MM 23: Poster II

Time: Tuesday 18:15–20:00 Location: P2/OG1+2

MM 23.1 Tue 18:15 P2/OG1+2

(ZnO) 42 Nanocluster: A Novel Visibly Active Magic Quantum Dot under First Principle Investigation — •Bijal Mehta and Debesh Roy — Materials and Biophysics Group, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India.

A systematic density functional investigation on the structural, electronic and optical properties of the growth of (ZnO) 6 cluster unit in the series of (ZnO) 6n for n=1*9 is performed in this report. Different electronic properties of (ZnO) 6n nanoclusters are analyzed in terms of HOMO-LUMO gap (HLG), ionization potential (IP), electron affinity (EA), chemical hardness (η), and electrophilicity index (ω) which all shows a zigzag behavior as the size of (ZnO) 6n clusters increases. The clusters' electronic energy gain (*E) identified an exceptionally stable *magic* nanocluster, viz. (ZnO) 42. Frontier orbitals analysis results indicate easy electron transfer in (ZnO) 42 nanocluster system. The optical absorption spectra confirm that the magic (ZnO) 42 nanocluster is active in electromagnetic radiation's visible range (λ=406.8 Å). Interestingly, similar optical switching towards the growth of (ZnO) 6 unit is also observed like zig-zag electronic properties. The simulation results of electronic properties as well as the infrared spectra of magic (ZnO) 42 cluster will open up a vista to the experimentalists for its possible synthesis, which in turn will help in the development of the visibly active magic (ZnO) 42 nanocluster with novel applications in the fields of quantum dots or assembled materials.

MM 23.2 Tue 18:15 P2/OG1+2

Investigation of the stability for AlB_2-type transition metal diborides from electronic structure — •Nebahat Bulut and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

Boron has huge chemical bonding diversity (metallic, ionic, and covalent bonds) because it provides fewer valence electrons compared to the number of orbitals it can form. Not surprisingly, intermetallic borides can crystallize in many different crystal symmetries, for example cubic, hexagonal or orthorhombic. The unit cell of the hexagonal AlB_2-type has two trigonal prisms in which borons are in the center surrounded by six metal atoms. Interestingly, not all twenty eight transition metals form the AlB_2-type crystal structure. The goal of the study is to understand the chemical bonding nature in detail in order to answer why some of these compounds are stable in AlB_2-type structure while others are not. We investigate the impact of the *d*-orbitals of the transition metals on the stability in order to provide a guideline to possible new transition metal diborides. The chemical bonding and charge transfer in these transition metal diborides is investigated by electronic structure calculations based on density functional theory as implemented in Quantum Espresso [1]. The study is focused on the analysis of the electron density together with the electron localization function (ELF) and provide thermodynamic information e.g. formation enthalpies, and mechanical properties.

[1] P. Giannozzi et al., J. Chem. Phys. 152 154105 (2020)

MM 23.3 Tue 18:15 P2/OG1+2

Trapping and detrapping of excess vacancies during natural ageing in Al-Cu — •Tobias Stegmüller, Johannes Berlin, Andreas Schuss, and Ferdinand Haider — University of Augsburg, Chair for Experimental Physics I, Universitätsstr. 1, 86159 Augsburg

A special feature of Al-Cu alloys is the occurrence of decomposition in supersaturated solid solutions by the formation of Guinier-Preston zones (GPZ) even at ambient temperature, where the equilibrium diffusion coefficient is far too low for any unmixing. A condition for this natural ageing is the existence of excess vacancies which remain in the material after quenching from the homogenisation temperature. As the ageing process proceeds for surprisingly long times (hours or days), the vacancies seem to be stabilised in the material and do not decay to the equilibrium value, which would stop the ageing.

Although there exist theories on the stabilisation of excess vacancies, there is no established and verified model to explain the effect. To illuminate the mechanisms behind the long term formation of GPZ we combine results from TEM and DSC measurements as well as Monte Carlo, molecular static and DFT simulations, which reveal that the GPZ themselves may act as temporal vacancy traps. Values for the trapping energy for vacancies in GPZ and on dislocations are estimated from simulations.

MM 23.4 Tue 18:15 P2/OG1+2

Proof of concept for micro pulling down growth of phase change materials in the example system of NiTi — •Lauritz Schnatmann, Timon Sieweke, and Gabi Schierning — University of Bielefeld

The micro pulling down growth method (mPD) is a common approach to synthesize small crystals for material screening in e.g. high-entropy oxides. Another interesting group of materials are phase change materials namely showing unique structural transitions interplaying with electronic and magnetic contributions. However, the interplay between the different contributions is strongly dependent on the composition of materials. We built up a micro pulling down set up for fast material screening of phase changing materials. We grew a NiTi- shape memory alloy to show the possibility of comparable easy growth of crystals by mPD. Hereby, we verified mPD as a powerful tool for the versatile fabrication of small crystals in the field of phase change materials.

