MM 18: Poster Session I

Time: Monday 18:15–20:00 Location: P4

MM 18.1 Mon 18:15 P4

Analysis of polymers and stainless steels by scanning and transmission electron microscopy — •Bernhard Kaltschmidt, Inga Ennen, and Andreas Hütten — Thin Films & Physics of Nanostructures, University of Bielefeld, Bielefeld, Germany

The mechanisms of material aging are investigated to have a better understanding of the durability of materials. The aim of this work was to investigate the molecular changes induced by material aging. We examined polypropylene with different fillers like glass fibers and talcum. Here we analysed the microstructure of polypropylene after etching and heating. The polypropylene samples were freeze fractured and ultramicrotomed in different orientations. The stainless steels examined were: 1.4016, 1.4301 and 1.4510. The effects of pitting corrosion under different chemical environments were analysed. The steel lamellas used for TEM analysis of steel were cut by Focused Ion Beam (FIB). Results from SEM and TEM were compared to determine which technique is best suited for the task.

MM 18.2 Mon 18:15 P4

Detection and characterisation of amorphous silicon nanoclusters in laser-annealed silicon-rich silicon oxide via STEM — •Lukas Richert[1], Christoph Flathmann[1], Tobias Meyer[1], Hendrik Voigt[1,2], and Michael Seibt[1] — [1]IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]currently at Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Low-dimensional silicon such as crystalline or amorphous silicon nanostructures exhibit room-temperature photoluminescence in the visible range, which may lead to low-cost optoelectronic integrated circuits and LED displays. Laser annealing of an amorphous silicon-rich silicon oxide (SRSO) film with laser powers of 40 to 50 mW results in the thermal decomposition of SRSO into silicon and silicon oxide.

As a result of annealing, three distinct morphologies can be identified. Laser damage results in a porous area, surrounded by a silicon nanocrystalline-rich material and, finally, a phase-separated amorphous region consisting of amorphous silicon nanoclusters (aSi-NCs) and silicon oxide. Cross-sectional TEM lamellae are analysed using fluctuation electron microscopy and electron energy loss spectroscopy to investigate the microstructure of the laser-annealed sample and verify the existence of aSi-NCs.

MM 18.3 Mon 18:15 P4

Time and temperature resolved in situ investigation of the metal-induced crystallization of amorphous carbon thin films — •Matthias Krause[1], Daniel Janke[1], Robert Wenisch[1], René Heller[1], David Rafaja[2], and Sibylle Gemming[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden — [2]Institute of Materials Science, TU Freiberg, 09599 Freiberg — [3]Institute of Physics, TU Chemnitz, 09126 Chemnitz

The metal-induced crystallization of amorphous carbon in thin film stacks with Ni was investigated in situ as a function of initial stacking order, temperature and time by Rutherford backscattering spectrometry and Raman spectroscopy. Four different bilayer and triple layer stacks were exposed to heating ramps up to 700 °C. Formation of turbostratic carbon occurred simultaneously with a layer exchange (LE) and was completed during the applied heating ramp up to 700 °C. The temperature resolved measurements allowed the determination of the onset temperatures and transition rates as a function of the annealing temperature and the stacking order. Finally, the activation energy for both LE directions was estimated. In combination with the thermodynamic calculations, this in situ study allows to identify the metal-induced crystallization via wetting and diffusion along grain boundaries, instead of dissolution/precipitation upon annealing as the responsible mechanism for crystallization of amorphous carbon with layer exchange in contact with Ni.

MM 18.4 Mon 18:15 P4

Phase Transformations in TiAl during Selective Laser Melting (SLM) studied by X-ray Diffraction — •Jan Rosigkeit, Peter Staron, Emad Maawad, and Florian Pyczak — Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany

Interest in SLM has dramatically expanded in the last several years, owing to the advantages of additive manufacturing (AM) compared to conventional manufacturing. The possibility to generate complex components just from CAD-data using a layer-by-layer process may reduce production costs, lead times and material consumption. Complex components can be produced without a mold, and structures can be generated that cannot be produced by other techniques. AM attracts strong attention in the area of high performance materials like intermetallic Titanium Aluminide (TiAl) alloys. They represent innovative materials for high-temperature applications in aviation or energy generation, e.g. turbines blades. However, the cyclic heating and cooling during SLM leads to heat treatments of the previous solidified layers changing the phase content and inducing large residual stresses. Therefore, TiAl has so far only been additively manufactured using electron beam melting, which easily facilitates substrate heating to the required temperatures. Nevertheless, SLM of TiAl can also be achieved with sufficient substrate heating. This study focuses on the phase transformations and residual stress build-up as a function of process parameters in order to understand cracking. For this, diffraction measurements with high-energy X-rays were performed in-situ using an SLM chamber developed for use at a synchrotron beamline.

MM 18.5 Mon 18:15 P4

Antiphase domain growth on cubic lattices: a Monte Carlo study — •Ulrike Zweck and Michael Leitner — Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching

The ordering process in binary alloys, following the quench from a disordered state, has a great influence on system properties, such as magnetism or hardness. Describing the atomic ordering process as well as its kinetics accurately is crucial for understanding the correlation of system properties and structural order. The most accessible quantity in measurements, for example in scattering and diffraction experiments, is the structure function $S(k)$.

To give a general model for describing the ordering process and the behavior of antiphase domains (APDs) growing isotropically on crystal structures we investigate systems on cubic lattices via Monte Carlo simulations. We study systems exhibiting two, three or four APDs during the ordering process in the Ising model, the simplest atomistic model, as well as the standard q-state Potts model, which allows us a more abstract view on the ordering process. To describe and compare the growth and coarsening of APDs we exploit the scaling behavior of the pair correlation function as well as its Fourier transform $S(k,t)$ and obtain a scaling factor L for each time step in the ordering process. We define a master curve describing simultaneously the scaled correlation functions as well as their scaled Fourier transforms $S(k)L(t)$ and determine the kinetics of APDs in terms of $L(t)$. Thereby we obtain an explicit and quantitative coupling of length scales in real and reciprocal space.

MM 18.6 Mon 18:15 P4

Analysis of Crystal Defects in Tungsten by Positron Annihilation Lifetime and Doppler-Broadening Spectroscopy — •Vassily Vadimovitch Burwitz[1], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Physik Department E21 and FRM II, TU München — [2]Max-Planck-Institut für Plasmaphysik, Garching bei München

The quantitative analysis of radiation defects in tungsten is important for the safe operation of future nuclear fusion reactions.

