

MM 18: Poster Session 2

Time: Tuesday 17:30–20:00

Location: P2

MM 18.1 Tue 17:30 P2

Thermal transport properties of sodium superionic conductors from molecular dynamics simulations — ●INSA DE VRIES, FREYA HALLFARTH, HELENA OSTHUES, and NIKOS DOLTSINIS — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany

Improvements of energy storage systems include the usage of sustainable and low-cost materials. In the case of electrolytes for solid state batteries, this is true for sodium superionic conductors due to the high availability of sodium especially compared to lithium based systems. A proper and safe integration of the electrolyte into battery cells also requires taking into account its thermal properties. Due to the ionic motion enabled by the open crystal structure of the electrolyte, in addition to electronic and phononic parts, a diffusive part also contributes to thermal transport. It is thus important to determine activation barriers for ionic motion and diffusion mechanisms, as they affect the thermal properties.

Equilibrium atomistic molecular dynamics simulations were performed of $\text{NaZr}_2\text{P}_3\text{O}_{12}$ and $\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ using a pair potential by Kumar and Yashonath [1]. Besides identifying ionic diffusion pathways, diffusion constants and thermal transport properties were calculated for various temperatures and compared to results from first principles molecular dynamics.

[1] P. P. Kumar and S. Yashonath, *J. Am. Chem. Soc.* **124**, 3828 (2002)

MM 18.2 Tue 17:30 P2

hiphive - Constructing and sampling higher order force constants for strongly anharmonic materials — ●ERIK FRANSSON¹, FREDRIK ERIKSSON¹, JOAKIM BRORSSON¹, ZHEYONG FAN², and PAUL ERHART¹ — ¹Chalmers University of Technology, Gothenburg, Sweden — ²Aalto, University Helsinki Finland

Higher order force constants (FCs) play a key role in lattice dynamics and are crucial for the analysis of many thermodynamic materials properties. Typically FCs have been extracted using the finite displacement method, which suffers, however, from poor scaling with order and system size. In this contribution we present updates to and applications of the python package hiphive, a tool that allows the efficient extraction of FCs via a regression approach, both up to high order and for low symmetry systems. Higher order FCs can be used to directly run molecular dynamics (MD) simulations, however for strong anharmonic materials these models can become unstable. To overcome this obstacle, we present a self-consistent (iterative) approach for training higher order FCs and demonstrate its effectiveness for multiple strongly anharmonic materials. We have furthermore interfaced hiphive with the GPUMD software, which enables large scale molecular dynamics simulations using FC expansion potentials. This allows for sampling of, e.g., thermal conductivity via Green-Kubo techniques. This approach of extracting higher order FCs and sampling thermal conductivity is demonstrated for two very anharmonic materials, SnSe and BaGaGe. Lastly, we also demonstrate the application of this approach to study the complex dynamics of inorganic halide perovskites.

MM 18.3 Tue 17:30 P2

High-throughput calculations for propriety maps of solids — ●DANIELA IVANOVA¹, DANIEL WORTMANN¹, STEFAN BLÜGEL¹, and MATTHIAS WUTTIG² — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — ²Department of Physics, RWTH Aachen University, Aachen, Germany

Over the last two decades, high-throughput computation has become a vital pillar of the scientific research and development process in the field of computational science. In order to forecast material properties for a larger sets of atomic configurations, Density Functional Theory (DFT) as a widely utilized and high-predictive-power first-principles approach, has become increasingly frequent to be used robust and automated. In this work, the DFT open-source of an integrated suite of codes for electronic-structure calculations, Quantum ESPRESSO is used as connected and deployed through the open source Automated Interactive Infrastructure and Database for Computational Science AiIDA framework to achieve automation. Aside from the existence of (1) covalent, (2) metallic, and (3) ionic bonding, as well as the two weaker forms of (4) hydrogen and (5) van der Waals bonding, compelling

evidence has been found that a new bonding mechanism prevails in crystalline phase change materials, termed as*(6)'metavalent bonding*. The materials data set chosen for high-throughput computing and calculation of the relevant materials properties supplies essential data for mapping distinctions between the bonding mechanisms. Such property maps can also lead to the conjecture of a sixth bonding mechanism (MVB).

MM 18.4 Tue 17:30 P2

High Performance Computing as enabler for condensed matter research — ●ANDREAS STRAUCH, JENS FÖRSTNER, THOMAS KÜHNE, and CHRISTIAN PLESSL — Paderborn University, Paderborn, Germany

The availability of High Performance Computing resources has enabled a wide range of high-impact science in the field of condensed matter physics in the last decades. We review the numerical research performed at the Paderborn Center for Parallel Computing (PC²) ranging from atomistic ab-initio-calculations to electromagnetic, optoelectronic, and quantum dynamical simulations. Combining in-depth knowledge on high performance computing and on heterogeneous hardware architectures with topical research has led to the development of high-level hardware-agnostic parallel-computing frameworks like HighPerMeshes [1] and to research on novel numerical methods, e.g. for molecular dynamics simulations [2,3].

[1] S. Alhaddad et al, "The HighPerMeshes framework for numerical algorithms on unstructured grids", *Concurrency and Computation: Practice and Experience* (2021), pp. e6616, DOI: 10.1002/cpe.6616 (2022)

[2] R. Schade et al, "Towards electronic structure-based ab-initio molecular dynamics simulations with hundreds of millions of atoms", *Parallel Computing* 111, doi:10.1016/j.parco.2022.102920 (2022)

[3] R. Schade et al, "Breaking the Exascale Barrier for the Electronic Structure Problem in Ab-Initio Molecular Dynamics", arXiv:2205.12182 (2022)

MM 18.5 Tue 17:30 P2

Computational studies of liquid chromophores — ●ERIC LINDGREN — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Liquid chromophores such as perylene and its derivatives constitute an important class of materials, with applications ranging as solvent-free dyes to increasing the efficiency of solar cells via photon conversion. Their structural and in particular dynamical behaviour on the molecular level is not very well known, yet crucial for their optical properties. In this work, we use molecular dynamics (MD) simulations to investigate the structural and dynamical properties of perylene and two of its derivatives (perylene-ethyl and perylene-diimide). Specifically, we extract the static and dynamical structure factors and the current correlation functions for various temperatures as well as for two different initial structural models of the systems, which in principle allows us to establish a direct link to experimental studies. Motivated by recent experimental work by Hultmark et al. (*Science Advances* 7.29 (July 2021)), we consider two structural models that differ with respect to the relative orientation of the molecules. Whereas in model 1 the molecules are more or less randomly oriented, model 2 features domains with pronounced pi-pi stacking. The latter configuration corresponds to a simplified representation of the supramolecular aggregates that some extended perylene derivatives have been observed to form experimentally. At the moment we have established our simulation protocol and verified the basic premise of this project. Next we will extend our study to derivatives with larger sidegroups and mixtures thereof.