MM 23.5 Tue 18:15 P2/OG1+2

The role of electrons during the martensitic phase transformation in NiTi-based shape memory alloys — •Alexander Kunzmann[1], Jan Frenzel[2], Ulrike Wolff[3], Jeong Woo Han[4], Lars Giebeler[3], David Piorunek[2], Martin Mittendorf[4], Juliane Scheiter[3], Heiko Reith[3], Nicolas Perez[3], Kornelius Nielsch[3,5], Gunther Eggeler[2], and Gabi Schierning[1] — [1]Bielefeld University — [2]Ruhr University Bochum — [3]IFW-Dresden — [4]University of Duisburg-Essen — [5]TU Dresden

The present work provides an experimental contribution to the investigation of the role of conduction electrons in the martensitic phase transition of Nickel-Titanium. This material, which is structurally very well studied due to its shape memory effect, still offers room for further knowledge more than 60 years after its discovery. For this purpose, a series of alloys within the equiatomic NiTi phase was characterized by temperature-resolved transport experiments, thermodynamic characterizations and structural investigations. In addition to the well-known resistivity anomaly, a reduction of the charge carrier density by 90% was measured, which has not been described before for this class of materials. Using a novel approach for structural materials, conclusions could be drawn about the entropy of the electronic system and a correlation with the phase transition temperature could be demonstrated. The obtained data allow an interpretation as the formation of a charge carrier density wave phase, which explains both the drastic reduction of charge carriers and the large electronic entropy contribution.

MM 23.6 Tue 18:15 P2/OG1+2

developing high-hardness, high-electrical conductivity and gradient structure of bulk Al-2.5Fe alloy by a new severe plastic deformation: high pressure torsion extrusion — •Rui Xu — Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

The effect of High Pressure Torsion Extrusion (HPTE) on microstructure, hardness and electrical conductivity has been investigated in the bulk Al-2.5Fe alloy. The equivalent strain accumulated in the samples after one pass of HPTE varied in a wide range between 0.9 and 24.8, depending on the processing parameters. HPTE led to the formation of a gradient microstructure in which the grain and Al6Fe intermetallic size decreased by increasing the distance from the central axis of the samples. With increasing the equivalent strain, which is below 5.7, the microhardness and the electrical conductivity simultaneously increased, from 53.7 HV to 87 HV, from 38% IACS to 47% IACS respectively. This can be attributed to the grain size and Al6Fe intermetallic size decreased. When the equivalent strain gradually increased to 24.8, the microhardness continuously increased from 87 Hv to 126 Hv, the electrical conductivity decreased from 47% IACS to 43% IACS. This is contributed to the grain and Al6Fe intermetallic transformed into nanometer size, which significantly increased the microhardness, and some Fe atoms into Al matrix, which decreased the electrical conductivity. The High Pressure Torsion Extrusion process can lead to gradient microstructure and simultaneously increase the

microhardness and the electrical conductivity of bulk Al-2.5Fe alloy..

MM 23.7 Tue 18:15 P2/OG1+2

In situ XRD measurements of a Si Li half battery cell — •Leonard Aue, Frederik Stender, Thomas Brede, and Cynthia Volkert — Georg-August-Universität Göttingen, Deutschland

Li-ion batteries have become an indispensable part of modern life. They enable the repeated storage of energy on a medium and small scale, for example in electric vehicles or mobile devices.

In addition to the commonly used graphite, silicon is gaining increasing attention as a suitable anode material due to its higher capacity. However, this capacity decreases rapidly in application and a significant increase of the internal resistance occurs. Both are mainly caused by the large volume changes during lithium uptake and release.

In this work, we investigate the amorphization process that first starts during loading in in-situ XRD measurements of Si-Li composite materials in a half-battery setup. This will give us insight into Si phase changes under direct control of critical parameters such as charge or discharge rates. This knowledge could help to understand and control the phase transformations and thereby improve Si anode performance.