Positron annihilation measurements were conducted in order to trace defect evolution through the treatment steps. All tungsten samples studied were cut by spark erosion from the same single-crystal rod with orientation (111), polished mechanically and electro-chemically before annealing at 2300 K under vacuum. One set of samples was irradiated by an MeV electron beam to different fluences, in order to produce Frenkel pairs as the predominant defect type. The other set was quenched from various temperatures close to the melting point in order to freeze in single vacancies at well-defined concentrations. This procedure provides a benchmark for single vacancies, thereby it is possible to determine if other defect types are present too. Positron annihilation lifetime (PALS) and Doppler-broadening spectroscopy (DBS) was performed simultaneously using a Na-22 source with two samples in sandwich geometry. First results are presented showing how different defect types in tungsten can be characterized by a combined analysis of DBS and PALS data.

MM 18.7 Mon 18:15 P4

Optical testing of phase change materials — •Simon von Oehsen, Maximilian Müller, Christoph Persch, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, 52074, Germany

Faster switching enables advances in information storage. The well established phase change materials have proven to be a promising candidate to increase the switching speed of non-volatile memory. Yet, after over two decades of research its kinetics are still not fully understood.

The phase change optical tester (POT) provides the possibilty to measure the reflectivity change during crystal growth in real time over 8 orders of magnitude down to 10^{-8} s. The sample temperature can be tuned by an underlying heater and a laser, whose different heating parameters open up a variety of measures to study phase transformations. It allows the examination of as-deposited material as well as melt-quenched systems. Many phase change compounds are continuously being studied this way.

The power of the employed laser is yet to be transformed to a temperature by simulation and calibration to the heater or differential scanning calorimetry in order to better access, compare and process the data in the well known time-temperature-transition (TTT) diagram.

MM 18.8 Mon 18:15 P4

Glass Dynamics and Crystallization Kinetics of the System GeSe:GeTe — •Maximilian Müller, Julian Pries, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, 52074, Germany

To optimize the application potential of phase-change materials (PCM) as random access memory switching speed from amorphous to crystalline phase has to be minimized. For a better understanding of the crystallization process of different materials it is important to clarify if crystallization occurs from the undercooled liquid phase or from a glassy phase and would be thereby depending on aging processes.

Because the glass transition of most phase change materials can not be observed in standard differential scanning calorimetric (DSC) measurements, a system of GeSe:GeTe was used to trace the stoichiometry dependence of glass transition from GeSe (non-PCM) for which glass transition is observable to GeTe (PCM) for which it is not. Additionally, ultra-fast DSC and standard DSC were used to explore the interplay of the glass transition and crystallization for heating rates in a range of more than 6 orders of magnitude.

From these data a lower boundary of the glass transition temperature of GeTe could be determined for a wide range of heating rates, especially for the standard glass transition heating rate of 20 K/min. The resulting dataset is also a promising starting point for further studies of glass dynamics and crystallization kinetics of GeTe.

MM 18.9 Mon 18:15 P4

Combining Atom Probe Tomography and Statistical Mechanics: Analysis of the Miscibility Gap in Copper-Nickel — •Marvin Poul, Rüya Duran, Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Deutschland

Although Copper-Nickel alloys are commonly used in technical applications, their alloying behavior at low temperatures is still controversial. Early theoretical and indirect experimental investigations indicated that the phase diagram may contain a miscibility gap. Nevertheless, direct experimental proof is missing due to the slow kinetics at low temperatures.

This work combines thin film Atom Probe Tomography measurements with a novel methodology based on statistical mechanics to extract T_c from histograms of thermodynamically inherent local concentration fluctuations annealed above T_c, i. e. in the region of complete miscibility, to side-step the slow kinetics. The same formalism allows access to relative chemical potential differences between samples with different mean concentration and the excess Gibbs free energy of mixing as a function of concentration, allowing direct approach to a Calphad parametrization.

The approach is showcased using Monte Carlo simulations and Atom Probe Tomography measurements of Copper-Nickel, yielding a T_c appreciably lower than the expected 600 K from current Calphad parametrizations and too low to be practically accessed in experiment.

MM 18.10 Mon 18:15 P4

Experimental investigation of the early stage precipitation reactions in Al-Cu alloys — •Johannes Berlin, Maximilian Gnedel, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg (Germany)

Due to their superior strength to weight ratio heat treatable Al-Cu alloys (2XXX-Series) are widely used particularly in aerospace industry. Although the occurring precipitates in these alloys are well known, the very early stages of formation and transformation mechanisms still are a topic of ongoing research. Transmission electron microscopy is used to investigate the influence of different parameters such as thermal history and additional plastic deformation on early stage precipitation in aluminum. Based on state-of-the-art transmission electron microscopy natural aging in form of growing GP-zones accelerated by excess vacancies can be examined, which was possible before only by diffraction experiments. In addition, DSC and hardness measurements are performed to evaluate the temper state of the specimens. The results are compared to numerical simulations. A better understanding of the precipitate formation mechanisms in these alloys for important future light-weight construction could be tuned more precisely regarding their intended use.

MM 18.11 Mon 18:15 P4

Analysis of grain boundary character and the resulting hardness distribution in High Entropy Alloys — •Lydia Daum, Bengü Tas, Martin Peterlechner, Sergiy Divinskiy, and Gerhard Wilde — Institute of Materials Physics

In this study four and five component alloys, CoCrFeNi and CoCrFeMnNi respectively, were prepared with different heat treatments to analyse their grain boundary character and their microstructures and mechanical properties. Thus, XRD, EBSD, EDX and Vickers microhardness indentation measurements have been carried out. The equiatomic distribution of the alloy components was shown with EDX maps for the polycrystalline alloys. A CoCrFe and a MnNi rich area was identified for the five component alloy which had been annealed at 500°C. An increase in hardness of about 8% was observed after annealing at temperatures between 500°C and 600°C for CoCrFeMnNi and CoCrFeNi, respectively. To compare each hardness value with respect to the grain orientation, a grid of hardness indentations were imprinted onto the sample surface and that surface was subsequently analyzed again by EBSD. Calculating for each hardness measurement the Schmid factor, a correlation between orientation and hardness was observed. Especially indentations in (1 1 1)-planes measured increased hardness values.

