster B3

Sulfation kinetics of high temperature corrosion in waste to energy plants — •Daniel Ott[1], Ferdinand Haider[1], and Ragnar Warnecke[2] — [1]Univ. Augsburg, Inst. f. Physik, 86135 Augsburg — [2]Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion leads especially in waste-to-energy-plants to massive problems. At prevalent temperatures around 500°C-600°C corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlorides.

This reaction requires an atmosphere containing SO_2, H_2O, O_2 and releases HCl/Cl_2. In this work we present results for the reaction kinetics, which depends on different parameters, like temperature, gas stream, gas components or (catalytic)additives. The conversion rate is strongly dependent on the transformation of SO_2 to SO_3, which is catalyzed by the presence of iron and iron oxides. In parallel to the study of the reaction rate it is possible to characterize the loss of

metall simultaneously. Furthermore the behaviour of chlorine during the process of the corrosion was investigated. Investigations (theoretical and practical) of real superheater deposits were conducted for a better understanding of the predominant reactions and comparability of laboratory experiments. Principles of the prevalent conditions and reactions in waste-to-energy-plants, especially at the superheaters, are shown and experiments regarding the kinetics are presented.

Project supported by: BMBF - MatRessource, project: VOKos

MM 15.13 Mon 18:00 Poster B3

Deoxidation of stainless steels during vacuum brazing — •Cornelia Kunz[1], Wolfgang Maus-Friedrichs[1], Simon Schöler[2,3], Ulrich Holländer[2,3], and Kai Möhwald[2,3] — [1]Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Germany — [2]Institut für Werkstoffkunde, Bereich Füge- und Oberflächentechnik (Fortis), , Leibniz Universität Hannover, Germany — [3]Institut für Werkstoffkunde, Leibniz Universität Hannover, Germany

Stainless steels are in widespread use due to their excellent mechanical and corrosion-proof properties. Corrosion resistance stems from native oxide layers formed on the surface of stainless steels, only a few nanometers thick and consisting of a mixture of chromium and iron oxides and hydroxides.

However, when choosing to join stainless steels by the means of vacuum brazing, the oxide layer prevents the wetting of the surface with braze, therefore inhibiting the joining process. Thus, deoxidation is a necessity. While procedural knowledge is abundant, fundamental understanding of thermophysical and chemical processes is lacking. Deoxidation is studied with two different stainless steels, AISI 304 and 446. Effect of heat treatment during vacuum brazing is recreated in laboratory scale by electron impact heating. Chemical analysis before and after heat treatment is carried out by XPS, AES and EDX/ WDX, optical and topographical properties are studied by CLSM. Bulk changes can be separated from surface changes due to different information depths of XPS/ AES and EDX/ WDX.

MM 15.14 Mon 18:00 Poster B3

Atomistic simulation of the early stages of precipitation in Al-Si-Mg alloys — •Daniele Giofrè and Michele Ceriotti — Laboratory of Computational Science and Modelling - EPFL, Lausanne, Switerland

In the solid state the ternary phases exist mainly outside the fields of their primary crystallization. In the compositional range of 6XXX series alluminum alloys all phases, which form during the solidification, are of eutectic origin and are generally the result of non-equilibrium solidification (quenching mode). Furthermore, their properties are determined by the formation of coherent precipitates containing Mg, Al, Si.

In order to control the aging mode, namely the final result, an analysis of the stability and kinetics of these precipitates is of great importance in the Al-metallurgical industry. For these reasons it is particularly advantageous to have a mastery of the little-known early stages of precipitation. Therefore we want to study these small nuclei in order to investigate the aggregation of solute atoms, the critical sizes of nano-particules of the β'' phase, and their associated driving forces.

In the regime of this process, we have used a first-principles theory to conduct both the strength and stability study of the finite-size embedded precipitates nuclei of the β'' phase in the Al-bulk. We have carried out all that in order to compare the results with the simulation of formation energy, and to discover which is the morphology and stability of early precipitates and their thermodynamic driving force.