MM 23.8 Tue 18:15 P2/OG1+2

High capacity thin film battery electrodes from lithium titanate — Yijie Tao, •Yug Joshi, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

Lithium titanium oxide is becoming an increasingly popular anode material for high-power Li-ion batteries due to their safe operating voltages and high cycle lifetime. The motivation to enhance the specific capacity of Li4Ti5O12 (LTO) is of practical significance. In this work, reactive ion beam sputtering is used to deposit the titanium-based metal oxide thin films. A Li2CO3 modification is introduced by mixing it with LTO and using the composite as a target material. The deposition conditions (i.e., reactive oxygen) and annealing treatment (i.e., under air or vacuum at varying temperatures) are explored to optimize the thin films for the best possible capacity. X-ray diffraction (XRD), X-ray photoelectron (XPS) and electron diffraction (TEM) are used to unravel the chemical and structural nature of the thin films. The films were electrochemically characterized using cyclic voltammetry with a broad potential window, much wider than conventional LTO (i.e., 2.5V to 0.1 V vs Li/Li+, whereas conventional electrode is generally limited to a lower voltage of 1V). The optimised film shows good cyclic stability at a relatively high rate of 1 mV/s and show an astounding maximum capacity of 101.4 μAh*cm-2*μm-1 after 50 cycles. To put this in context, conventional LTO shows theoretically 60.8 μAh*cm-2*μm-1 and 91 μAh*cm-2*μm-1 when cycled down to 1 V and 0.1 V vs Li/Li+, respectively.

MM 23.9 Tue 18:15 P2/OG1+2

high-rate and long-duration Sodium Storage Enabled by Sodiation-Driven Reconfiguration — •Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Vanadium sulfides, with various crystal structures, such as VS2, V2S3, V3S4, V5S8, and VS4 have attracted increasing attention because they could provide high theoretical specific capacity. Nevertheless, such vanadium-based sulfides frequently suffer significant mechanical pulverization during long-term cycling as a result of volume expansion caused by sodization/desodization, which result in severe irreversible capacity degradation, poor initial coulombic efficiency, reduced rate capability, and inappreciable cycling stability. Here, we demonstrate a carbon-free 3D micro-nano flower-like VSx heterostructure electrode material that is synthesized by a facile hydrothermal process for SIB applications. The 3D micro-nano flower-like structure can well prevent the accumulation of nanosheets during electrochemical cycles and ensure full contact between the active material and the electrolyte. Therefore, 3D micro-nano flower-like VSx electrode that finally achieves an ultrahigh-rate capacity (613.8 mAh/g at 10 A/g) and an ultra-long cyclability (more than 1500 cycles) by sodiation-driven reconfiguration for sodium ions batteries. This work presents a general approach for preparing super-high specific capacity and rate capacity electrode materials for further improving the SIBs performance.

MM 23.10 Tue 18:15 P2/OG1+2

Detection of Lithium in potential electrode materials — •Patrick Kirscht and Hans Hofsäss — II Physikalisches Institut, Georg August Universität, Göttingen, Deutschland

Nuclear reaction analysis is used to quantify light elements such as lithium in a sample. The advantage of NRA is the isotope specific measurement of elements in a sample. In the current investigations we demonstrate the detection limits and sensitivity of a new setup for the detection of lithium via its nuclear reaction with protons p(7-Li,alpha)alpha with Q=17MeV. For this purpose an external proton beam with 2.5MeV is used. To determine the detection limit, lithium was implanted into silicon and ta-C near the surface by ultra-low energy ion implantation at 100eV. Furthermore, the depth profile and penetration depth were simulated using Imintdyn and SRIM and were compared with the measurements. For the measurement of diffusivity of lithium, the samples were baked at different temperatures. For comparison, MD simulation was performed using LAMMPS. These investigations are the starting point of measurements on graphene and biological materials like wood, which are considered for possible applications as electrode materials in batteries.

MM 23.11 Tue 18:15 P2/OG1+2

High-resolution measurement of displacement field from gold nanoparticules tracking — •Antoine Ollivier, Nicholas Blanchard, Antonio Pereira, Loïc Vanel, and Döme Tanguy — Institut Lumière Matière-UMR 5306, Université Claude Bernard Lyon 1, 6 rue Ada Byron, 69622 Villeurbanne cedex

A new method has been developped to measure displacement field during a tensile test with both high resolution ($\sim$ 50 nm) and good precision ($\sim$ 1nm). This method has been applied on the reduced activation ferrito-martensitic steel Eurofer97. Gold nanoparticules are created by pulsed-laser induced dewetting of a nanofilm. This technique does not modify the structure of the steel below. Nanoparticules are then observed with a scanning electron microscope during tensile test. Their tracking allows to see displacement field *in situ*. This method is particularly adapted for locating heterogeneities in the displacement field and it could be very useful to understand how fracture appears.