MM 18.12 Mon 18:15 P4

Electronic structure and stability studies on random configurations of silicon-germanium carbon alloys — •Willi Roscher[1], Florian Fuchs[2,3,4], Christian Wagner[5], Jörg Schuster[2,3,4], and Sibylle Gemming[4,5] — [1]Leibniz Institute for Solid State and Materials Research Dresden, D-01069 — [2]Fraunhofer Institute for Electronic Nano Systems, D-09126 — [3]Center for Microtechnologies, Technische Universität Chemnitz, D-09126 — [4]Institute of Physics, Technische Universität Chemnitz, D-09126 — [5]Helmholtz-Zentrum Dresden-Rossendorf, D-01328

One important application of silicon-germanium carbon are heterojunction-bipolar transistors (HBTs). Current research aims to reduce the device dimensions, making fluctuations on the atomic scale a serious concern. We therefore study the statistical distributions of the electronic properties in bulk $Si_{1-x-y}Ge_xC_y$. The entire composition range $0 \leq x \leq 1$ including small carbon concentrations is considered. Density functional theory is used in this study.

We demonstrate fluctuations of the band gap, which are in the range of about 10 %. These fluctuations occur in bulk SiGeC on a local scale, and they will become observable in down-scaled devices. Further properties, such as the lattice constant, the formation energy, and the change of Gibbs free energy are studied as well. Entropic contributions decrease the Gibbs free energy of mixed systems, which stabilize SiGeC at room temperature. Finally, local changes of the band gap in an HBT due to a spatially varying germanium concentration are presented.

MM 18.13 Mon 18:15 P4

On the complex structure and phase boundaries in Fe-Al binary alloys — •Subhamoy Char and Dasari Prasad — Department of Chemistry, Indian Institute of Technology Kanpur, UP-208016, India

Although elemental Fe and Al are simple metals in their respective

ground states, the solubility of one in another with varying composition leads to a series of intermetallic Fe_xAl_y phases consists of wide variation in structure, electronic, magnetic, and mechanical properties. The phases are dressed-up with full of complexities that are often challenged the computations to comprehend the structure-property relationship. This is mostly attributed due to the fact that the structures undergo temperature driven order-disorder phase transformations, thermal vacancies, antisite defects, and ambiguous phase segregation between different Fe-Al phases. Therefore, it is indispensable to correctly model the phase diagram by predicting the Fe-Al structures at finite temperature. While the DFT is more effective in calculating total energies and forces of such alloys, it is computationally quite an arduous task in predicting the structures across the temperature verses the compositional structure state-space of Fe-Al phase diagram. Here, we have adopted a hybrid data-driven, stochastic and evolutionary crystal structure prediction approach coupled to DFT electronic energy calculations to predict thermodynamically viable structural solutions and thereby the Fe-Al phase boundaries are constructed. It is found that the vibrational entropy essentially steers the inexplicable phase segregations in Fe-Al binary alloys.

MM 18.14 Mon 18:15 P4

Analyse und vergleichende Synthese von anodischen Aluminiumoxidschichten auf technischen Aluminiumlegierungen — Ivan Zadyraka, Stefan Ostendorp, Martin Peterlechner und •Gerhard Wilde — Institut für Materialphysik und CeNTech, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, D-Germany

Bauteile aus technischen Aluminiumlegierungen finden in vielen Bereichen Anwendung. Die Oberflächenvergütung mittels Anodisierung stellt hierbei ein wichtiges Mittel dar, um sowohl die mechanische als auch chemische Resistenz der Bauteile zu gewährleisten. Ziel dieser Arbeit ist die Untersuchung vermeintlich vergleichbar oder ähnlich hergestellter Aluminiumoxidcoatings auf verschiedenen Aluminiumlegierungen mit einem Fokus auf den strukturellen und chemischen Eigenheiten dieser Schichten. Mit Hilfe von elektronenmikroskopischen Untersuchungen inkl. EDX-basierter Elementanalysen sollen Korrelationen zwischen mikroskopischen Eigenschaften und der makroskopisch ermittelten chemischen Resistenz der untersuchten Schichten hergeleitet werden. Zum Vergleich wird Rohmaterial der entsprechenden technischen Legierungen in variierenden Oxal- und Phosphorsäure-basierten Elektrolyten unter DC-Potential und potentiostatischen Bedingungen im Labormaßstab anodisiert. Analog zu den kommerziellen Produkten wird anschließend ein Heißwasser-Sealing angewendet. Analysen dieser Coatings zeigen Unterschiede zu kommerziellen und somit gebräuchlichen Schichten auf und erlauben die Diskussion über einen optimierten Herstellungsprozess für solch schützende Aluminiumoxidschichten.

MM 18.15 Mon 18:15 P4

Copper Precipitates in Aluminum Alloys studied by Positron Annihilation Spectroscopy — •Leon Chryssos, Thomas Gigl, and Christoph Hugenschmidt — Physics Department E21 and Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München

Aluminum alloys are an integral part of modern engineering. However, due to its poor welding properties and rigidity, pure aluminum is not suitable for most industry applications. Therefore, most of the shortcomings of pure aluminum can be mitigated by alloying percentage amounts of copper. The formation of copper precipitates in the aluminum lattice introduces strain and, hence, improves rigidity. Due to its, in comparison to Al, greater positron affinity, Cu clusters can be detected in AlCu alloys using Coincident Doppler Broadening Spectroscopy (CDBS). To better understand the precipitation process the Al alloy EN AW-2219 T87 was treated under different conditions ,i.e. samples were prepared using different artificial aging procedures. Afterwards they were analysed using the CDB Spectrometer at NEPOMUC/FRMII of the TU München. With this method it was possible to determine optimal aging parameters for the alloy. A summary of the investigated procedures will be presented, giving an insight into the Cu precipitation process and dissolution of precipitates under different annealing conditions.

MM 18.16 Mon 18:15 P4

DFT characterization of β- and δ- intermetallic Al-Fe-Si phases — •Nebahat Bulut[1], Hanka Becker[2], Andreas Leineweber[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, Germany

The β-$Al_{4.5}FeSi$ and δ-Al_3FeSi_2 phases are known stable phases of Fe-containing Al-Si alloys. Despite the known stoichiometry of the β- and δ- phase the positions of the Al and Si atoms in these Al-Fe-Si intermetallic phases could not be uniquely determined experimentally [1]. Therefore possible positions of Si atoms in these intermetallic phases were investigated using the density functional theory (DFT) code Quantum Espresso, which is based on plane waves and pseudopotentials [2]. For all calculations the PBE exchange-correlation functional has been used.