MM 15.15 Mon 18:00 Poster B3

Theoretical investigation of BiTeX (X=Cl,Br,I): Crystal structure and optical conductivity — •René Wirnata[1], Sebastian Schwalbe[1], Giulio A.H. Schober[2], Jens Kortus[1], and Ronald Starke[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]University of Heidelberg, Institute for Theoretical Physics, Germany

Recently, the group of bismuth tellurohalides (BiTeX, X=Cl,Br,I) has been discovered to show a giant bulk Rashba splitting [1] that can be used e.g. in spintronics applications or magneto-optical devices [2,3]. Starting from X-ray data [4], we have constructed mono and double layer models of the experimental crystal systems. Using density functional theory, we discover a graphene/graphite-like band-crossing, which can also be observed in the low-frequency region of the optical response tensor. This may provide a new method for structural characterization by performing optical conductivity measurements.

Furthermore, this materials class shows a layered electron localization around the X and Te atoms, which manifests itself in the form of an increased conductivity in this plane.

[1] Bahramy, M. S. et al., Phys. Rev. B, vol. 84, p. 041202
[2] Lee, J. S. and Schober, G. A. H. et al., PRL, vol. 107, p. 117401
[3] Demkó, L. and Schober, G. A. H. et al., PRL, vol. 109, p. 167401
[4] Shevelkov, A. V. et al., J. Sol. St. Chem., vol. 114, pp. 379 - 384

MM 15.16 Mon 18:00 Poster B3

A fast Fermi orbital based self-interaction correction: Analytic 2nd order derivatives — •Charlotte Vogelbusch, Lenz Fiedler, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

One of the widely used electronic structure theories, density functional theory (DFT), is still limited due to systematic errors, e.g. the self-interaction error [1]. A new approach of a self-interaction correction (SIC) using Fermi orbitals has been initiated by Pederson, Ruzsinszky and Perdew [2].

The optimization of the Fermi orbital positions calculated with well established methods like the conjugate gradient results in high computational effort. In order to accelerate the slow convergence, some preconditioning for the numerical optimization of the SIC energy is needed. In this context the calculation of its derivatives is useful. The first order derivative of SIC energies has been investigated analytically by Pederson [3].

For preconditioning, the diagonal elements of the second order derivative have been analytically calculated. In the present work, this analytic approach has been benchmarked against numerical results for a set of small molecules.

[1] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

MM 15.17 Mon 18:00 Poster B3

A fast Fermi orbital based self-interaction correction: A preconditioned Conjugate Gradient algorithm — •Lenz Fiedler, Charlotte Vogelbusch, Torsten Hahn, and Jens Kortus — TU Freiberg, Institute for Theoretical Physics, Germany

In order to optimize methodical errors of density functional theory (DFT), a sufficient self-interaction correction (SIC) is needed. A possible approach is realized by the construction of localized orbitals such as Fermi orbitals, which can be obtained from Kohn-Sham orbitals. A full theoretical description of such a Fermi orbital based SIC is given by Pederson [1,2] drawing on previous results by Perdew and Zunger [3]. The implementation of this approach in a DFT code causes some numerical problems, due to the slow convergence in the optimization of the Fermi orbital positions.

Therefore we present an implementation of a conjugate gradient algorithm that is likely to improve the convergence of the calculation and therefore decreases the computational time. This is done by using a preconditioner which is composed of the diagonal elements of the Hessian of the energy function. These diagonal elements have been implemented both analytically and numerically. We show benchmarks against each other for a set of small molecules.

[1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[2] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[3] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)

MM 15.18 Mon 18:00 Poster B3

Kondo effect in Dirac and Weyl semimetals — •Andrew Mitchell and Lars Fritz — Institute for Theoretical Physics, Utrecht University, 3584 CE Utrecht, The Netherlands

Magnetic impurities in three-dimensional Dirac and Weyl systems are shown to exhibit a fascinatingly diverse range of Kondo physics. When the Fermi level is precisely at the Dirac point, Dirac semimetals are in fact unlikely candidates for a Kondo effect due to the pseudogapped density of states. However, the influence of a nearby quantum critical point leads to the unconventional evolution of Kondo physics for even tiny deviations in the chemical potential.

Separating the degenerate Dirac nodes produces a Weyl phase: Time-reversal symmetry breaking precludes Kondo physics due to an effective impurity magnetic field, but different Kondo variants are accessible in time-reversal invariant Weyl systems. We study the distinctive spectroscopic signatures expected from scanning tunneling spectroscopy (STS), and also quasiparticle interference (QPI) where

Kondo scattering is confined to surface Fermi arcs.