MM 23.12 Tue 18:15 P2/OG1+2

Electronic Properties of Self-assembled 1D Gold Nanoparticle Chains — •Stefan M. Schupp[1], David J. Schupp[2], Emil Schwarz[2], Rebecca Köser[2], Helmut Cölfen[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, Germany

1D nanoparticle (NP) assemblies exhibit unique electronic properties due to their directional charge transport. In addition, the usage of stabilizing ligands enables a further possibility to add new functionalities and tune their conductivities. However, the assembly and characterization of 1D NP chains remains a challenge to this day. Here, we present a study on thiol-induced dipoles on gold (Au) nanoparticle surfaces which result in chain-like assemblies in solution under ambient conditions. Thereby, 1D assemblies of 40 nm Au-NPs with different shapes and thiolated ligands could be achieved. Afterwards, a developed transfer technique allows the electrical characterization of individual 1D NP chains through prefabricated gold electrodes. In this configuration, the temperature-dependent resistance of different NP assemblies is investigated to understand the underlying conduction mechanisms. With the gained knowledge it should be possible to generate 1D Au NP chains with controllable electronic conductivities for future applications.

MM 23.13 Tue 18:15 P2/OG1+2

Local hydrogen absorption in Pd nanoparticles observed with in-situ TEM — •Svetlana Korneychuk[1], Stefan Wagner[1], Georgian Melinte[2], Darius Rohleder[3], Phillipp Vana[3], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]King Abdullah University of Science and Technology, Saudi Arabia — [3]Institute of Physical Chemistry Georg-August-University Göttingen, Göttingen, Germany

The mechanism of the hydrogen absorption in metals is of a high interest for many areas of hydrogen technology, such as hydrogen storage, hydrogen detection and catalysis. Palladium is an ideal model system to study hydrogen absorption in metals due to its extreme affinity to hydrogen. Nanoscale systems, such as nanoparticles and thin films, are of the high interest to hydrogen technology due to their faster interaction with hydrogen. In this work, we investigate the behavior of a model system, Pd nanoparticles, in real time with in-situ H2-gas TEM. With the special gas holder from Protochips it is possible to reach pres-

sures up to 1 atmosphere and study the particles at elevated temperatures within the stability limit of the nanoparticles up to 200°C. We can observe initial stages of hydrogen absorption in Pd nanoparticles and local formation of PdHx at different temperatures and pressures by using EELS. We support our observations with the in-situ strain measurements carried out with nanobeam electron diffraction. Finally, we propose a mechanism of hydrogen absorption in metallic nanoparticles based on the local PdHx formation and strain measures at different loading conditions.

MM 23.14 Tue 18:15 P2/OG1+2

Investigation of the MoS_2 crystallization process in thin films — •Annika Korn, Thomas Brede, and Cynthia A. Volkert — Institut für Materialphysik, Göttingen, Germany

Crystalline transition metal dichalcogenide thin films show interesting potential in various application areas (e.g. optoelectronics and data storage). Crystallization of amorphous sputtered thin films is one way to produce large crystalline regions suitable for the application [1]. The aim of this work is to follow the structure of the thin films over the course of crystallization and to characterize them in different intermediate states. In this way, the process and properties of the transition can be studied and better understood. Specifically, various methods (XRD, SEM, EDX, XPS, AFM, TEM) will be used to analyze the microstructures and compositions of the samples. In addition, DSC and TGA will be used to directly measure the crystallization and possible decomposition processes.

[1] Krbal, Milos, et al.: Amorphous-to-Crystal Transition in Quasi-Two-Dimensional MoS2: Implications for 2D Electronic Devices. In: ACS Applied Nano Materials 2021 4 (9), 8834-8844. DOI: 10.1021/acsanm.1c01504

MM 23.15 Tue 18:15 P2/OG1+2

Towards measuring fatigue-generated vacancies in thin copper films using nanoindenter creep tests — •My Nguyen, Thomas Brede, Jan Verhoeven, and Cynthia Volkert — Institute for Materials Physics, Georg-August University of Göttingen

Vacancies can be created in metals during cyclic loading, however, they have been only rarely directly detected. In this study, we develop an experimental set-up to detect fatigue generated vacancies by measuring their contribution to creep deformation. Our methodology involves performing nanoindenter creep tests on thin metal films while they are being fatigued by cyclic loading. The fatigue is realized using delay line structures, with thin copper films on top, on which standing surface acoustic waves are generated. Contributions from thermal drift during the creep tests have been minimized using a continuous stiffness measurement method.