For both β- and δ- phase different arrangements of Si atoms in the Al-Fe-Si intermetallics were considered. We compare the energies of these arrangements (1) relaxing the atomic positions keeping the unit cell volume constant and (2) fully relaxing atomic positions and unit cell shape and volume. As result we find that arangements where the Si atoms are not nearest neighbours are energetically favored. Further, we analyze the electronic structure and investigate the bonding.

[1] Becker et al., JAC 780:917-929, (2019)
[2] P. Giannozzi et al., J.Phys.Condens.Matter 21, 395502 (2009)

MM 18.17 Mon 18:15 P4

Ab initio opto electronic properties of magnesium silicide alloys — •Juan Guerra, Marcel Giar, Carsten Mahr, Michael Czerner, and Christian Heiliger — Justus Liebig University Giessen, Institut für Theoretische Physik, Giessen, Germany

Due to an increasing interest in the use of environmentally friendly materials for energy conversion, we present a comprehensive ab initio analysis of the opto electronic properties of magnesium silicide materials. These materials have shown an enhancement in the thermoelectric performance when alloyed by Sn as consequence of the convergence of the conduction bands and the reduction of thermal transport. Mg2Si and Mg2Ge have also be shown to be thermodynamically unstable when alloyed by Sn for compositions between the so-called miscibility gap. Our calculations are based on the full-relativistic Green's function Korringa, Kohn and Rostocker (KKR) formalism, within the coherent potential approximation (CPA). We perform total energy calculations to obtain optimal structural properties and relative formation energies to interpret the material's instability. Using the Bloch spectral density function (BSF), we interpolate and map the electronic bands to extract relevant parameters for transport, e.g., band gaps and effective masses within the single parabolic band approximation. We also provide calculations of the contributions to the dielectric function due to direct interband transitions via the joint density of states (JDOS).

MM 18.18 Mon 18:15 P4

Lattice Dynamics of W-Cr Alloys by Ab Initio Calculations — •Michal Farana, Andrzej Piotr Kadzielawa, and Dominik Legut — IT4Innovations, VSB - Technical university of Ostrava, 17.listopadu 2172/15, CZ 708 00 Ostrava - Poruba, Czech Republic

Tungsten alloys are promising candidates to replace the currently favored choice - pure tungsten [1] in the first wall applications in future fusion facilities. The main goal of the alloying of tungsten is to gain additional properties such as self-passivation under accidental conditions [2,3]. According to the W-Cr phase diagram [4], the single solid BCC solution experiences tendency for phase separation within the miscibility gap to reach thermodynamic equilibrium. We applied the Density Functional Theory both within the Special Quasirandom Structure and Virtual Crystal Approximation frameworks to obtain a realistic model of Tungsten-Chromium alloy, with the elastic (via deformation of the crystal) and thermodynamic (via the phonon spectra within the Quasiharmonic Approximation) properties to be compared with experimental data. Based on our results we promote a possible route to enhance both melting temperature as well as the miscibility gap in the Cr-W alloys.

References:

[1] M. Kaufmann Fusion Eng. and Des. **82** 521-527 (2007)
[2] F. Koch, H. Bolt. **T128**, 100-105 (2007).
[3] M. Vilémová, K. Illková, F. Lukáč. **127**, 173-178 (2018).
[4] W-Cr phase diagram, Bul. of Alloy Phase Diagr. Vol. 5 No. 3 1984.

MM 18.19 Mon 18:15 P4

Computational prediction of solubility limits in selected solid solutions — •Ondřej Fikar and Martin Zelený — Faculty of Mechanical Engineering, Brno University of Technoloty, Brno, Czech

Republic

We provide a theoretical study of the phase stability of solid solutions in Al-Ge, Al-Pb, Ag-Au, Ag-Ge and Ag-Pb alloys, in which there are no intermediate phases across the whole composition range. Solubilities of Au, Ge and Pb in Ag and Al were determined using temperature-dependent free energies of pure elements and corresponding Al- and Ag-rich solid solutions obtained from ab initio calculations based on density functional theory. Contributions of vibrational free energy calculated from phonons, electron free energy and configuration entropy were considered. The temperature, at which a solid solution become stable, was estimated from the free energy difference between solid solution and mixture of pure elements. In case of the Al-Ge alloy, quasi-harmonic approximation was employed to include also the effect of volume expansion. For this system we employed more precise approach where mixture of Ge and Al-rich solid solution with maximum solubility were considered instead of mixture of pure elements. Predicted solubilities were compared with experimental ones in phase diagrams provided by the CALPHAD method. The results qualitatively agree with experimental observations. However, the exact temperatures at which the solid solutions become stable are underestimated.

MM 18.20 Mon 18:15 P4

Impact of magnetism on the energy of stacking faults in the *C*14 $NbFe_2$ Laves phase — •Ali Zendegani, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The stacking fault energy (SFE) is a key descriptor for predicting plastic deformation mechanisms of materials. In Laves phases basal synchroshear-formed stacking faults (BSSF), which locally transform the hexagonal $C14$ into the cubic $C15$ Laves phase, support the propagation of dislocations. The calculation of the BSSF in $NbFe_2$, however, results in a negative energy, if a ferrimagnetic ground state configuration is used for the *ab initio* supercell. The underlying reason is that ferrimagnetic $C15$ is more stable than ferrimagnetic $C14$ in this system [1].

Considering the very low magnetic ordering temperature of 10 K we, therefore, performed computationally challenging paramagnetic calculations. In this case $C14$ has the lower energy as compared to $C15$. A transfer of this method to the more complex BSSF containing supercells is not yet feasible. Instead, we present an alternative analytical approach [2], which correlates the SFE with the difference of the $C14$ and $C15$ bulk energies and thus allows to determine the energy of the complex BSSF in $NbFe_2$ properly including the magnetic contribution [1].

[1] M. Šlapáková, et al. *Acta Materialia* 183 (2020):362-376.

[2] F. Chu, et al. *Philosophical magazine letters* 72.3 (1995): 147-153.