[1] A. K. Mitchell and L. Fritz, Phys. Rev. B **92**, 121109(R) (2015)

MM 15.19 Mon 18:00 Poster B3

Hydrogen sorption kinetics in magnesium and titanium hydride thin films — •Efi Hadjixenophontos, Lukas Michalek, and Guido Schmitz — University of Stuttgart, IMW, Heisenbergstrasse 3, 70569 Stuttgart Germany

Magnesium hydride is a model material which is intensively studied for hydrogen sorption in the last few years. Beside its favorable abundance, it is known for its high weight capacity of about 7 wt.% of hydrogen (H). It's a reversible storage system. However, it suffers from slow kinetics which makes it operational at only high temperatures. Research has shown that transition metals (TM) can improve this properties. In this work, we focus on the H-sorption behavior in thin films of thicknesses between 50-400nm in different conditions. The focus is to compare the kinetic properties and diffusion coefficients between TiH2 and MgH2 and multilayers thereof. Mg requires a thin Palladium (Pd) film on top for the hydrogenation to take place. Pure Mg/Pd and Ti metals were deposited by ion beam sputtering on Si/SiO2 substrates. Hydrogenation of these layers followed at different temperatures (RT-300°C) and for different duration of times (10-600min) at 1-20 bars of H atmosphere. Full dehydrogenation of the samples has been tested and is shown to be more challenging for the TiH2 because of its stability. Microstructure was studied by TEM. SEM was used for surface analysis. XRD is applied to quantify the hydrogen-sorption process and diffusion coefficients. Quantitative measurements and evaluation at different temperatures will be presented that allow determination of diffusivity and surface reaction coefficients.

MM 15.20 Mon 18:00 Poster B3

Ion-Beam Sputtered Thin Li_xSi Films and Atomic Transport — •Florian Strauss[1], Harald Schmidt[1], and Paul Heitjans[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Leibniz Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, Deutschland

Thin films of lithium-silicon compounds as well as of pure silicon, both in the amorphous and the crystalline state, are promising high capacity anode materials for future battery applications. An investigation of atomic and ionic transport processes in these materials is needed for an optimisation of charging/discharging properties and power densities. Li_xSi can either be deposited from a segmented target consisting of elemental Si and metallic Li by reactive co-sputtering as shown in [1] or directly from a bulk Li-Si alloy target. While no value for x below 1 is achievable for Li-Si alloys, segmented targets have been shown to produce films with a value of $0.03 < x < 0.6$. Experiments with SIMS, XPS and XRD were used to further characterise the sputtered layers. Measurements of transport parameters can be done by a neutron reflectometry based method, recently proposed by Hüger et al. [2].

[1] F. Strauß et al., RSC Adv. 5, 7192 (2014).
[2] E. Hüger et al., Nano Lett. 13, 1237 (2013).

MM 15.21 Mon 18:00 Poster B3

Identification of structural bottlenecks for sodium ion transport in solid state sodium ion conductors — •Kaustubh Bhat, Stefan Blügel, and Hans Lustfeld — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Sodium ion conductors offer significant advantages for applications in large scale-energy storage systems. It was observed that the ionic conductivity of NASICON [1] materials is correlated to certain areas that were proposed to be structural bottlenecks to sodium ion transport [2]. We use density functional theory along with the Nudged Elastic Band Method [3] to calculate the energy barrier for transport pathways in the NASICON material sodium scandium phosphate $Na_3Sc_2(PO_4)_3$. We apply stress to the crystal to calculate the change of the energy barrier with changing strain [4]. Using a constrained gradient descent method, we quantify the effect of the following structural features on the energy barrier: (a) interatomic distances, (b) areas between neighboring atoms and (c) volumes around mobile ions. This enables us to identify all relevant structural bottlenecks. – We acknowledge fruitful discussions with our experimental colleagues F. Tietz and M. Guin toward this work.

[1] Hong H.Y.P., MRB **11**, 173-182 (1976).
[2] Winaud J.M. *et al.* J.Mater. Sci. **25**, 4008-4013 (1990).
[3] Henkelman G. *et al.* JCP **113**, 9901-9904 (2000).
[4] Hirschfeld J.A. *et al.* PRB **84**, 224308 (2011).