MM 23.16 Tue 18:15 P2/OG1+2

Optical Modulation and Phase Distribution in LiCoO2 upon Li-ion De/Intercalation — Sanaz Banifarsi, •Yug Joshi, Robert Lawitzki, Gábor Csiszár, and Guido Schmitz — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

The optical modulation of sputter deposited thin-films of LiCoO2 upon de-/lithiation is probed in reflectance geometry. The thin-films of LiCoO2 (LCO) are sputter-coated using ion-beam sputtering, onto mirror-like platinum current collectors. A reversible electrochemical and electrochromic behavior is obtained from the in-operando electrochemical and optical measurements. The optical constants (using ex-situ optical spectroscopy) are obtained by modelling the obtained spectra using Clausius-Mossotti relation. The model parameters reveal a dominant resonant wavelength at 646 nm for the fully intercalated LCO. For the delithiated state, Li0.5CoO2, a much broader and more intense absorption peak is obtained. This broad and intense peak is correlated to the conducting nature of the delithiated state. The obtained complex refractive index (CRI) are justified by prior reported calculations of the density of states. With the evolving CRI, the variation in the imaginary and real part of the dielectric constant is understood by a layered phase propagation. This is due to (i) the faster diffusion between the layers of CoO6 octahedra of the layered structured LCO and, (ii) the alignment of these octahedral planes almost perpendicular to surface of the electrode as a result of the identified growth texture (due to the deposition and the subsequent annealing).

MM 23.17 Tue 18:15 P2/OG1+2

Simulations of two-dimensional amorphous materials based on force fields and ab initio calculations — •Emel Gurbuz and Biplab Sanyal — Uppsala University, Uppsala, Sweden

In recent times, low dimensional crystalline structures and van der Waals(vdW) solids have attracted a lot of attention for their huge potential in device applications.However, the exploration of two-dimensional(2D) amorphous forms is less explored. Here, we present a detailed study of structural, electronic and thermal properties of 2D amorphous graphene(A-Gra), silicene(A-Si) and silicon carbide(A-SiC) by Classical Molecular Dynamics (CMD) simulations for structure generation, stability tests, thermal conductivity and vibrational analysis along with density functional theory (DFT) calculations for the electronic structure.We find that A-Gra is planar and metallic with a thermal conductivity around 55.30 W/Km whereas the monolayer A-Si has a much lower thermal conductivity (2.68 W/Km). Among our studied materials, A-SiC's thermal conductivity is found to be the highest (70.29 W/Km).Vibrational analysis shows that the heat carriers in A-Si and A-SiC are extendons, especially diffusions in the absence of localized vibrational modes. Bilayer and trilayer structures of amorphous structures resulted respectively, in vdW bonding of A-Gra layers; covalent bonding of A-Si layers and weak bonding of SiC layers through only Si atoms. Finally, the observed uneven charge distributions can lead to the designing future electronic devices by tuning the local functionalities of 2D-amorphous structures.

MM 23.18 Tue 18:15 P2/OG1+2

Effect of micro-alloying and structural relaxation on the nanoindentation behavior of Pd-based metallic glasses — •Richard von Destinon, Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

Two methods rising in interest to modify the mechanical properties of metallic glasses consist of micro-alloying as well as relaxation. We study the influence of structural relaxation and 1 at.% additions of Fe or Co on the well-researched metallic glass $Pd_{40}Ni_{40}P_{20}$. The relaxation states are created by quenching from temperatures above T_g with different cooling rates. The samples are analyzed using nanoindentation with force ranges up to 1 mN. Correlations between the change in mechanical properties, such as hardness and young's modulus, and the shear deformation behavior through the pop-in distribution are investigated in detail. The results indicate that both, micro-alloying and relaxation increase the hardness of the material significantly, while the pop-in frequency remains insensitive to either.

MM 23.19 Tue 18:15 P2/OG1+2

Orientation-tunable Rod-shaped Liquid Crystal Under Surface Acoustic Wave — •Zhuoqing Li[1], Pai Zhao[1], Patrick Huber[2], and Robert Blick[2] — [1]TU Hamburg Institut für Material- und Röntgenphysik, Hamburg, Germany — [2]Center for Hybrid Nanostructures, University of Hamburg, Hamburg, Germany

Surface acoustic waves (SAW) are widely used in both industry and science, while liquid crystals are unique fluids exhibiting long-rang order and self-organization. In this work, a combination of SAW and rod-shaped nematic liquid crystals will be studied to explore the tunablility of liquid crystal orientations under SAW. Surface acoustic waves are introduced into miniatured solid-state devices on piezoelectric LiNbO3 substrates by interlocking metallic gates called interdigitated transducers (IDT). When a high-frequency sinusoidal signal is applied to the IDT, a mechanical deformation wave will propagate along the surface of the substrate and the induced shear strain will influence the orientation of the nematic liquid crystals on the surface of the substrate. A feature of the nematic phase is that the anisotropic rod-shaped molecules are collectively orientated in preferred directions. Considering the optical anisotropy of rod-shaped liquid crystals, the collective orientation change of liquid crystal molecules under SAW can be analyzed through birefringence measurements. By studying the tunability of the liquid crystal orientation under SAW induced shear component of the wave, we will be able to develop a novel wireless LC-based optical modulator controllable by acoustic stimuli.