MM 18.21 Mon 18:15 P4

Large-scale simulations of plasticity in nanocrystalline Iron — •Hoang-Thien Luu and Nina Gunkelmann — Institute of Applied Mechanics, TU Clausthal, Germany

Shock compression is widely used to investigate the mechanical responses of iron under dynamic loading. It has been long known that α-iron transforms to ϵ-iron under high pressure. Recently, molecular dynamics simulations have shown that plasticity occurs just before the parent phase transforms into ϵ-iron. To provide insights into the interplay of elastic and plastic activities during shocks in iron, we performed atomistic simulations of shock compression of nanocrystalline iron with a mean grain size of 20 nm comprising a total number of 267.5 million atoms. We observed elastic and plastic deformations before the phase transformation takes place. The plastic state is metastable and highly depends on the deformation rate. After a relaxation process of a few picosecond, the structure transforms to a quasi-3D compressed state in which the new phase is stable. The process is ramp time-dependent. In addition, we found that with increasing ramp time of the piston, the period of plasticity is longer.

MM 18.22 Mon 18:15 P4

Electronic and Optical Properties of Bismuthene on a SiC Substrate — •Armando Consiglio and Domenico Di Sante — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

The work focuses on the study of the electronic and optical properties of a material based on a monolayer of Bismuth atoms in an honeycomb structure, known as Bismuthene, supported by an insulating Silicon Carbide (0001) bilayer substrate that stabilizes the system and that contributes to the electronic properties. As the high atomic number of Bismuth atoms leads to an high Spin-Orbit Coupling, and so to large values of the energy gap, this material is promising in the framework of the Quantum Spin Hall systems. Here we show our results based on first principles calculations, obtained via Density Functional Theory and GW methods, and we compare them with experimental results.

MM 18.23 Mon 18:15 P4

Self-consistent implementation of meta-GGA functionals in the (L)APW code Wien2k — •Jan Doumont, Fabien Tran, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

We present a self-consistent implementation of meta-GGA functionals in a full-potential (linearised) augmented plane-wave density functional theory (DFT) code. Because the exchange-correlation (xc) potential is not multiplicative the generalised Kohn-Sham (gKS) formalism was used. To evaluate the energy and potential of the functionals, Libxc was used. We will discuss the novel (compared to a GGA functional) contributions to the matrix elements of the hamiltonian and discuss their implementation. Furthermore we present some convergence and performance tests of the meta-GGAs compared to PBE.

MM 18.24 Mon 18:15 P4

Theoretical Description of Non-linear Processes in magnetic material — •Shalu Rani and Valérie Veniard — École Polytechnique, Institute Polytechnique de Paris, Palaiseau, France

Chromia is an anti-ferromagnetic insulator and an ideal material to demonstrate ultra-fast control of demagnetization at higher speed. Ultra-fast control on magnetic state could have the strong impact on magnetic recording technology.

Second harmonic generation (SHG) is used to study the optical properties of materials. SHG is forbidden in centro-symmetric materials and it is possible to obtain a structural and electronic characterization for these systems. However, the absence of time-inversion symmetry in antiferromagnetic materials leads to new contributions in second harmonic generation, thus revealing the arrangement of spins in the solid. SHG becomes a powerful tool to study of ultra-fast demagnetization processes. Chromia is centrosymmetric, but SHG occur because symmetry broke due to the spin.

There are few satisfactory theoretical descriptions for SHG in magnetic materials, since spin-orbit coupling, electron-electron interactions and local field effect must be treated on the same footing. The project is to calculate the Second order response function of chromia using Time-Dependent Density Functional Theory, and taking into account the many-body effects through an exchange-correlation kernel derived from the Bethe-Salpeter equation (BSE) for the linear response.

Results will be shown for the linear response, the GW corrected band gap for the Chromia and for the BSE calculations

MM 18.25 Mon 18:15 P4

Ab initio studies on NbO_2 — •Kathrin Kulmus, Sibylle Gemming, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz

The insulator-metal transition (IMT) of niobium dioxide occurs at T_c = 1080K with changing the crystal structure. It is found experimentally[1] as well as theoretically[2], that NbO_2 behaves like a one-dimensional conductor in its metallic phase. Regarding excitonic effects, we analysed the dielectric function, the partial density of states and the bandstructure (fat bands) in an all-electron ab-initio calculation, each directionally resolved. We further examined the recently found photoinduced IMT at temperatures below T_c[3], i.e. the separation of the thermal and the electronic phase change.

The all-electron DFT code Questaal[4] was employed for the calculations; we acknowledge many valuable discussions with the developer team.

[1] G. Bélanger et al., Can. J. Phys. **52**, 2272(1974)

[2] A. O'Hara et al., J. Appl. Phys. **116**, 213705(2014)

[3] R. Rana et al., Phys. Rev. B. **99**, 041102R(2019)

[4] www.questaal.org

MM 18.26 Mon 18:15 P4

Towards all-optical spectroscopy of ordered and disordered phononic crystals — •Tobias Claus, Sina Ludewig, and Henning Ulrichs — I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

On this poster we report on our recent progress regarding the conceptual realization, fabrication and optical spectroscopy of disordered and ordered phononic metamaterials. Besides applications in acoustics and heat conduction, such materials can generally be used as macro- to nanoscale toy models for physical phenomena based on wave interference. Note that topological spectral properties are nowadays of great scientific interest mainly regarding electronic structure. But also bosonic excitations like magnons and the here addressed phonons can acquire unconventional properties like localization due to symmetry breaking [1] or due to disorder-induced omnidirectional band gaps. [2] Here, we present our design strategy for metamaterials targeting elastic dynamics from the MHz to GHz spectral range. This strategy is based on FEM modelling of the sample and of the finally envisaged all-optical pump-probe experiment. Secondly, we discuss our experimental setup and first measurements on a sample structured by the focussed ion beam experimental technique. We acknowledge financial support by the DFG within the SFB 1073.

MM 18.27 Mon 18:15 P4

Atomistic study of the influence of oxide shell layers on the material properties of aluminum nanowires — •Hoang-Thien Luu[1], Yudi Rosandi[2], and Nina Gunkelmann[1] — [1]Institute of Applied Mechanics, TU Clausthal, Germany — [2]Department of Geophysics, Universitas Padjadjaran, Indonesia

For materials with high oxygen affinity, oxide layers will significantly change the material properties. At aluminum surfaces, an oxide layer may form in seconds, even under vacuum conditions. Recent studies show that thin amorphous oxide shell layers on aluminum surfaces significantly change the responses of the material. However, the relations between the thickness of the oxidized layer, the temperature and the mechanical response of nanowires have not been investigated intensively. In this study, we use a ReaxFF potential to analyze the influences of oxide shell layers on the material responses of the nanowires under uniaxial loading at different strain rates. We conduct simulations within a wide range of strain rates and temperatures varying between 10K and 500K. The Al-O interface leads to an increased defect nucleation rate at the oxide interface preventing localized deformation.