MM 15.22 Mon 18:00 Poster B3

Quantum Oscillation Signatures of Pressure-induced Topological Phase Transition in BiTeI — •Joonbum Park[1,2], Kyung-Hwan Jin[3], Geunsik Lee[4], Youn Jung Jo[5], Eun Sang Choi[6], Woun Kang[7], Erik Kampert[8], Jong-Soo Rhyee[9], Seung-Hoon Jhi[10], and Jun Sung Kim[10] — [1]Max-Planck-Institute for Chemical Physics of Soilds, Dresden, Germany — [2]Max Planck Center for Complex Phase Materials, Pohang, South Korea — [3]University of Utah, Salt Lake City, Utah, USA — [4]UNIST, Ulsan, South Korea — [5]Kyungpuk University, Daegu, South Korea — [6]National High Magnetic Field Laboratory, Tallahassee, Florida, USA — [7]Ewha Womens' University, Seoul, South Korea — [8]Dresden High Magnetic Field Laboratory, Dresden, Germany — [9]Kyung-Hee University, Suwon, South Korea — [10]POSTECH, Pohang, South Korea

We report the pressure-induced topological quantum phase transition of BiTeI single crystals using Shubnikov-de Haas oscillations of bulk Fermi surfaces. Above a critical pressure $P \sim 2$GPa, the Shubnikov-de Haas frequency for the inner Fermi surface increases unusually with pressure, and the Shubnikov-de Haas oscillations for the outer Fermi surface shows an abrupt phase shift. In comparison with band structure calculations, we find that these unusual behaviors originate from the Fermi surface shape change due to pressure-induced band inversion. These results clearly demonstrate that the topological quantum phase transition is intimately tied to the shape of bulk Fermi surfaces enclosing the time-reversal invariant momenta with band inversion.

MM 15.23 Mon 18:00 Poster B3

Atomic structure and dynamic viscosity of liquid GeTe — •Hans Weber[1,2], Mathias Schumacher[3], Pál Jóvári[4], Werner Skrotzki[2], Riccardo Mazzarello[3], and Ivan Kaban[1] — [1]IFW Dresden, Institute for Complex Materials, PO Box 270116, 01171 Dresden, Germany — [2]Technische Universität Dresden, Institut für Strukturphysik, 01062 Dresden, Germany — [3]RWTH Aachen University, Institute for Theoretical Solid State Physics, 52056 Aachen, Germany — [4]Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, PO Box 49, 1525 Budapest, Hungary

The atomic structure of GeTe liquid alloy is studied by X-ray diffraction and neutron diffraction in the temperature range from 750 to 850 °C. Its dynamic viscosity is measured from 1000 to 680 °C, which is 55 °C below the solidification point, using an oscillating-cup viscometer. The structural parameters of liquid GeTe show small changes and the dynamic viscosity behaves in accordance to the Arrhenius law. The experimental structural data are modeled with the reverse Monte-Carlo simulation technique. Ge atoms are found to be mainly coordinated by Te atoms and to a less extent by Ge atoms. The formation of a small number of Te-Te bonds is also probable. The results obtained are in agreement with ab-initio molecular dynamics simulations.

MM 15.24 Mon 18:00 Poster B3

Phase Transformation in Alloyed Nanowires — •Manuel Roussel, Martin Schellenberger, Tim Lehmann, and Guido Schmitz — Institute for Materials Science, Stuttgart, Germany

Since the discovery of giant magnetoresistance, for which Albert Fert and Peter Grünberg have been awarded the 2007 Nobel Prize, thin magnetic films have attracted much interest. More particularly, multi-layered nanowires consisting of magnetic and nonmagnetic layers (FeNi/Cu, Ni/Cu, Fe/Cr, Co/Cu...) have been proven to exhibit outstanding properties which have straightforward applications: M-RAM (magnetic random access memories), nano-sensors, data storage... Most of the time, the bottle neck for the usage of such nanostructures is that their synthesis is not reliable, especially when it comes to producing very small wires, in the range of a few tens of nanometers diameter. We are exploring alternative synthesis routes in order to find a new self-ordering way of producing multilayered or core-shell nanowires which would be only based on diffusion processes and phase separation. Simply put, we would like to create a plain alloyed nanowire and provoke the formation of layers just by a well-designed heat treatment. We will first present our approach to grow alloyed metallic nanowires of various compositions. In order to do so, we adopted a process based on electro-deposition in porous membranes. Later on we will focus on the influence of the nanowire geometry on phase transformation during annealing.