MM 18.6 Tue 17:30 P2

Edge states in proximitized graphene ribbons and flakes in a perpendicular magnetic field: Emergence of lone pseudohelical pairs and pure spin-current states — ●YAROSLAV ZHUMAGULOV, TOBIAS FRANK, and JAROSLAV FABIAN — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Graphene influenced by the valley-Zeeman intrinsic spin-orbit coupling through proximity effects provides signatures of pseudohelical edge states. Analyzing the band structure of a zigzag graphene nanoribbon in the presence of proximity induced spin-orbit interaction and an external magnetic field, we have discovered the effect of stabiliza-

tion of intervalley edge states and removal intravalley edge states by the external magnetic field. Stabilization of states is associated with the closing/reopening of the bulk bandgap between nonzero Landau levels. The magnitude of the external magnetic stabilization field was estimated both numerically and analytically. Finally, we have found that stabilized intervalley edge states in the presence or in the absence of a spin-flip hopping through the armchair edge form pseudohelical states or pure spin current states, respectively. The states of pure spin current are formed in wide graphene flakes and are protected from scattering by defects on the zigzag edges of graphene flakes. This work was supported by DFG SPP 2244, DFG SFB 1277 and EU Graphene Flagship.

MM 18.7 Tue 17:30 P2

Modelling mechanical bond scission of amine cured Epoxy resins under stress — ●SAMPANNAI PAHI¹, MATTIA LIVRAGHI¹, CHRISTIAN WICK^{1,2}, and ANA-SUNCANA SMITH^{1,3} — ¹PULS Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — ²Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany — ³Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bosković Institute, 10000 Zagreb, Croatia

Epoxy resins are widely used thermoset polymers in manufacturing processes. Understanding of fracture propagation in cured epoxy resins is pivotal in determining the bulk level properties of the material. In this paper, a scale-bridging approach that links atomistic molecular dynamics (MD) simulations with DFT based Quantum Mechanical (QM) criterions has been implemented to model bond breakage in Quantum level. In our approach, we create smaller model systems for each bond and implement COGEF procedure to determine optimal bond breakage criterion. Furthermore, a hybrid on-the-fly QM/MM method is described and its ability to capture bond scission on cross linked polymer system with no predetermined fracture site is demonstrated. Using QM bond breakage criterion, bond scission in MD run is identified and checked using presence of spin contamination. Our study provides insights into the molecular mechanisms governing the fracture mechanism of epoxy resins and demonstrates the success of utilising atomistic molecular simulations towards predicting bulk properties.

MM 18.8 Tue 17:30 P2

Solvation effects on proton irradiation of DNA — ●DANIEL MUÑOZ-SANTIBURCIO¹, BIN GU², and JORGE KOHANOFF¹ — ¹Instituto de Fusión Nuclear “Guillermo Velarde”, Universidad Politécnica de Madrid, Spain — ²Department of Physics, Nanjing University of Information Science and Technology, China

Proton irradiation of DNA is of utmost importance for many fields, from radiation damage in space to medical applications for cancer treatment. Ab initio simulations are highly valuable tools for understanding such process, but they are cumbersome due to the required level of theory. These involve simulating the non-adiabatic propagation of the electronic subsystem of the target material, and to date have been restricted to DNA systems in absence of water, or at most with few solvating molecules. Here we present the results of large-scale ab initio (RT-TDDFT) simulations of proton irradiation of a realistic DNA system in bulk water, where we have determined different important aspects of the proton irradiation process such as the stopping power of the system, the spacial distribution of the holes in terms of the depopulations of the maximally localized Wannier functions, and more importantly the influence of the surrounding water. We will show that water is neither a mere spectator on the process nor a simplistic reducing or enhancing agent of the excitation process. Instead, water qualitatively changes the excitation landscape of the proton-irradiated DNA, making the hole population on the different atoms and bonds qualitatively different in the solvated vs. the dry DNA case.

MM 18.9 Tue 17:30 P2

Resistometric determination of GP-zone formation and growth — ●FABIAN MILLER, JOHANNES BERLIN, TOBIAS STEGMÜLLER, and FERDINAND HAIDER — Universität Augsburg, Institut für Physik, 86135 Augsburg, Deutschland

Aluminium alloys are of crucial importance in today's economy, therefore the deeper understanding of their mechanical and electrical properties is important. These properties can be influenced by precipitate formation. In this work we focused in the Al*Cu system with samples containing around 4 wt.% of Cu. They were homogenized at the eutectic temperature and rapidly quenched to ambient temperature. After-

wards 4-point-resistance measurements were conducted during natural and artificial aging. Due to formation of Guinier Preston zones, the resistivity first increases, then slowly decreases, allowing to monitor the unmixing for different temperatures and for different quenching conditions. Further experiments with other alloying metals than Cu will be conducted and variations of the homogenisation temperature are planned to be inspected.

MM 18.10 Tue 17:30 P2

Dealloying and nanoscale structure formation at crystal-melt coexistence — ●ZHONGYANG LI¹, NINA PETERSEN¹, LUKAS LÜHRS¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology — ²Institute of Materials Mechanics, Hybrid Materials Systems, Helmholtz-Zentrum Hereon

Recent work on Ti-Ag alloy has shown that a bicontinuous microstructure can be formed via peritectic melting, which could further transform to open porous Ti or Ag networks through selective etching. Several factors including the large solubility difference of two alloy elements in liquid phase, large composition difference and the volume fraction of the solid and liquid phases are considered to be criteria for this phenomenon. However, the formation mechanism of this particular microstructure during peritectic dealloying is still not fully known.

In this work, alloy systems including Bi-Ni, Fe-Sn and Mn-Sn, are chosen, which satisfy part or all of the aforementioned criteria. With SEM and diffraction experiments of these samples after peritectic melting, we investigate the morphology of different phases, and discuss the dominant factor for the formation of bicontinuous structure. The effect of parameters for thermal treatment, including temperature and duration of heat treatment, are also studied using SEM, in order to find the optimized combination that could produce finer microstructure. With the research in these two aspects, we discuss the possibility of broadening the application of this new dealloying method from peritectic dealloying to dealloying at liquid-solid coexistence state.

MM 18.11 Tue 17:30 P2

Structural and Textural Transitions of Discotic Ionic Liquid Crystals in Nanoporous Solids — ●ZHUOQING LI¹, PATRICK HUBER¹, SABINE LASCHAT², AILEEN RAAB², ANDREAS SCHÖNHALS³, and MOHAMED A. KOLMANGADI³ — ¹Institute for Materials and X-Ray Physics, Technische Universität Hamburg, Hamburg, Germany — ²Institut für Organische Chemie, Universität Stuttgart, Stuttgart, Germany — ³Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Discotic ionic liquid crystals (DILCs) derived from 3,4-dihydroxyphenylalanine (DOPA) have synergetic properties of liquid crystals and ionic liquids. Driven by the $\pi^*\pi$ interactions among the aromatic cores, DILCs may self-organize, leading to a hexagonal ordered columnar liquid crystalline mesophase. Embedding of DILCs in nanoporous solids allows one to design hybrid materials with 1-D ionic conductivity pathways on the single-nanopore scale and tailorable photonic properties. The structural organization of confined DILCs is determined by an interplay of geometrical constraints and interfacial interactions at the pore wall and thus depends on pore size, temperature treatment and molecular wall anchoring. The optical birefringence experiments and small angle X-ray scattering results indicate ordered liquid crystalline mesophases of different collective orientations as a function of anchoring of the DILC discs at the pore surface. In particular, these experiments suggest that depending on the pore size a transition from the formation of circular concentric ring structures to an arrangement, where the columns are aligned parallel to the pore axis occurs.