MM 18.28 Mon 18:15 P4

Investigation of electrostatic and elastic grain interactions in ferroelectric ceramics using the self-consistent mesoscopic switching model — •Ruben Khachaturyan[1], Anna Grünebohm[1], and Yuri Genenko[2] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum — [2]Institute of Materials Science, Technische Universität Darmstadt

The self-consistent mesoscopic switching model simulates polarization kinetics of polycrystalline ferroelectrics taking into account electrostatic interactions [1]. The model is now improved to take into account elastic interactions between grains. This improvement allows for polarization and strain kinetics description taking into account local strains and electric fields. Having a switching barrier as one of the input parameters the model promises to become a bridge between polycrystalline materials and atomistic simulations.

[1] **Correlated polarization-switching kinetics in bulk polycrystalline ferroelectrics. II: Impact of crystalline phase symmetries**, R. Khachaturyan, Y.A. Genenko,*Physical Review B.*, **98(13)**, 134106, (2018)

MM 18.29 Mon 18:15 P4

Impact of pressure on bulk diffusion in TiN: a combined ab initio and molecular dynamics study — •Ganesh Kumar Nayak[1], Ilia Ponomarev[2], Paolo Nicolini[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700, Leoben, Austria — [2]Department of Control Engineering - K335, Faculty of Electrical Engineering, Czech Technical University in Prague, Karlovo náměstí 13, 121 35, Prague 2, Czech Republic

Cutting tools protected with hard coatings have been successfully employed in the industry for almost 50 years. In our project, we investigate Ti(Si)VN nanostructured coatings with the aim to control the formation of V2O5 surface oxide acting as a solid lubricant in order to extend the lifetime of cutting tools. In the present work, we report on state-of-the-art DFT and Molecular Dynamics calculations of diffusion barrier for V and Ti in the crystalline TiN matrix. Special attention is paid to the impact of pressure on the diffusion properties, an effect experimentally relevant since the physical-vapor deposited coatings often exhibit compressive stresses. Interestingly, the preliminary results show no significant impact of pressure on the barrier heights obtained using the nudged-elastic-band method. Detailed analysis of these results as well as discussion of different diffusion scenarios (pathways) will be presented.

MM 18.30 Mon 18:15 P4

Calorimetric Study of Low Melting Eutectics in Chlorine-induced High Temperature Corrosion Environment — •Sophie Winkler, Sebastian Pentz, and Ferdinand Haider — Chair of Experimental Physics I, University of Augsburg, 86135 Augsburg

Waste incineration power plants provide an energetic usage of the produced heat by thermal composition. Complex systems in the exhaust stream are used for the heat extraction at prevalent temperatures of 400–600 °C. These steel pipes are exposed to the flue gas and therefore subject to a high degree of corrosion. The main damage is caused by the chlorine induced high temperature corrosion. Sulfation reactions of the sulfur dioxide with solid alkali chlorides in the flue steam occur which results in a release of chlorine or chlorine compounds in close proximity of the metallic components like superheaters or boiler walls. The released Cl_2 or HCl attack the iron under formation of $FeCl_2$ or $FeCl_3$ leading to a massive removal of the steel material.

The resulting deposits of the steel pipes are then subjected to different methods of thermal and elemental analysis to determine the composition and chemical reactions happening in the corrosion process. Using Differential Scanning Calorimetry, it is possible to construct the phase diagrams of the participating sulfates ($CaSO_4$, K_2SO_4, Na_2SO_4) and to analyse the occurring low melting eutectics that accelerate the corrosion process.

MM 18.31 Mon 18:15 P4

Study of the evaluation of NanoBeam Electron Diffraction Patterns from Bulk Metallic Glasses — •Manuel Lindenblatt, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

An approach to obtain knowledge about the properties of a material is to analyze its structure with diffraction experiments such as in a transmission electron microscope (TEM) done with electron diffraction. Using these experiments to evaluate the structure of a metallic glass proves to be a challenge, since no long range order (LRO) is available. However, the structure of glasses may be characterized by the specific medium range order (MRO) that is present. One possibility to analyze the MRO to evaluate a nanobeam electron diffraction pattern (NBDP) concerning the radial distribution function (RDF).

With the sample being a bulk metallic glass (Vitreloy105, $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ in at%) the focus of the present work is on analyzing the MRO structure of a shear band via obtaining the NBDP (by [1]). This task was approached for each relating parameter individually at first. One significant improvement done by this work is a method to find reliable and reproducible center coordinates for any elliptical undistorted single NBDP. Another contribution relates to the measured background intensity. This work discusses the physical meaning of the parameters relating to the obtained RDFs and discusses also the reliability of information obtained through the RDF analysis concerning the real-space structure of glasses.

[1] S. Hilke et al, Acta Materialia, 171:275-281, 2019.

MM 18.32 Mon 18:15 P4

Investigations on the relaxation of metallic glasses using fast scanning calorimetry — •Maximilian Demming[1], Mark Stringe[1], Martin Peterlechner[1], Gerhard Wilde[1], and Benedikt Bochtler[2] — [1]IMP Uni Münster — [2]LMW Uni Saarland

During isothermal annealing below the glass transition, all glasses, and thus also metallic glasses, show relaxation effects that resemble the underlying trajectory in phase space towards metastable equilibrium. Using fast scanning calorimetry (FSC) it becomes feasible to investigate such phenomena over a wide range of rates and at very high controlled heating or cooling rates. The tremendous advantage of FSC in comparison to a conventional differential scanning calorimeter (DSC) is, that here one can reach cooling and heating rates up to several 10000 K/s, which makes in-situ quenching possible. Another advantage is that a large number of measurements can be performed in small time intervals. This makes the FSC quite interesting for experiments in thermic cycling with controlled heating and cooling rates. One special method is the so-called cryogenic cycling, which means, that a sample is periodically quenched and reheated between room and a cryogenic temperature. According to literature, this treatment, that has been

termed as *cryogenic rejuvenation* could lead to markedly changed properties of the metallic glass. The materials investigated here are AuCuSiAg and PdNiS due to their low glass transition temperature and melting point. Here different relaxation states achieved by in-situ quenching via FSC are examined and compared to the relaxation behavior observed at conventional rates.