MM 23.20 Tue 18:15 P2/OG1+2

Strain-coupled polar textures in ferroelectric nanocylinders — •Svitlana Kondovych[1] and Igor Lukyanchuk[2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Laboratory of Condensed Matter Physics, University of Picardie, 80039 Amiens, France

We consider ferroelectric $PbTiO_3$ nanocylinders of various size hosting strain-coupled polarization vortices. Depending on the cylinder

height and radius, the polarization either swirls around the *c*-oriented cylinder axis (*c*-vortex) or falls into the state with the *a*- or *b*-oriented vortex core (*a*-vortex). The emergence of vortices occurs due to the competition of elastic and electrostatic interactions and complies with the Arnold theorem for divergenceless vector fields, which exist as two types of topological excitations, either vortices or Hopfions [2]. In $PbTiO_3$ cylinders, we observe the geometry- and temperature-induced vortex axis rotation and corresponding transition between the *c*- and *a*-vortex states. The resulting phase diagram, obtained by phase-field modeling in line with analytical calculations, illustrates the variety of polar textures in nanocylinders, applicable for the efficient design of ferroelectric-based device components.

S.K. acknowledges the support from the Alexander von Humboldt Foundation.

[1] S. Kondovych, et al., arXiv:2112.10129v3 (2022).

[2] I. Luk'yanchuk, et al., Nat. Commun. 11, 2433 (2020).

MM 23.21 Tue 18:15 P2/OG1+2

Tuning porous silicon's pore geometry and its influence on laser-excited guided waves — •Marc Thelen[1], Nicolas Bochud[2], Manuel Brinker[1], Claire Prada[3], and Patrick Huber[1,4,5] — [1]MXP, TUHH, Hamburg, Germany — [2]MSME, UPEC, Creteil, France — [3]Institut Langevin, ESPCI Paris, Université PSL, CNRS, Paris, France — [4]CXNS, DESY, Hamburg, Germany — [5]CHyN, UHH, Hamburg, Germany

Nanoporosity in silicon leads to entirely new functionalities of this mainstream semiconductor with a wide range of applications. In a recent study, we investigated the complex mechanics and the influence of the pores' conicity [1]. This provided the basis for predictable applications in robust on-chip devices and evidence that recent breakthroughs in laser ultrasound technology open up entirely new possibilities for non-destructive in-situ mechanical characterization of dry and liquid-functionalized porous materials. The pores' conicity, which is unintentionally generated during the electrochemical synthesis of porous silicon, can be actively influenced by the process parameters and, within certain limits, arbitrary pore profiles can be generated. This is used, for example, in the production of Bragg mirrors. By tuning the pore shape, we are now investigating its influence on guided waves further, with the goal of developing a phononic material.

[1] Thelen, M., Bochud, N. et al., Nat Commun., 12, 3597 (2021)

MM 23.22 Tue 18:15 P2/OG1+2

Unraveling Fluid Phase Behavior in Geometrically Disordered Nanoporous Materials — •Henry R. N. B. Enninful and Rustem Valiullin — Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstraße 5, 04103, Leipzig, Germany.

Mesoporous solids exhibit structural disorder which strongly influence confined fluid properties. This renders quantification of structural disorder and its correlation with physical properties of confined matter a necessary step towards their optimization in practical applications.

In this work, we present advances made in the understanding of correlations between the phase state and geometric disorder in a series of nanoporous solids with variable morphologies. We overview the recently developed statistical theory for phase transitions in a minimalistic model of disordered pore networks represented by the linear chains of pores with statistical disorder. Furthermore, we show that correlating its predictions with various experimental observations, the model gives notable insights into collective phenomena in phase-transition processes in disordered materials and is capable of explaining self-consistently the majority of the experimental results obtained for gas*liquid and solid*liquid equilibria in mesoporous solids. We also show how a newly-introduced interconnectivity parameter of the pore network can be assessed to describe the morphology of porous solids.