MM 18.12 Tue 17:30 P2

Laughlin topology on fractal lattices without area law entanglement — ●MANI CHANDRA JHA — MPI-PKS

Laughlin states have recently been constructed on fractal lattices, and the charge and braiding statistics of the quasiholes were used to confirm that these states have Laughlin type topology. Here, we investigate density, correlation, and entanglement properties of the states on a fractal lattice derived from a Sierpinski triangle with the purpose of identifying similarities and differences compared to two-dimensional systems and with the purpose of investigating whether various probes of topology work for fractal lattices. Similarly to two-dimensional systems, we find that the connected particle-particle correlation function decays roughly exponentially with the distance between the lattice sites measured in the two-dimensional plane, but the values also depend on the local environment. Contrary to two-dimensional systems, we find that the entanglement entropy does not follow the area law if one de-

finds the area to be the number of nearest neighbor bonds that cross the edge of the selected subsystem. Considering bipartitions with two bonds crossing the edge, we find a close to logarithmic scaling of the entanglement entropy with the number of sites in the subsystem. This also means that the topological entanglement entropy cannot be extracted using the Kitaev-Preskill or the Levin-Wen methods. Studying the entanglement spectrum for different bipartitions, we find that the number of states below the entanglement gap is robust and the same as for Laughlin states on two-dimensional lattices.

MM 18.13 Tue 17:30 P2

A study of the local fields in bismuth ferrite by using different radioactive tracer ions — •THANH T. DANG¹, JULIANA SCHELL^{1,2}, MARIANELA E-CASTILLO¹, DANIIL LEWIN¹, ASTITA DUBEY¹, ANDREA G. BOA^{2,3}, REINHARD BECK⁴, CORNELIA NOLL⁴, JOÃO N. GONÇALVES⁵, DMITRY ZYABKIN⁶, KONSTANTIN GLUKHOV⁷, IAN C. J. YAP⁸, ADELEH M. GERAMI^{2,9}, KOEN V. STIPHOUT¹⁰, GEORG MARSCHICK¹¹, EDGAR M. S. D. REIS^{1,2}, SOBHAN M. FATHABAD¹, and DORU C. LUPASCU¹ — ¹University of Duisburg-Essen — ²European Organization for Nuclear Research — ³Technical University of Denmark — ⁴University of Bonn — ⁵Universidade de Aveiro — ⁶TU Ilmenau — ⁷Uzhhorod National University — ⁸Universität Göttingen — ⁹School of Particles and Accelerators — ¹⁰Georg-August-Universität Göttingen — ¹¹Vienna University of Technology

This work presents the study of the local electric and magnetic fields in multiferroic bismuth ferrite using Time Differential Perturbed Angular Correlation spectroscopy. The measurements were carried out at a wide range of temperatures up to 850°C, after the implantation of various radioactive tracer ions: 181Hf, 111In and 111mCd. The experimental results reflect the obedience to Landau theory and Brillouin-Weiss equation of local electric polarization and magnetization, respectively. Particularly, a huge coupling between local electric and magnetic fields has been investigated in anti-ferromagnetic order. With the support of ab-initio DFT simulations, we can conclude that 111mCd is located at Bi-atom, 181Hf and 111In substitute Fe-atom.

MM 18.14 Tue 17:30 P2

Partitioning of transition metals to the γ and γ' phase of Co-based superalloys — •ISABEL PIETKA¹, ANDREAS FÖRNER², MANUEL KÖBRICH², STEFFEN NEUMEIER², RALF DRAUTZ¹, and THOMAS HAMMERSCHMIDT¹ — ¹Ruhr-Universität Bochum, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science & Engineering

Single-crystal Co-base superalloys are a promising class of materials in high-pressure high-temperature applications such as blades of gas turbines or jet engines. The superior mechanical properties at high temperatures are a consequence of the underlying γ/γ' microstructure. The improvement of the mechanical properties of these alloys is therefore closely tied to an understanding of the influence of alloying elements on the microstructure. In this work, we describe the γ/γ' partitioning of different alloying elements, i.e. their preference for the γ matrix or the γ' particles of the microstructure. In particular, we determine the energy difference of nearly all 3d, 4d, 5d transition metals (TMs) in $\text{Co}_3(\text{Al}/\text{W})$ by density functional theory calculations. In very good agreement with results from wavelength-dispersive X-ray spectroscopy and atom probe tomography, we find a preference of early TMs for the γ' phase while mid to late TMs show no clear preference. We demonstrate that the findings can be rationalized in terms of band-filling and atomic size differences by moment analysis from bond order potential theory.

MM 18.15 Tue 17:30 P2

The oxidation of TNM alloy at 700°C and 760°C — •HENG ZHANG^{1,2} and YONGFENG LIANG² — ¹Institute of Materials Physics, University of Münster, Germany — ²State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing, China

The TNM sample morphology and components of the oxides are measured with SEM, EDS and XPS after oxidation until 200 hours at 700°C and 760°C respectively. Al_2O_3 is the main oxides at 700°C combined with a little TiO_2 , MoO_2 and MoO_3 , while the oxides are TiO_2 , MoO_2 and MoO_3 at 760°C, exhibiting a good oxidation resistance under 700°C.

MM 18.16 Tue 17:30 P2

Reactive Surface Corrosion of Stainless Steel studied with Atomic Force Microscopy and Kelvin Probe Force Microscopy — •JULIAN CREMER¹, SINAN KIREMIT², BERNHARD KALTSCHMIDT³, THOMAS KORDISCH², ANDREAS HÜTTEN³, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience (BINAS), Bielefeld University — ²Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences — ³Thin Films & Physics of Nanostructures, Bielefeld University

The pitting surface corrosion of three different stainless steels (1.4016, 1.4510 and 1.4301) used for industrial applications was investigated by exposition to oxidative liquids. Here, we focus on the investigation of the origin of the pitting using Kelvin probe force microscopy (KPFM) and on the prevention of corrosion by surfactants using high-resolution atomic force microscopy (AFM). KPFM allows to determine the work function of a sample with high spatial resolution. We found that the initiation of a pit can be caused by an abnormal anodic site (low work function) surrounded by a normal surface which acts as a cathode, or by the presence of an abnormal cathodic site (high work function) surrounded by a normal surface. In order to test whether KPFM can predict where and why pitting corrosion occurs, we use a micro corrosion liquid cell that allows live observation of the previously scanned area during corrosion. Additionally, we study the surface activity of surfactants acting as corrosion inhibitors on stainless steels regarding adsorption dynamics and layer thickness in different temperature-controlled solutions.