MM 18.33 Mon 18:15 P4

Investigating the short-range order (SRO) of glassy $Ge_{15}Te_{85}$ and GeSe obtained by TEM diffractometry — •Christian Stenz, Julian Pries, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany

In contrast to the crystalline phase, in the amorphous glassy and undercooled-liquid phase atoms show no long-range order and have no periodic structure. Still, atoms in amorphous solids exhibit a certain short-range order (SRO), which can be inferred from diffractometry. Here, transmission electron microscopy (TEM) is utilized in order to acquire selective area electron diffraction (SAED) patterns of as-deposited amorphous $Ge_{15}Te_{85}$ and GeSe. The 2D diffraction patterns acquired are circularly integrated to obtain 1D diffraction profiles. From these diffraction profiles the pair distribution functions (PDFs) are calculated using *SUePDF* providing insight on the SRO. After background substraction, algebraic redefining and normalization, the PDF is obtained by a Fourier transformation of the 1D diffraction pattern. The PDFs are compared to the expected atomic distances of the crystalline phase by a *MATLAB* program, which outputs the corresponding PDF computed from the unit cell.

MM 18.34 Mon 18:15 P4

Effects of annealing and thermal history of glassy materials — •Alexander Heinrich, Julian Pries, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany

The relaxation dynamics of glassy materials can vary dependent on its thermal history and of the material itself. To understand structural relaxation dynamics more, this process is simulated according to Hodge and Berens. They published their simulating scheme as early as 1981. This simulation uses the expression of Tool Narayanaswamy Moynihan (TNM). This simulation numerically solves the TNM-equation of the fictive temperature T_f for discrete temperature steps. Thereby the normalized heat capacity is calculated by deviating the fictive temperature by temperature. By reproducing this simulation and results of Hodge and Berens, the simulation can be used to simulate the cooling and heating cycle of a glassy material. The simulation enables the prediction of glass dynamics close to the glass transition for different thermal histories.

MM 18.35 Mon 18:15 P4

Signatures of quasiparticle transport in excitonic insulator candidate: Ta_2NiSe_5 — •Yuan-Shan Zhang[1], Jan Bruin[1], Yosuke Matsumoto[1], Masahiko Isobe[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany — [3]Department of Physics, Univerisity of Tokyo, Japan

Ta_2NiSe_5 is a narrow gap semiconductor which is electronically quasi-one-dimensional and undergoes a transition to an excitonic insulator at T_c=328K[1], where the electron-hole pairs condense into a many body ground state. Thermal conductivity is a useful probe for the quasiparticle states as well as the relevant phonons in excitonic insulators.

Here, we present the temperature dependence of thermal conductivity $\kappa(T)$ of single crystals of Ta_2NiSe_5 around the transition temperature, measured along both parallel and perpendicular to the quasi-one dimensional chain direction. We observed a clear anomaly in $\kappa(T)$ at T_c: a kink followed by a raid decrease below T_c for the chain direction and a pronounced dip for the perpendicular to the chain direction.

We argue that, while the former originates predominantly from the quasi-particle contribution, the latter represents the phonon contributions scattered by the shear-mode soft phonons coupled strongly to the excitonic state.

[1] Y. F. Lu et al. Nat. Commun., **8** 14408(2017)

MM 18.36 Mon 18:15 P4

Monte Carlo simulation of the energy distribution in laser-irradiated solids under the influence of a magnetic field — •Xavier del Arco, Julia Amann, Pavel N. Terekhin, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Strasse 46, 67663 Kaiserslautern, Germany

The complex phenomenon arising after irradiation of a solid with ultrashort laser pulse is studied using a Monte Carlo simulation. Two possible electron interactions are considered: inelastic scattering and impact ionization. The influence of the external homogeneous magnetic field on the energy exchange between the electron and lattice subsystems is investigated. The results of this simulation contain the information about the evolution of the electron density, electron and lattice energy distributions. The developed approach can be used to study the influence of the magnetic field on the energy deposition and develop optimal strategies to improve ablation processes in solids.

MM 18.37 Mon 18:15 P4

Interdiffusion and atomic mobility in Mo-Zr and Mo-Nb-Zr bcc phase alloys — •Baixue Bian[1], Yong Du[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Gemany — [2]State Key Laboratory of Powder Metallurgy, Central South University, 410083 Changsha, China

Accurate kinetic characteristics of refractory alloys are critical for understanding and tuning the phase transformation and microstructure evolution during homogenization and precipitation. In this work, the diffusion couple technique, Bltzmann-Matano and Matano-Kirkaldy methods were applied to measure the interdiffusion coefficients of bcc phase Mo-Zr binary alloys and Mo-Nb-Zr ternary alloys at 1423-1523 K, respectively. Subsequently, on the basis of the presently obtained interdiffusivities together with the thermodynamic descriptions for bcc Mo-Nb-Zr system, the atomic mobility parameters of Mo, Nb and Zr elements were assessed by means of DICTRA software package. Moreover, the comprehensive comparisons between the experimental diffusion properties (i.e., interdiffusivities, composition profiles, and diffusion paths) and the calculated /model-predicted data due to the present atomic mobilities were conducted in order to verify the reliability of the mobility values. The present atomic mobilities for bcc Mo-Nb-Zr system are shown to provide the accurate interdiffusivity matrix over a wide composition range.

MM 18.38 Mon 18:15 P4

Investigation of Hydrogen Isotopologue Sorption in Ti/Pd Films — •Sonja Schneidewind[1], Sebastian Vetter[1], Christian Goffing[1], Max Aker[1], Marco Langer[3], Andreas Fleischmann[2], Loredana Gastaldo[2], Andreas Reifenberger[2], and Magnus Schlösser[1] — [1]IKP, KIT, Karlsruhe, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg, Germany — [3]ITEP, KIT, Karlsruhe, Germany

Certain metals can solve hydrogen isotopes in their lattice structure and can subsequently form metal hydrides. Out of these materials, Ti has one of the lowest dissociation pressures which allows for quasi-irreversible hydrogen isotope capture. However, the Ti surface tends to form an oxide layer in air which acts as effective permeation barrier. The oxidation can be prevented by a thin Pd film on top allowing for gas permeation through the Pd layer into the Ti getter. This technique can be used to build effective passive hydrogen isotopologue pumps or by employing the radioactive isotopologue, tritium, one can build dedicated radioisotope heat sources, e.g. for calibration purposes.

We perform sorption experiments by using a quartz crystal micro balance with nanogram resolution to determine the dependence of absorbed gas amount and durability of absorbed gas in Ti/Pd films on loading parameters. Films coated on QCMs are exposed to hydrogen isotopologue gas. XRD and resistance measurements are used to study phase transformations and to verify the absorbed gas amount. The sorption of tritium by the films is investigated by Beta-Induced X-Ray Spectrometry combined with simulations using GEANT4.