MM 15.25 Mon 18:00 Poster B3

Low-temperature heat capacity and magnetization of CoCr-

FeNi and CoCrFeNiMn high-entropy alloys — •Josua Kottke[1], Martin Peterlechner[1], Mayur Vaidya[1,2], Blazej Grabowski[3,4], Fritz Koermann[3,4], Jörg Neugebauer[3], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Westfälische Wilhelms-Universität Münster, Germany — [2]Indian Institute of Technology Madras, Chennai, India — [3]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [4]Materials Science and Engineering, TU Delft, Delft, Netherlands

High entropy alloys, i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as a potential structural material due to attractive mechanical and physical properties. We report on the first measurements of low-temperature heat capacity of four- (CoCrFeNi) and five-component (CoCrFeNiMn) high-entropy alloys in the temperature interval from 1.9 to 400 K. The measurements were performed with and without application of a magnetic field (8T). Furthermore, room-temperature hysteresis loop and magnetization were measured in these alloys. The experimental data are compared with density-functional-theory-based calculations and a close agreement is seen. The deviations between the mean-field based theoretical results and direct experimental data are discussed in terms of probable ordering effects.

MM 15.26 Mon 18:00 Poster B3

Corrosion scale dynamics — •Markus Tautschnig, Nicholas Harrison, and Michael Finnis — Imperial College London

The presence of solid corrosion products, such as iron sulphides and iron carbonates, can lead to a significant reduction in the corrosion rate. Therefore, a fundamental understanding from the atomistic to the continuum level of their formation, stability and growth behaviour is vital for the oil and gas field equipment sustainability.

A "hexagonal slab" mesoscale growth model is being developed. This model has been created in order to predict the growth rate for scales with mesoscale morphology in various chemical environments. Assuming a dense and adherent scale, grain boundaries are considered as preferential pathways for the transport of charged point defects through the scale. The model includes the long range Coulomb interaction between the moving charged defect species. Migration-reaction-diffusion is simulated for the model geometry. The equations for the mobile species are solved numerically with a novel C++ code. Time dependent concentration profiles throughout the grain boundaries can be calculated.

MM 15.27 Mon 18:00 Poster B3

Wurtzite to rocksalt phase transitions in binary compounds — •Ning Wang, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

A pressure-induced wurtzite-to-rocksalt phase transition is observed in many binary compound semiconductors, such as CdSe, GaN and w-SiC. We analyzed this transition with the generalized solid-solid nudged elastic band method and determined the enthalpy landscape with first-principles calculations. Our results show that at both lower pressure and higher pressure, CdSe, GaN, and w-SiC prefer the tetragonal transition path to the hexagonal path. Furthermore, at lower pressure, the tetragonal-sliding and tetragonal-compression paths have almost the same transition barrier due to a similar intermediate tetragonal structure. At higher pressure, this metastable structure cannot be stabilized and the tetragonal-sliding path becomes energetically more favorable. We furthermore test the performance of two force fields for CdSe, and find that neither of them is able to describe the enthalpy landscape with good accuracy.

MM 15.28 Mon 18:00 Poster B3

Integration of a Fast-Scanning Calorimeter into a He-cryostat — •Daniel Gaertner, Martin Peterlechner, Christian Simon, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

The Fast-Scanning Calorimeter (FSC), also known as Chipcalorimeter, is a power compensated and small scaled Differential-Scanning Calorimeter. Typically, sample up to several micrometers in diameter can be investigated with high heating rates exceeding 10000 K/s. Two FSC sensor chips are used simultaneously, one sensor is used as a reference and the other for the sample. Depending on the thermal bath temperature it is expected to achieve even higher cooling rates under high vacuum in a He-cryostat, the Physical-Properties-Measurement-System (PPMS, QD-LOT). Another advantage is a switchable magnetic field up to 9 Tesla. The technical approach of this custom build system will be presented including calibration procedures. The present approach allows in-situ quenching of metallic glasses, and measurements of the magnetic contribution to the specific heat of high-entropy alloys.