MM 18.17 Tue 17:30 P2

Reactive Surface Corrosion of Polypropylene studied with Atomic Force Microscopy — •JULIAN CREMER¹, BERNHARD KALTSCHMIDT², ANDREAS HÜTTEN², and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience (BINAS), Bielefeld University — ²Thin Films & Physics of Nanostructures, Bielefeld University

The surface corrosion of various polypropylene samples used for industrial applications was investigated by exposition to oxidative liquids. The samples are formulated by different additive packages and include fillers such as talc or glass fibers for reinforcement. In particular, we study the aging and corrosion of these polypropylene samples in oxidative liquid media, analyzing the influence of temperature and oxidants. Contrary to aging induced by UV radiation, aging in oxidative liquids is rarely studied. Shedding some light on this research area, we placed the polypropylene samples in an oxidative test solution at 95°C, which was constantly renewed. In total, the samples were examined after ten different time steps up to 4000h. Mainly, we used atomic force microscopy (AFM) to image the samples and to determine the Young's modulus, which is a decisive parameter for the age of plastic materials. In some cases, we observe a growth of a fibrous structure on the surface covering nearly the whole sample. To determine the chemical composition of the bloomed structure and follow the aging on a chemical level, attenuated total reflection infrared spectroscopy was performed (ATR-FTIR). We present structural and chemical changes of aged industrial polypropylene as well as the consequence of additive blooming.

MM 18.18 Tue 17:30 P2

High-Pressure Torsion Deformed Magnesium: Microstructure Evolution and Hydrogen Diffusion — •SABINE SCHLABACH^{1,2,3}, BINGYU WU¹, GIORGIA GUARDI¹, STEFAN WAGNER¹, JULIA IVANISENKO^{2,3}, and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology, Institute for Applied Materials, Karlsruhe, Germany — ²Karlsruhe Institute of Technology, Institute of Nanotechnology, Karlsruhe, Germany — ³Karlsruhe Institute of Technology, Karlsruhe Nano Micro Facility, Karlsruhe, Germany

Magnesium (Mg) is one of the materials considered as a solid state storage material for Hydrogen (H) as it is capable of storing up to 7.6 wt.% of H while forming magnesium hydride (MgH_2). However, the volume diffusion rate of H in MgH_2 is low, and thus the sorption rate of H is rather slow. As grain boundaries are suggested as fast diffusion paths, an increasing volume fraction of grain boundaries by reducing the grain size is aimed. Starting from polycrystalline bulk Mg, this can be done, e.g., by high-pressure torsion, one method of severe plastic deformation. The deformation induced microstructure evolution is investigated by using electron backscatter diffraction depending on different process parameters like imposed pressure and number of revolutions. Special attention is taken on local misorientations as a measure of dislocation density and their possible influence on H-diffusion. The related H loading capability of the deformed Mg samples is tested at room temperature utilizing gas volumetry. In a first step, H-diffusion

in the α -Mg phase is assessed as model system. Thus, the maximum H concentration is kept below the solid solution limit.

MM 18.19 Tue 17:30 P2

Co(OH)₂@FeCo₂O₄ as high-performance electrode material for supercapacitors — •ZIDONG WANG^{1,2}, YUDE WANG², HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²School of Materials and Energy, Yunnan University, 6500504 Kunming, Peoples Republic of China

Spinel-type MCo₂O₄ (M = Zn, Ni, Fe, *) are regarded as a partial replacement of Co₃O₄ without crystal structure changes, and they provide advantages of lower cost and improved performance compared with Co₃O₄. Particularly, the variable valence of Fe in FeCo₂O₄ benefits the energy storage capability. However, previous works indicate that the attainable performance of FeCo₂O₄ is still limited. Herein, a 2D planar morphology design is proposed to optimize the performance of FeCo₂O₄ as active materials of supercapacitors. In this work, nano-sized Co(OH)₂ were composited on FeCo₂O₄ nanosheets skeleton by a simple one-step hydrothermal process. Due to the synergistic effect, the sample achieves outstanding performances with the specific capacitance of 1173.43 F g⁻¹ at a current density of 1 A g⁻¹ and 95.4% capacitance retention after 5000 cycles. It indicates that nanostructured Co(OH)₂@FeCo₂O₄ would have hopeful prospects in energy storage applications.

MM 18.20 Tue 17:30 P2

Quantitative investigation of reversible Li₂O formation on Germanium battery anodes — •KE WANG and GUIDO SCHMITZ — Chair of Materials Physics, Institute for Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany

Lithium-ion batteries (LIB) serves as efficient energy storage devices in many aspects of our life. Anodes belonging to the Group IV (Si, Ge and Sn) are promising candidates to replace commercially applied graphite (372 mAh g⁻¹) owing to their high theoretical capacity (3850 mAh g⁻¹ for Si, 1570 mAh g⁻¹ for Ge, and 990 mAh g⁻¹ for Sn). But, the respective mechanisms of Li storage and the formation of solid electrolyte interface (SEI) are still not clearly. In this work, cyclic voltammetry has been conducted in combination with a quartz crystal microbalance to measure the SEI mass, and the amount of eventual reversibly processed species. Similar to Si and Sn, also with Ge anodes, the QCM mass spectroscopy identifies Li₂O as a reversibly processed species that contributes a significant part to the electrochemical capacity. The amount of reversibly stored Li₂O decreases weakly with increasing cycling rate, but increases significantly with the thickness of the Ge anodes. Interestingly, the amount of Li₂O decreases if pronounced anode cracking appears, which is probably attributed to the fact that the fracture introduces short circuit transport paths deep into the volume of the Ge which accelerates lithiation. Thermodynamically, Li₂O should form before Li is inserted. But in the experiment simultaneously formation of Li₂O and Li_xSn_y is observed on Sn, probably attributed to lateral heterogeneity introduced by surface roughness.

MM 18.21 Tue 17:30 P2

Recycling of anode graphite from spent lithium-ion batteries and reused in heat transfer medium — •YU QIAO^{1,2}, ZHONGHAO RAO^{3,4}, HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²School of Electrical and Power Engineering, China University of Mining and Technology, 221116, Xuzhou, China — ³School of Energy and Environmental Engineering, Hebei University of Technology, 300401, Tianjin, China — ⁴Hebei Key Laboratory of Thermal Science and Energy Clean Utilization, Hebei University of Technology, 300401, Tianjin, China

Lithium-ion batteries (LIBs) have been widely employed in fast-growing mobile devices, stationary storage devices and electric vehicles. However, LIBs face a large wave of retirement because of a certain life. Graphite is the most common anode material in LIBs, amount of waste graphite will also be produced with the retirement of spent LIBs. Anode graphite (AG) from spent LIBs has the characteristics of large layer spacing and ease of being intercalated due to reducing the interlamination force after repeated charge and discharge cycles. In this study, two-dimensional graphite flakes (GFs) were prepared from spent AG through a freeze-thaw ultrasonic-assisted circulation method. The heat transfer ability of as-obtained GFs dispersed in ethylene glycol was investigated experimentally. The results indicated that GFs could enhance the heat transfer coefficient and the maximum enhancement

is about 30%.

MM 18.22 Tue 17:30 P2

Mild-temperature solution-assisted encapsulation of phosphorus into ZIF-8 derived porous carbon as lithium-ion battery anode — •CHENGZHAN YAN¹, SHUN WANG², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany. — ²Key Laboratory of Carbon Materials of Zhejiang Province, Institute of Materials and Industrial Technologies, Wenzhou University, Wenzhou, Zhejiang, 325027, China.