MM 23.23 Tue 18:15 P2/OG1+2

Negative Poisson's Ratio in Hierarchical Nanoporous Gold — •Haonan Sun[1,2], Lukas Lührs[2], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of crack-free monolithic hierarchical nested network nanoporous gold enables the investigation on the benefits of hierarchy in the aspect of mechanical properties [1]. It has been demonstrated that hierarchical nanoporous gold (HNPG) can achieve a substantially reduced solid fraction and enhanced specific stiffness and strength compared with non-hierarchical nanoporous gold. However, the role of the hierarchical structure on Poisson's ratio is not explored yet. In this work, we synthesize mm-sized HNPG samples out of a Ag93Au7 master alloy with a dealloying-coarsening-dealloying method. We then explore the elastic and plastic Poisson*s ratios of HNPG by using digital image correlation during compression testsing. Remarkably, we find Poisson*s ratio of HNPG is negative for a given strain regime, which suggests their potential application as auxetic materials. Furthermore, the effect of ligament size at both hierarchy levels on Poisson*s ratio is also investigated. [1] S. Shi, Y. Li, B.-N. Ngo-Dinh, J. Markmann and J. Weissmüller, Scaling behavior of stiffness and strength of hierarchical network nanomaterials, Science 371 (6533), 2021.

MM 23.24 Tue 18:15 P2/OG1+2

Mechanical actuation of nanoporous metal driven by electroactive self-assembled monolayers — •Matts Olga and Mameka Nadiia — Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous (np) metals fabricated by alloy corrosion are emerging as promising functional materials for (bio-)chemical sensing and actuation. The actuation with np metals exploits the electrocapillary phenomena of metal surfaces, in which surface stress responses to changes of the surface state (e.g. due to adsorption). As the surface stress is coupled with stresses of opposite sigh in the metal bulk [1], its variations manifest themselves through macroscopic movements of the entire solid [2].

Due to high surface area, surface-functionalized np metals offer an ideal platform for highly sensitive sensing and actuation technologies. Here, were report reversible electroactuation of unimodal and hierarchical np-Au modified with an electroactive ferrocene-terminated self-assembled monolayer (SAM). In our experiment utilizing in situ dilatometry in electrolyte, an electrode potential is imposed on np-Au modulates redox transformations of SAM by oxidation and reduction of the ferrocene moiety. We find pronounced actuation strain variations that accompany the monolayer structural transformations triggered by potential. We discuss an origin of the phenomena in view of surface stress change of gold surfaces functionalized with the redox-active SAM. [1] Weissmüller, Cahn. Acta Mater. 45(5) 1899 (1997). [2] Kramer, et al. Nano Lett. 4(5) 793 (2004).

MM 23.25 Tue 18:15 P2/OG1+2

Importance of symmetry for the collapse of nanowire arrays — •Malte Grunert, Chengzhang Yhang, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau

We present numerical results highlighting the importance of symmetry considerations in the capillary collapse of nanowire arrays. For many of the envisaged applications of nanowire arrays, for example as a novel electrode material in lithium-ion batteries [1], maximizing the aspect ratio of the individual nanowires is one of the main goals. However, collapse occurs for wet-chemical fabrication processes after a critical aspect ratio is exceeded. As the length of the nanowires is increased, the torque resulting from surface tension during the drying step is increased as well, leading to collapse. In literature, only systems consisting of few nanowires are considered [2]. We show using multi-physics FEM simulations that a perfectly symmetric periodic nanowire array does not collapse, as the forces acting on the nanowires exactly cancel out. However, we also show that even slight length variations below the currently achievable experimental precision suffice to break the symmetry enough to load to the collapse of the entire array.

[1] L. Liang, Y. Xu, C. Wang, L. Wen, Y. Fang, Y. Mi, M. Zhou, H. Zhao, and Y. Lei, Large-scale highly ordered Sb nanorod array anodes with high capacity and rate capability for sodium-ion batteries, Energy & Environmental Science, 8, (2015).

[2] D. Chandra and S. Yang, Stability of high-aspect-ratio micropillar arrays against adhesive and capillary forces, Accounts of Chemical Research, 43, (2010)

MM 23.26 Tue 18:15 P2/OG1+2

Architecting Nanoscaffolds to Ward Off Agglomeration of Nanowire arrays: Achieving Reliable Length Retention — •Chengzhan Yan, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany.

Nanowire arrays with well-defined arrangements and high aspect ratios are of particular interest for energy storage systems. To this end, one

prevailing strategy is to combine ordered porous templates with wet chemical techniques. However, nanowires with high aspect ratios have a more severe tendency to self-agglomerate because of uneven capillary forces, which leads to poor arrangement reliability and degrades the electrochemical performance. Herein, an ultra-thin honeycomb alumina nanoscaffold (HAN) is constructed to ensure the structural stability of nanowire arrays, achieving a four-fold increase in the aspect ratio over the restriction. Within the integrated architecture, each nickel nanowire is individually separated by HAN so that the capillary forces around the nanowire cancel each other out during drying. Moreover, MnO2 and polypyrrole are further electrodeposited on these free-standing nanowires to form a vertically aligned core-shell 1D nanostructure arrays as cathodes and anodes for assembling micro-supercapacitors (MSCs). Attributed to the high specific surface area and low charge diffusion resistance, the assembled MSCs attain remarkably improved energy density, rate performance and lifespan.