MM 18.39 Mon 18:15 P4

Nanoscale heat transport in heterostructures — •Jan-Etienne Pudell[1], Marc Herzog[1], Alexander von Reppert[1], Gregory Malinowski[3], Matthias Rössle[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Institut Jean Lamour, Université Lorraine, Nancy, France

The transport of heat (or energy in general) in nanoscopic heterostructures is of great interest on a fundamental as well as a technological level, e.g. in the context of thermal management in devices or heat-assisted magnetic recording. In metal heterostructures, heat can be

conducted by electrons, which are in- or out-of-equilibrium with lattice vibrations. Using time-resolved x-ray diffraction, we investigate the thermal transport through a 100 nm Cu layer sandwiched by thin Pt and Ni films on a glass substrate on picosecond time scales after femtosecond laser excitation. A time-dependent diffusive transport model accurately reproduces our experimental data and thus verifies the efficient transport channel from the laser excited Pt-layer to the Ni-layer via hot electrons. The results imply dominant diffusive instead of ballistic electron transport.

MM 18.40 Mon 18:15 P4

Synthesising high-T_c hydrides for the electrical transport measurements — •Takaki Muramatsu[1], Israel Osmond[1], Owen Moulding[1], Jonathan Buhot[1], Oliver Load[2], and Sven Friedemann[1] — [1]School of Physics, University of Bristol, UK — [2]School of Earth Science, University of Bristol, UK

A series of high-T_c superconductors (LaH_x, YH_x, and ThH_x) have been reported in hydrogen-rich hydrides under extreme high pressures since 200 K superconductivity was discovered in H_3S in 2015 [1-6]. The hydrides are synthesised under high pressure above 100 GPa by using laser-heated diamond anvil cell (DAC) technique and the superconducting transitions are detected by electrical transport measurements in the DACs. However, these techniques are established only in a limited number of groups so far. Therefore, we pursued to acquire the experimental techniques to observe the high-T_c superconductivity of the hydrides. Recently we successfully synthesised the hydrides (H_3S, LaH_x and YH_x) and observed the resistance drops in the temperature dependence of electrical resistance. The resistance drops were confirmed to be superconducting transitions as the temperatures of the drops shift to lower temperature with applied magnetic field. Our study now focuses on synthesising high quality samples and observing zero resistance of the superconductors.

MM 18.41 Mon 18:15 P4

The study of non-linear Hall effect via semiclassical theory — •Botsz Huang[1] and Ching-Hao Chang[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan 701, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan

Ordinary Hall effect is driven by an applied magnetic field that provides Lorentz force on a charge carrier and thus leads to charge accumulation perpendicular to the current direction. While anomalous Hall effect occurring in magnetic materials does not require any external magnetic field. It is driven by the Berry curvature that acts an effective magnetic field in momentum space. Based on the mechanics of anomalous Hall effect, non-linear Hall effect due to Berry curvature fluctuation is predicted and also observed in non-magnetic material without any magnetic field. In this talk, a numerical approach solution is presented to study the non-linear Hall effect driven by the magnetic field. The equation of motion of electron is

$$\dot{\mathbf{r}} = -\frac{1}{\hbar}\frac{\partial \mathcal{E}(\mathbf{k})}{\partial \mathbf{k}} + \mathbf{k} \times \mathbf{\Omega}(\mathbf{k})$$
$$\hbar\dot{\mathbf{k}} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)$$

based on the semi-classical transport theory. According to the equation of motion, the test particle method is employed to trace particle trajectories and to determine the transportation. This work opens a new avenue to investigate the transport in semiclassical region and establishes a connection between ordinary Hall effect and non-linear Hall effect.

MM 18.42 Mon 18:15 P4

Thermal conduction in epitaxial $LaMnO_3$/$SrMnO_3$ superlattices — •Daniel Metternich[1], Dennis Meyer[1], Roland Potthast[1], Jan-Phillip Bange[1], Marius Keunecke[1], Robert Gruhl[1], Vladimir Roddatis[2], Vasily Moshnyaga[1], and Henning Ulrichs[1] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Helmholtz-Zentrum Potsdam Deutsches GeoForschungsZentrum

We report on experimental and theoretical investigations of the thermal conduction in $LaMnO_3$ (LMO) / $SrMnO_3$ (SMO) epitaxial superlattice structures, grown by metal-organic aerosol deposition (MAD).

The thermal conductivity of our samples is measured with a transient thermoreflectivity setup - a method that uses a pulsed laser to heat the sample whilst a continuous wave laser measures the surface reflectivity (TTR), and thereby the surface temperature in the time domain. A comparison between samples of different periodicities and LMO/SMO-ratios in particular reveals an unexpected behaviour of the contribution of LMO to the thermal conduction: In single LMO films we find a thermal conductivity close to the amorphous limit, whereas when integrating the LMO into a superlattice, its contribution to the conductivity strongly increases. We relate this finding to a structural modification of the LMO layers in the superlattice.

In addition, we compare our findings with theoretical first-principles calculations regarding the structural configuration of the multi-layered system as well as the phononic contributions to the heat transfer. We acknowledge financial support by the DFG within SFB 1073.

MM 18.43 Mon 18:15 P4

Synthesis and luminescence properties of Ca(1-x)Eu(x)AlSiN3 — Norovsambuu Tuvjargal[1], Chao Kefu[2], Ojied Tegus[2], and •Jav Davaasambuu[1] — [1]Department of Physics, National University of Mongolia, Ulaanbaatar, Mongolia — [2]Inner Mongolia Key Laboratory for Physics and Chemistry of Functional Materials, Inner Mongolia Normal University, Hohhot, China

Ca(1-x)Eu(x)AlSiN3 is currently one of the best known red-emitting materials for LED applications. We will present the experimental results of structural and optical properties of Ca(1-x)Eu(x)AlSiN3 samples. Ca(1-x)Eu(x)AlSiN3(x=0.02, 0.04, 0.06, 0.08, 0.1) samples were successfully synthesized by the high-temperature solid state reaction method. The structure and luminescence properties of samples were investigated by x-ray diffraction and spectroscopic measurements. The Ca0.96Eu0.04AlSiN3 sample shows the strongest red fluorescence emission peak at 670nm under the excitation wavelength of 450nm.

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