Phosphorus in the form of polyphosphides anions (PP) is encapsulated into ZIF-8 derived porous carbon through a solution-assisted etching diffusion process under a mild temperature, and the composites with a high phosphorous content of 30 wt% exhibit a high capacity, improved cycling stability as well as a good rate performance as a lithium-ion battery anode. Herein, a series of morphological and structural characterizations are applied to analyze the differences between individual MOF-derived carbon hosts with the whole body that has PP inside the pore. Subsequently, their electrochemical performance is also compared. The results of the above-mentioned material analysis and application practices jointly confirmed the superiority of this mild temperature solution-assisted encapsulation of phosphorus method. In summary, this work provides a new strategy to design and fabricate phosphorus-based electrodes for batteries beyond lithium-ion batteries.

MM 18.23 Tue 17:30 P2

Optimization of flash sintering input parameters for obtaining 8YSZ dense samples — •FÁBULO R. MONTEIRO¹, GUSTAVO C. DACANAL¹, JOÃO V. CAMPOS², LILIAN M. JESUS², ADILSON L. CHINELATTO³, and ELIRIA M. J. A. PALLONE¹ — ¹University of São Paulo, Pirassununga, Brazil — ²Federal University of São Carlos, São Carlos, Brazil — ³University of Ponta Grossa, Ponta Grossa, Brazil

Flash sintering has been widely investigated due to its technological potential, since it allows very rapid densification of different ceramic materials. The literature still lacks studies assessing how the electrical parameters of the technique (electric field and current density) involved in the process affect material densification since these parameters may vary depending on furnace type and, especially, sample geometry. Thus, this study used the response surface technique to analyze and relate, in a multivariate way, a few flash sintering variables. A mathematical model was proposed to optimize the densification of 8YSZ cylindrical and dog-bone samples. For this, a complete second order factorial planning with three central points was used in combination with the response surface methodology. The results obtained allowed us to predict electric field and electric current density values to optimize the densification of 8YSZ samples in the two geometries used and to understand how electric field and electrical current density values affected onset and sample temperatures (estimated by the black body radiation model).

MM 18.24 Tue 17:30 P2

The effect of crystallinity of layered transition metal disulfide on the performance of potassium-ion batteries: The case of molybdenum disulfide — •YULIAN DONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Layer-structured transition metal dichalcogenides (LS-TMDs) are being studied in potassium-ion batteries owing to their structural uniqueness and electrochemical mechanisms. In this work, the dependence of electrochemical performance on the crystallinity of LS-TMDs has been investigated. Taking MoS₂ as an example, lower crystallinity can alleviate diffusional limitation in 0.5*3.0 V, where intercalation reaction takes charge in storing K-ions. Higher crystallinity can ensure the structural stability of the MoS₂ layers and promote surface charge storage in 0.01*3.0 V, where conversion reaction mainly contributes. The low-crystallized MoS₂ exhibits an intercalation capacity (118 mAh/g) and great rate capability (41 mAh/g at 2 A/g), and the high-crystallized MoS₂ delivers a high capacity of 330 mAh/g at 1 A/g and retains 161 mAh/g at 20 A/g. It shows that when intercalation and conversion reactions both contribute to store K-ions, higher crystallinity ensures the structural stability of the exfoliated MoS₂ basal layers and promotes surface-controlled charge storage.

MM 18.25 Tue 17:30 P2

Magnetic Hardening of Nd-Fe-B Permanent Magnets —

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Nd-Fe-B alloys used for permanent magnets provide highest performance and energy density and are therefore used in numerous energy and high-tech applications. The superior intrinsic properties of the hard magnetic Nd₂Fe₁₄B phase are translated by a controlled production processes leading to a specific micro- and grain boundary structure and high coercivity. In this work, we take a different approach and show a novel magnetic hardening mechanism in such materials. This mechanism has the potential to be incorporated into existing manufacturing processes and to be adapted to novel production routes for Nd-Fe-B permanent magnets such as Additive Manufacturing. As an example, we demonstrate how the microstructural transformation from metastable Nd₂Fe₁₇B_x phase to the hard magnetic Nd₂Fe₁₄B phase by controlled annealing leads to a significant increase in coercivity from 250 kAm⁻¹ to 700 kAm⁻¹ in Nd₁₆Fe_{bal-x-y-z}Co_xMo_yCu_zB₇ alloys. This approach offers also a promising opportunity for the fabrication of nano composite magnets.

MM 18.26 Tue 17:30 P2

Spin fluctuations and Wigner thermal transport in thermoelectric skutterudites — •ENRICO DI LUCENTE¹, MICHELE SIMONCELLI², and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne 1015, Switzerland — ²TCM Group, Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge, CB3 0HE UK

Skutterudites are highly promising functional materials due to their peculiar thermoelectric and magnetic properties. We elucidate the complex phenomenology that takes place in these materials both in terms of spin fluctuations and in the crossover from a Peierls-Boltzmann to a Wigner thermal transport regime, where tunneling of phonon wavepackets emerges. We first study the electronic structure using the state-of-the-art DFT+Hubbard theory to uncover multiple self-consistent magnetic and charge disproportionated configurations. While the lowest energy state is antiferromagnetic but metallic, paramagnetic fluctuations captured through a special quasi random structure open a small gap of 61 meV, in good agreement with experiments. Moreover, in going from the parent compound to the related filled skutterudite, a transition from a Peierls-Boltzmann to a Wigner thermal transport regime arises, where, at working temperature of the devices, the tunneling of phonon wavepackets becomes as relevant as the drifting diffusion.

MM 18.27 Tue 17:30 P2

Freezing and melting of water in nanopores: A temperature-dependent X-ray scattering study — •LARS DAMMANN^{1,2}, STELLA GRIES^{1,2}, MILENA LIPPMANN¹, and PATRICK HUBER^{1,2} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany — ²Hamburg University of Technology, Institute for Materials and X-Ray Physics, Eißendorfer Straße 42, Hamburg 21073, Germany

The crystallization of water in extreme spatial confinement of nanoporous media plays a pivotal role in many natural and technological processes, ranging from frost heave to modern materials processing. However, the induced interfacial stresses in the porous medium during melting and crystallization and the crystalline structures of nanoconfined water are still subject of scientific discussions. Here we present simultaneous temperature dependent small and wide angle X-ray scattering (SAXS/WAXS) measurements of water in ordered silica nanopores of diameters around 3 nm and 7-8 nm in a temperature range from 300 K to 150 K. With SAXS we investigate the crystallization induced strain on the pore network and with WAXS the structure of water ice in nanoconfinement. A complete analysis of the measurements is yet to be conducted, however, promising first results of the SAXS measurements show a strong dependence of pore strain on freezing in the pores especially for the smaller pores. As a next step we aim to compare the SAXS data to the measured WAXS signal to investigate the structure of the crystallized confined water.

MM 18.28 Tue 17:30 P2

Liquids in Atom Probe Tomography — •TIM MAXIMILIAN

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Frozen liquids are challenging and rather new in the investigation by atom probe tomography. However, recent progress in instrumentation, especially the introduction of cryo transfer shuttles, and the development of the required preparation routes to shape nanometric needles of frozen liquids enable measurements of sufficient quality and size of data sets to discover the typical features of this material class. The field evaporation of liquids resembles more the behaviour of weakly cross-linked polymers than that of metals. So frozen liquids, stabilized by weak hydrogen or van der Waals bonds, typically evaporate in large molecular fragments which raises general questions about spatial resolving power and chemical sensitivity of the atom probe tomography. At the example of saturated glucose solutions, we investigate the accuracy of the chemical analysis and the spatial resolution in localizing dissolved molecules. The direct comparison to the field evaporation of solid bulk glucose demonstrates in water a matrix-assisted field desorption that enables the detection of the chemical structure of larger organic molecules. One step further natural honey, which is a super-saturated solution consisting of a mixture of different monosaccharides and higher sugars in water, can be investigated on the nanoscale.