MM 15.29 Mon 18:00 Poster B3

Atomistic study of the growth of a B33 NiZr crystal from the melt: Observation of five- and tenfold twinning — •M. Guerdane — Karlsruhe Institute of Technology (KIT), IAM-CMS, Karlsruhe

The crystallization of Ni50Zr50 from the melt is studied by means of molecular dynamics simulation. We consider pseudo-two-dimensional growth by setting up cylindrical crystalline NiZr seeds with a CrB-type structure (B33) and which can grow freely in all directions perpendicular to the cylinder axis. The crystallization is characterized by the formation of a high density of almost stress-free twins. The structure of the twins is reminiscent of that of FeB-type as predicted by Parthe earlier [1]. Moreover, fivefold and tenfold twinning is observed. The twins-formation mechanism is discussed and compared with that in pure materials as well as with the recently observed tenfold (quasicrystalline) twinned dendritic microstructure in the NiZr system [2].

1. E. Parthe, Acta Cryst. (1976). B32, 2813
2. W. Hornfeck et al., arXiv:1410.2952 [cond-mat.mtrl-sci].

MM 15.30 Mon 18:00 Poster B3

pressure induced phase transition in XeF2 — •Gang Wu[1], Xiaoli Huang[2], Yanping Huang[2], Xin Li[1], Fangfei Li[1], and Tian Cui[1,2] — [1]National Laboratory of Superhard Materials, Jilin University, Changchun 130012, P.R. China — [2]College of Physics, Jilin University, Changchun 130012, P.R. China

It is well known that high pressure will bring materials some unique properties such as metallization or superconductivity. XeF2 was reported to metalize under pressure. However, there is still controversy on its high pressure structure between the recent experimental and theoretical research. In this study, in-situ Synchrotron X-ray diffraction, Raman spectra and theoretical calculations are used to investigate the structure of XeF2 up to 94GPa. The experimental and theoretical Raman spectra results indicate that the ambient structure of XeF2 (I4/mmm) transforms into a Immm structure at 26GPa, and then high pressure phase (space group Pnma) appears at 56GPa. In the XRD study, the rietveld refinement results show that the I4/mmm structure (a=3.8242Å, c=6.7882Å, Z=2, 7.5GPa) changes into Immm at 26GPa(a=3.3789Å, b=3.4056 Å, c=6.5883Å, Z=2), and stabilizes with the pnma structure at 60GPa (a=4.5275Å, b=4.5025Å, c=6.4703Å, Z=4), which is in accordance with our Raman study.

MM 15.31 Mon 18:00 Poster B3

On the influence of temperature and dopant concentration on Cu-Si phase formation — •Honeyeh Matbaechi Ettehad[1,3], Stefan E. Schulz[1,2], and Alexander Heinrich[3] — [1]Technische Universität Chemnitz, Center for Microtechnologies, D-09107 Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (Fraunhofer ENAS), Technologie-Campus 3, D-09126 Chemnitz, Germany — [3]Infineon Technologies AG, Wernerwerkstr. 2, D-93049 Regensburg, Germany

One of the reliability issues of semiconductor devices is the interaction between Copper (Cu) and Silicon (Si) while contacting the solder material with the side wall of the semiconductor die. Cu from the lead frame can diffuse into Si by diffusing through the solder material. So, this could lead to crack or failure of the device due to strain that result from volume increase. Nucleation and growth of CuSix precipitates in Si has been studied by thermal treatment of copper layer in the range of 250-450°C on various commercially available silicon substrates, high-doped and low-doped. For all of the base materials the reaction between Cu and Si starts at lower temperatures in the range of 300-350°C, and leads to the formation of Cu3Si. Number density and diameter of precipitates for different base materials and annealings were assessed experimentally and characterized by means of FIB, SEM and optical microscope. The influence of different base materials on number density of the CuSi precipitation was investigated. Significant differences in number density and size of precipitates are seen for various temperatures and dopant concentrations and will be discussed.

MM 15.32 Mon 18:00 Poster B3

Phase-Field Study of Anisotropic γ'-Coarsening Kinetics in Ni-Base Superalloys with Varying Re and Ru Contents —

•Leslie Tafadzwa Mushongera, Micheal Fleck, Julia Kundin, Frank Querfurth, and Heike Emmerich — Material- und Prozesssimulation Universität Bayreuth, Universität Bayreuth, Germany

The coarsening kinetics of γ'-precipitates in single crystalline Ni-based superalloys is studied using phase-field simulations. At first, we discuss interdiffusion-limited γ'-coarsening in technologically relevant superalloys with the explicit inclusion of up to nine chemical components. The simulations show that an additional influence from the coherency strain leads to a substantially faster coarsening-evolution compared to the predictions from the LSW-theory. Second, we perform a virtual experiment to determine the influence of varying rhenium (Re) and ruthenium (Ru) additions on the temporal evolution of the γ-γ' microstructure under thermo-mechanical loads. We observe that a change in the Re content strongly alters the coarsening kinetics. On the contrary, it is found that Ru variations have no significant effect on the coarsening kinetics.