MM 18.29 Tue 17:30 P2

Fractal abnormal grain growth in nanocrystalline Pd-Au at the atomistic level — •JOHANNES WILD¹, TORBEN BOLL¹, JULES DAKE², DOROTHÉE VINGA SZABÓ¹, STEFAN WAGNER¹, CARL E. KRILL², and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — ²University of Ulm, Institute of Functional Nanosystems, Ulm, Germany

Nanocrystalline (NC) Pd-10 at.% Au (PdAu) prepared by inert gas condensation (IGC) shows an unconventional manifestation of abnormal grain growth upon heat treatment. This unusual growth mode leads to complex and highly convoluted boundaries resembling those of fractal shapes. Furthermore, the microstructure shows a bimodal grain size distribution with regions of NC grains bordering grains in the micron range. This phenomenon is unique to this NC PdAu as conventionally prepared samples showed normal grain growth for the same heat treatment. In this study, we investigate the abnormal grain boundaries of heat-treated IGC PdAu using atom probe tomography (APT) and field ion microscopy (FIM). The position-specific APT samples are produced by targeted sample preparation with focused ion beam lift-out methods at chosen regions of interest that are identified beforehand by high-resolution electron backscatter diffraction imaging. We also use FIM, which has a higher lateral resolution than APT. This research is financially supported by the Deutsche Forschungsgemeinschaft (DFG) via project number 461632490, DFG PU131/18-1, DFG KR1658/10-1 and Karlsruhe Nano Micro Facility (KNMFi).

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Formation porous metal nanosystems under near-equilibrium condensation conditions in plasma-condensate system — •ANNA KORNYUSHCHENKO^{1,2}, VYACHESLAV PEREKRESTOV¹, and GERHARD WILDE² — ¹Sumy State University, Laboratory of Vacuum Nanotechnologies, Sumy, Ukraine — ²WestfälischeWilhelms-Universität, Institute of Materials Physics, Münster, Germany

It is known, that porous structures depending on morphology can possess unique physical properties which can determine areas of their application. In the proposed work a new technique for synthesizing metal porous micro- and nanostructures has been developed. This approach is based on the phase transition of sputtered substances into the condensed state under conditions close to thermodynamic equilibrium. The low dimensional metal systems (Cr, Zn, Cu, Ti, Ni, Al) have been obtained in the different morphological forms, such as network structures, nanowires, agglomerations of weakly-bound crystals, columnar structures consisting of prolonged crystals with approximately identical habitus, etc. The results confirm the important new opportunities for size, shape and physical property tuning of nanostructured materials that are given by deposition near thermodynamic equilibrium conditions. It has been established that the growth mechanism under conditions close to thermodynamic equilibrium possesses principally new peculiarities and possibilities in comparison with traditional methods of condensation from vapor state and consequently can contribute to a new zone in the structure zone model.

MM 18.31 Tue 17:30 P2

Self-detachment and sub-surface densification of dealloyed nanoporous thin films — ●GIDEON HENKELMANN¹, DIANA WALDOW¹, MAOWEN LIU¹, LUKAS LÜHRS¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — ²Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

This work highlights experimental observations showing microstructural gradients at interfaces in nanoporous gold, and it explains those observations as a consequence of gradients in a laterally averaged mean curvature of the pore surfaces. Nanoporous gold can be covered by a densified layer at its external surfaces. Furthermore, as we report, thin films of the material often spontaneously detach from massive gold base layers that are intended to enhance adhesion to the substrate. Those phenomena appear intrinsic to the material, as they are naturally reproduced by our kinetic Monte Carlo (KMC) simulation of dealloying and of the subsequent microstructure evolution. Our results suggest that spontaneous densification or decohesion at interfaces may be generic features of nanoscale porous network materials that evolve by curvature-driven surface diffusion.

MM 18.32 Tue 17:30 P2

Structural-mechanical property correlation in hierarchical nanoporous gold — ●LUKAS RIEDEL¹, SHAN SHI^{1,2}, JÜRGEN MARKMANN¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany — ²Institute of Material Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Implementing a structural hierarchy in nanoporous metals has been demonstrated as an efficient way to achieve lightweight and enhanced mechanical performance. So far, several aspects of the correlation between structure and mechanical behavior are not clearly proven. Here, hierarchical nanoporous gold (HNPG) with tunable ligament size at each hierarchy level is synthesized out of Ag₉₀Au₁₀ via a dealloying-coarsening-dealloying strategy. The structural analysis is conducted with scanning electron microscopy, small-angle X-ray scattering (SAXS) and ultra small-angle X-ray scattering (USAXS). We demonstrate that SAXS and USAXS are valued as advantageous methods for the determination of the structural size of HNPG. In particular, USAXS is very useful for the description of nanoporous structures with a ligament size of several hundred nanometers. It is observed that the mechanical behavior of HNPG is highly dependent on the ligament size at both the upper and the lower hierarchy level. Moreover, HNPG made out of Ag₉₀Au₁₀ shows improved stiffness in comparison to HNPG made out of Ag₉₃Au₇ even though they have similar feature sizes. The results represent an evidence for the development of the connectivity during coarsening in relation to the solid fraction.

MM 18.33 Tue 17:30 P2

Hierarchical-structural effect on creep of nanoporous gold — ●HANSOL JEON¹, SHAN SHI^{1,2}, JÜRGEN MARKMANN^{1,2}, and ERICA LILLEODDEN³ — ¹Helmholtz-Zentrum Hereon, Institute of Materials Mechanics, 21502 Geesthacht — ²Hamburg University of Technology, Institute of Materials Physics and Technology, 21073 Hamburg — ³Fraunhofer Institute for Microstructure of Materials and Systems, 06120 Halle (Saale)

Nanoporous gold (NPG), a bi-continuous structure composed of ligaments and pores, is highly attracting attention in application fields due to its high surface area and chemical inertness. In addition, hierarchical nested-network nanoporous gold (N3PG) has been developed as an even lighter and faster functional material. With respect to mechanical properties, the research on the time-dependent deformation as called creep for NPG and N3PG is scarce while there have many studies of tension, compression, and nanoindentation. In this study, we performed compressive creep tests for NPG and N3PG pillars in order to investigate the creep behavior under control of the electrochemical potential. We prepared N3PG samples with the same higher-level ligament size and with different lower-level ligament-sizes and a non-hierarchical NPG sample according to the higher-level ligament size so that we analyzed the effect of lower-level ligament-size on N3PG as well as the effect of the hierarchical structure itself on creep. In addition, by controlling the electrochemical potential, we controlled the surface status in order to check on the size effect of the relationship between creep behavior and surface state.