MM 15.33 Mon 18:00 Poster B3

Microstructure development of aluminum based alloys in additive manufacturing revealed from differential fast scanning calorimetry and metallographic studies — •Bin Yang[1], Olaf Kessler[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Rostock, Germany

To obtain the desired additive manufacturing (AM) fabricated aluminum-based alloy parts, the rapid solidification processes need to be investigated in-situ. Based on the calorimetric method (differential fast scanning calorimetry) developed for the study of metal particles, the solidification process of aluminum-based alloy powder-particles, i.e. AlSi10Mg, was studied, for the very first time, under AM relevant heating and cooling rate conditions. A preliminary series of DFSC heating and cooling experiments was conducted, applying cooling rates as high as 80,000 K/s. The differential fast scanning calorimeter traces revealed that the material undergoes a two-stage melting and solidification processes depending on heating and cooling rates. In particular, the solidification structure of the real time quenched single droplet was observed and analyzed with focused ion beam (FIB), scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). This research proposed a new approach to research the solidification structure of single aluminum-based alloys particles used in AM technologies with precisely controlled size and extreme cooling rate.

MM 15.34 Mon 18:00 Poster B3

Cluster dynamics modelling for the precipitation in Al–Cu — •Tobias Stegmüller and Ferdinand Haider — Univ. Augsburg, Inst. f. Physik, 86135 Augsburg

A key role in the production of modern metal alloys is to understand the precipitation processes occuring during thermal treatments, by which many material parameters like hardness or corrosion resistance can be controlled. A lot of these processes are qualitatively well understood controlled by empirical approaches. Nevertheless there is still a lack of knowledge in the quantitave understanding of the evolution of precipitates.

One approach for the simulation of such processes is the so-called cluster dynamics. In this approach the precipitate size distribution evolves with time. For that the precipitates are divided into classes, which are characterized only by the number of solute atoms n they contain. The temporal evolution is done by solving an initial value problem for the concentration c_n of precipitates belonging to class n.

Up to now the model has already several times been successfully applied to the formation of a single precipitate phase in binary alloys in literature. Our aim is to extend the model for an application to a system with multiple precipitate phases. For this purpose the Al-Cu system was chosen due to its well known precipitation sequence: the system decomposes via the formation of GP-Zones and different metastable phases. For the modelling a size distribution for each phase is needed and the distributions have to be linked to one another to gather the precursor–successor relationships between the phases.

MM 15.35 Mon 18:00 Poster B3

Microstructure Effects on Nanometric Cutting Behavior of Silicon — •Alexander Stukowski[1] and Saurav Goel[2] — [1]Technische Universität Darmstadt — [2]School of Mechanical and Aerospace Engineering, Queen's University, Belfast, UK

Silicon is being used extensively in both single crystal and polycrystalline form for a wide range of applications. To enable the production of ultra-thin wafers for future microelectronic applications, it is vital to fully understand the mechanical response of the material at small length scales.

We use direct molecular dynamics simulation to study the mechanisms of plasticity during cutting of monocrystalline and polycrystalline silicon. Our simulations are based on an improved long-range potential, providing a more accurate picture of the atomic-scale mechanisms of fracture, ductile plasticity, and structural changes in Si.

The simulation results show a unique phenomenon of brittle cracking inclined at an angle of 45° to 55° to the cut surface, leading to the formation of periodic arrays of nanogrooves in monocrystalline Si, which provides new insights into previously published experimental results. Furthermore, during cutting, silicon is found to undergo solid-state directional amorphisation without prior Si-I to Si-II phase transformation, which is in direct contrast to many previously published MD studies on this topic. Our simulations also predict that the propensity for amorphisation is significantly higher in single crystal silicon than in polysilicon, signifying that grain boundaries ease the material removal process.