MM 18.34 Tue 17:30 P2

Fabrication of hierarchical porous silicon and amorphous silica by means of silver nanoparticle catalyzed chemical etching — ●STELLA GRIES^{1,2,3}, MANUEL BRINKER^{1,2,3}, and PATRICK HUBER^{1,2,3} — ¹Institute for Materials and X-Ray Physics, Hamburg University of Technology, 21073 Hamburg, Germany — ²Center for X-Ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — ³Center for Hybrid Nanostructures CHyN, University of Hamburg, 22607 Hamburg, Germany

Many biological tissues and materials exhibit a multiscale porosity with small, often nanoscale pores as well as large, macroscopic pores or capillaries in order to achieve simultaneously large inner surfaces in combination with an optimized mass transport capability. Achieving such a hierarchical porosity in artificial porous media is a very active research field. Here we present a novel approach based on silver nanoparticle-assisted chemical etching (MACE) of electrochemically fabricated macroporous silicon for the synthesis of wafer-scale, single-crystalline silicon with a bimodal pore size distribution. With MACE macroporous silicon membranes can be porosified into hierarchical porous silicon (hp-Si). The resulting semiconducting material offers good hydraulic permeabilities and simultaneously a large inner surface for potential applications in energy harvesting or conversion or for on-chip sensorics and actuorics. Finally, the hp-Si membranes can be transformed by thermal oxidation at temperatures above 800°C to hierarchical porous amorphous silica a material that could be of particular interest for opto-fluidic and photonic applications in the visible.

MM 18.35 Tue 17:30 P2

In situ X-ray spectroscopic and scattering studies on the emergence of CoO nano-assemblies in solution — ●CECILIA ZITO¹, LUKAS GROTE^{1,2}, KILIAN FRANK³, ANN-CHRISTIN DIPPEL², PATRICK REISBECK³, KRZYSZTOF PITALA⁴, KRISTINA KVASHNINA⁵, STEPHEN BAUTERS⁵, BLANKA DETLEFS⁵, OLEH IVASHKO², PALLAVI PANDIT², MATTHIAS REBBER¹, SANI HAROUNA-MAYER¹, BERT NICKEL³, and DOROTA KOZIEJ¹ — ¹University of Hamburg, Germany — ²Deutsches Elektronen-Synchrotron, Hamburg, Germany — ³Ludwig-Maximilians-Universität München, Germany — ⁴AGH, University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland — ⁵European Synchrotron Radiation Facility ESRF, Grenoble, France

The key to fabricating complex, hierarchical materials is the control of chemical reactions at various length scales. The classical crystallization theory is insufficient to properly describe the chemical reaction leading to monomer formation, the evolution of small primary particles, and how they assemble into superstructures. Here, we illustrate how the combination of advanced X-ray spectroscopic and scattering in situ studies probe length scales all the way from atomic to macroscopic, and shed light on the formation mechanism of CoO nanocrystal assemblies in solution. Utilizing HERFD-XANES, we directly access the molecular level of the nanomaterial synthesis. We reveal that initially Co(acac)₃ rapidly reduces to square-planar Co(acac)₂ and coordinates to two solvent molecules. Furthermore, we track subsequent structural changes with in situ total X-ray scattering and atomic pair distribution function analysis, pinning down the transition from the dissolved Co complex to crystalline CoO. Ultimately, SAXS uncovers the assembly process of the crystallites into distinct spherical superstructures. The concomitant growth and assembly of crystallites into a superstructure differentiates the investigated pathway from a classical mechanism. The combination of X-ray spectroscopy and scattering can elucidate the emergence of assemblies in solution with a broad perspective.

MM 18.36 Tue 17:30 P2

Hierarchical materials mimicking mechanical behaviour of human bone synthesized by additive manufacturing and dealloying. — ●ALEKSANDR FILIMONOV¹, LUTZ MÄDLER^{1,2}, and ILYA OKULOV^{1,2} — ¹Faculty of Production Engineering, University of Bremen, Badgasteiner Str. 1, 28359 Bremen, Germany — ²Leibniz Institute for Materials Engineering-IWT, Badgasteiner Str. 3, 28359 Bremen, Germany

The close match between the elastic properties of an implant material and bone is crucial to avoid the stress-shielding effect. Therefore, low modulus biomaterials are desirable for biomedical implants that ensure rapid healing of hard tissue. Due to its complex hierarchical structure, bone features moderate strength similar to some metals and low elastic modulus like polymers. Implant materials for bone fixation should be several times stronger compared with that of bone. However, the general relation between strength and elastic modulus of man-made materials suggest that stronger materials typically possess higher elastic

modulus including metals - usual candidates for bone fixation. In this work, novel hierarchical metal-polymer composite materials "breaking" the general trend between strength and elastic modulus were synthesized by additive manufacturing and liquid metal dealloying. The large digital porosity of metallic scaffold was synthesized by additive manufacturing and its fine porosity is a result of materials self-organization upon dealloying. The results suggest that these novel composite materials mimicking the structure and mechanical behaviour of bone are potential candidates for biomedical applications.

MM 18.37 Tue 17:30 P2

Peculiarities of electron transport and resistive switching in point contacts on TiSe₂ and TiSeS. — DMYTRO BASHLAKOV¹, ●OKSANA KVITNITSKAYA¹, YULIYA SHEMERLIUK², SAICHARAN ASWARTHAM², DMITRI EFREMOV², BERND BÜCHNER^{2,3}, and YURI NAIDYUK¹ — ¹B. Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine, Kharkiv, Ukraine — ²Institute for Solid State Research, IFW Dresden, Dresden, Germany — ³Institut für Festkörper- und Materialphysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Dresden, Germany

We report resistive switching in voltage biased point contacts (PCs) based on the transition metals chalcogenides TiSe₂ and TiSeS. The switching is taking place between a low resistive *metallic-type* state and a high resistive *semiconducting-type* state by applying bias voltage (<0.4V), while reverse switching takes place by applying voltage of opposite polarity. The difference in resistance between these two states can reach of about two orders of magnitude at helium temperature. The origin of the effect can be attributed to the electric field induced change of stoichiometry in PC core due to drift of Se vacancies. Additionally, we demonstrated, that heating takes place in PC core, which can facilitate the electric field induced effect. At the same time we did not find any evidence for CDW spectral features in our PC spectra for TiSe₂. The observed resistive switching allows to propose TiSe₂ and TiSeS as the promising materials, e.g., for non-volatile resistive random access memory (ReRAM) engineering.

MM 18.38 Tue 17:30 P2

Electron-phonon interaction and point contact enhanced superconductivity in trigonal PtBi₂ — DMYTRO BASHLAKOV¹, ●OKSANA KVITNITSKAYA¹, GRIGORY SHIPUNOV², SAICHARAN ASWARTHAM², OLEG FEYA^{2,3}, DMITRI EFREMOV², and BERND BÜCHNER^{2,4} — ¹B. Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine, Kharkiv, Ukraine — ²Institute for Solid State Research, IFW Dresden, Dresden, Germany — ³Kyiv Academic University, Kyiv, Ukraine — ⁴Institut für Festkörper- und Materialphysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Dresden, Germany

PtBi₂ is a Weyl semimetal, which demonstrates superconductivity with low critical temperature $T_c \sim 0.6$ K in the bulk. Here, we report our study of electron-phonon interaction (EPI) in trigonal PtBi₂ by the Yanson point contact (PC) spectroscopy and presenting the observation of PC enhanced superconductivity. We show, that the Yansons PC spectra display a broad maximum around 15 meV, indicating, apparently, EPI mechanism of Cooper pairing in PtBi₂. Moreover, we discovered a substantial increase of T_c up to ~ 3.5 K in PCs. The observed T_c is sufficiently higher than the bulk value, as well as detected at hydrostatic pressure. We calculated the phonon density of states and Eliashberg EPI function in PtBi₂ within the framework of the density functional theory. A comparison of experimental data with theoretical calculations showed acceptable agreement. The theoretical T_c is 3.5 K, which corresponds to the experimental value.