MM 15.36 Mon 18:00 Poster B3

Push-Out Behavior of Tungsten Fiber-Reinforced Tungsten — •Bruno Jasper[1], Stephan Schönen[2], Jan W. Coenen[1], Till Höschen[3], Johann Riesch[3], Rudolf Neu[3,4], and Christian Linsmeier[1] — [1]FZ Jülich GmbH, IEK4 - Plasmaphysik, Jülich, GER — [2]FZ Jülich GmbH, ZEA1 - Engineering und Technologie, Jülich, GER — [3]IPP, Garching, GER — [4]TU München, Garching, GER

Tungsten (W) with its many beneficial properties, ranging from low hydrogen retention to low erosion yields during plasma exposure, is the candidate material for first-wall application in future fusion powerplants. The major drawback when working with W is its high ductile to brittle transition temperature. To circumvent this and to improve the overall mechanical properties, a tungsten fiber-reinforced tungsten (W_f/W) composite material is under development. W_f/W is composed of a drawn W wire, coated with an interface layer, and a W matrix. If a crack is introduced into the material energy dissipation mechanisms are enabled by the interface. They lower the crack tip energy, leading to extrinsic toughening and therefore to a pseudo-ductile behavior of the material.

For better understanding and more insight into the underlaying micro-mechanisms, push-out tests on single-fiber W_f/W samples were performed. This experimental work, that also covers the influence of sample geometry, sample preparation and test setup, is compared to results of dedicated finite element models.

MM 15.37 Mon 18:00 Poster B3

Mono-energetic Positron Source (MePS) — •Thu Trang Trinh[1], Oscar Liedke[1], Wolfgang Anwand[1], Andreas Wagner[1], and Reinhard Krause-Rheberg[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Martin-Luther Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Positron annihilation lifetime spectroscopy serves as an excellent tool for studies of open-volume defects in solid materials such as vacancies, vacancy agglomerates, dislocations, pores and voids. The intense mono-energetic positron beamline (MePS) at the ELBE accelerator developed for positron lifetime and conventional Doppler Broadening experiments offers a non-destructive investigation method to study of porous media as well as thin films as a function of thickness.

MM 15.38 Mon 18:00 Poster B3

Friction under active control — •Victor Pfahl[1], Walter Arnold[1,2], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Universität Göttingen — [2]Department of Materials Science, Saarland University

Dissipation of mechanical and kinetic energy at a sliding contact – better known as friction – strongly depends on the topological structure and chemistry of the contact and on the dissipation mechanism of the underlying material. But instead of varying these internal mechanisms we are using external acoustic excitations – which is called sonolubricity – to control friction actively.

Friction is measured with the lateral force microscopy (LFM) mode of an atomic force acoustic microscope (AFAM) with the simultaneous excitation of the contact resonance frequency of the AFAM cantilever. The cantilever is moving periodically resulting in a reduced average

contact force and therefore the friction coefficient is reduced as well.

We investigated the reduction of friction of Si, PdCuSi, and LaSrMnO as a function of amplitude of the cantilever at different temperatures. We report a reduction of friction up to 100% on every sample. Due to a metal-insulator transition near 350K especially temperature dependent measurements on LaSrMnO are interesting. A different reduction – amplitude relation is found in the metallic phase in comparison to the insulating phase.

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MM 15.39 Mon 18:00 Poster B3

Influence of thermal and mechanical pre-treatment on the properties of bulk metallic glasses — •Niklas Olschewski[1], Moritz Stolpe[2], Christian Simon[1], Harald Rösner[1], Ralf Busch[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Chair for Metallic Materials, Department of Materials Science, Saarland University, Germany

Metallic glasses provide many advantageous properties such as high elasticity, wear resistance and yield strength. Despite these features and the possible merits for the use of metallic glasses in applications, the evolution of the microstructure in glasses upon external influences such as mechanical stress or temperature is still not fully understood. An example is the formation of so called shear bands, which evolve in glasses after a certain degree of deformation: the microscopic origin of such unit shear events is still unresolved.

The presented work focuses on the impact of mechanical predeformation and thermal treatment by calorimetry at different rates on the state of a bulk metallic glass. In particular the dependence of the materials properties on different strain rates during linear and cyclic deformation as well as the behavior of the glass-transition for various heating rates was investigated. The results of these investigations lead to an improvement in understanding; that is, how the history of a glass, whether mechanical or thermal, is linked to its macroscopic properties.