MM 18.39 Tue 17:30 P2

Quantification of intrinsic surface charges on MgO nanocubes using off-axis electron holography — ●YAN LU^{1,2}, FENGSHAN ZHENG¹, QIANQIAN LAN¹, MICHAEL SCHNEIDER¹, PHILIPP EBERT¹, and RAFAL E. DUNIN-BORKOWSKI¹ — ¹Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C 1) and Peter Grünberg Institute (PGI 5), Forschungszentrum Jülich, Jülich, Germany — ²Beijing Key Lab and Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing, China

Metal oxide nanoparticles exhibit outstanding catalytic properties, believed to be related to the presence of oxygen vacancies at the particle surface. However, little quantitative is known about concentrations of point defects inside and on surfaces of these nanoparticles due to the challenges in achieving an atomically resolved experimental access.

By employing off-axis electron holography, we demonstrate exemplarily using MgO nanoparticles as a methodology, which allows us to discriminate between mobile charges induced by electron beam irradiation and immobile charges associated with deep traps induced by point defects as well as distinguish between bulk and surface point defects. Counting the immobile charges provides a quantification of the concentration of F²⁺ centers induced by oxygen vacancies at the MgO nanocube surfaces.

MM 18.40 Tue 17:30 P2

3D Printed One Piece Surface Alteration Sensor with Galvanic Isolation — ●MICHAEL FEIGE and SONJA SCHÖNING — Bielefeld Institute for Applied Materials Research (BIFAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences and Mathematics

More recently it is possible to combine conductive and non-conductive materials in one 3D print process. This allows printing of complex structures like PCBs, 3D coils, transformers, capacitors or high frequency components like antennas or transmission lines. Furthermore it is possible to combine those components to build highly specialized sensors in one production step.

We developed a concept for a sensor which, in its specialized form, could be used for detection of mechanical, chemical or biological alteration of surfaces such as abrasion, material degradation or separation. The detection method is based on an electrical, inductive readout while maintaining a sufficient galvanic isolation between the sensing area and the readout circuit.

In this contribution an actual sensor device capable of detecting corrosion is presented, which was designed, printed and tested with successful results. The sophisticated design outweighs the lack of high electrical conductivity and high magnetic permeability within the range of printable materials by the ability of the printer to precisely integrate the conductive material into the insulating material.

MM 18.41 Tue 17:30 P2

A first study on the current-controlled flash sintering experiments on 3YSZ-Ni composites — ●PRANAV RAI and DEVINDER YADAV — Department of Metallurgical and Materials Engineering, Indian Institute of Technology Patna, Bihta, Patna 801106, India

Flash sintering involves densification of ceramic bodies in few seconds at relatively low furnace temperatures. The normal flash sintering experiments are characterized by a non-linear rise in the electrical conductivity of the sample. In the present work, flash sintering experiments were conducted in the current-controlled mode where the current is made to increase linearly through the sample at a constant rate. The sample sinters progressively as the current increases. Composites of 3YSZ and Ni, with different Ni contents (5wt.%, 10wt.%, and 20wt.%) were flash sintered at a constant current rate of 600 mA/min with a target current density of 100 mA/mm², at a furnace temperature of 900°C. The total span of the experiments was 50 s. The extent of densification decreased with increase in Ni content. In addition, the samples with higher Ni content started to densify at a higher current density. XRD revealed oxidation of Ni in all the samples, post flash sintering. However, complete oxidation of Ni to NiO in conventional sintering of the same composites occurred at 1450°C after a hold time of 2 hours. The flash sintered microstructure of 3YSZ phase was characterized by relatively fine grains with narrow grain size distribution. The 3YSZ-20Ni samples exhibited a microstructure with percolating network of the NiO phase. The processed samples can have possible applications in designing the anode materials for solid oxide fuel cells.

MM 18.42 Tue 17:30 P2

Electrospun Electroluminescent CsPbBr₃ Fibers: Flexible Perovskite Networks for Light-Emitting Application — ●KHAN LÉ¹, FLORIAN VON TOPERCZER², FERAY ÜNLÜ¹, THOMAS FISCHER¹, KLAS LINDFORS², and SANJAY MATHUR¹ — ¹Institute of Inorganic Chemistry, University of Cologne, Greinstr. 6, 50939 Cologne, Germany — ²Institute of Physical Chemistry, University of Cologne, Greinstr. 4-6, 50939 Cologne, Germany

Organic-inorganic and all-inorganic lead halide perovskites (APbX₃) have continuously attracted research interest and went through significant improvements towards highly efficient photovoltaic technologies and LEDs. Most lead-halide perovskite devices are based on thin films or quantum dots while reports on alternative morphologies are scarce. We prepared CsPbBr₃@polymer composite nanofibers by one-step electrospinning and characterized them by scanning electron microscopy, transmission electron microscopy, X-ray diffractometry,

UV/vis and photoluminescence spectroscopy. As a proof-of-concept, we subsequently integrated the fiber mats as active layers in electrically driven light emitting devices. While the synthesis of perovskite nanofibers is not new, to the best of our knowledge we would be the first to report on electroluminescence of such fibers. In addition, all preparations were conducted under ambient atmosphere and the perovskite precursor ink was prepared with low toxicity solvents (H₂O/EtOH/ionic liquid). This work could pave the way towards cost effective and flexible optoelectronic fiber- or yarn-based lead-halide perovskite devices by an up-scalable method.

MM 18.43 Tue 17:30 P2

Raman spectra of Arsenopyrite: Experiment and Theory —
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Arsenopyrite (FeAsS) is a semiconductor with a small bandgap and a common source for arsenic (As) mineral. Chemical and structural information on this material is still of interest. The crystal structure is, monoclinic with space group $P2_1/c$, derived from orthorhombic marcasite (FeS₂) [1]. Here we present a combined experimental and theoretical study on the vibrational properties of arsenopyrite, which have to our knowledge not yet been reported. Raman spectra have been recorded experimentally by means of a LabRam HR800 spectrometer from HORIBA Jobin Yvon using 633 nm laser as the excitation source. Additionally, Raman spectra were calculated using Quantum Espresso [2] with norm-conserving pseudopotential and PZ exchange-correlation functional. The comparison of experimental and theoretical data shows good agreement and allows for symmetry assignment of the Raman peaks.

[1] Bindi, L.; Moelo, Y.; Leone, P.; Suchaud, M. *Can. Mineral.* 50, 471*479 (2012).

[2] P. Giannozzi et al., *J.Phys. Condens. Matter* 21, 395502 (2009)