MM 23.27 Tue 18:15 P2/OG1+2

Porous alumina membranes: how close to perfection? — •Marine Bossert[1], Panayotis Spathis[2], Pierre-Étienne Wolf[2], Laurent Cagnon[2], Isabelle Trimaille[3], and Étienne Rolley[4] — [1]Institut of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institut Néel, Grenoble, France — [3]Institut des NanoSciences de Paris, Paris, France — [4]Laboratoire de Physique de l'École Normale Supérieure, Paris, France

Alumina, and to a lesser extent, silicon porous membranes are considered often as model systems made of straight and independent pores, and, as such, porous alumina is used as templates for the synthesis of magnetic or thermoelectric materials [1].

In order to assess to which extent this ideal picture is valid, we have carried out extensive sorption measurements on membranes of different thicknesses, either native or with a pore aperture reduced by Atomic Layer Deposition. For porous silicon membranes, we find constrictions along the pore axis for all samples and interconnections between neighbouring pores when the latter are longer than 2 microns [2]. For alumina membranes, the pores are independent, but conical in shape rather than cylindrical, and rough rather than smooth. Moreover, their average diameter (along their length) is distributed from pore to pore.

We present quantitative estimates of these deviations to ideality, and discuss how to minimize them. [1] Lee and Park Chemical Reviews 2014 114 (15), 7487-7556 [2] Bossert et al, Langmuir 2021 37 (49), 14419-14428

MM 23.28 Tue 18:15 P2/OG1+2

Freezing of water in 3 nm silica nanopores: A molecular dynamics study — •Lars Dammann[1,2], Robert Horst Meissner[2,3], and Patrick Huber[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany — [2]Hamburg University of Technology, Am Schwarzenberg-Campus 1, Hamburg 21073, Germany — [3]Institute of Surface Science, Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, Geesthacht 21502, 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 crystallization, the crystalline structures of nanoconfined water and the lower bounds of pore sizes that still permit phase transitions are subject of scientific discussions. Molecular dynamics simulations might support the investigation of open questions about the phase transitions of water in nanoporous systems. However, liquid to solid phase transitions of bulk water are difficult to simulate since the nucleation process is energetically hindered. In strong confinement the phase transition of water is further frustrated which makes a brute force approach computationally unfeasible. Additionally it is difficult to find collective variables for enhanced sampling techniques without knowledge about the target structure. We present our ongoing investigation on if and how MD simulations about the freezing of water in nanoporous media can be conducted with an exemplary silica nanopore structure of 3 nm pore diameter.

MM 23.29 Tue 18:15 P2/OG1+2

Mechanical properties of bicontinuous Ti networks formed via peritectic melting — •Nina Petersen[1], Zhongyang Li[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute of Materials Mechanics, Helmholtz-Zentrum hereon, Geesthacht

Recent work has shown, that bicontinuous networks can be obtained from TiAg alloys by peritectic melting. These microstructures can then be transformed to open porous networks by selective etching of the Ti or Ag phase. For open porous Ti networks, the ligament size as well as the morphology can be influenced by variation of the melting parameters like temperature and duration of the heat treatment.

In this work, the microstructure of open porous Ti samples was analysed by scanning electron microscopy. The samples were then mechanically tested using continuous compressive loading as well as loading-unloading protocols. The strain was analysed with digital image correlation. The samples exhibit strength values of over 150 MPa that increase with the duration of the heat treatment. This research links the mechanical performance of these Ti networks to the morphological evolution of the microstructures during heat treatment.

MM 23.30 Tue 18:15 P2/OG1+2

Time-resolved EBSD investigation of abnormal grain growth in the aluminum alloy AA5252 — •Karolína Holíková[1], Jules M. Dake[1], Madlen Atzen[1], Thomas Wilhelm[2], Lukas Petrich[2], Orkun Furat[2], Volker Schmidt[2], Baptiste Flipon[3], Marc Bernacki[3], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]Institute of Stochastics, Ulm University, Germany — [3]MINES ParisTech, PSL University, France

Heat treatment causes changes in the microstructure of polycrystalline materials, with growth of the average grain size being a prominent example. The driving force is the reduction in free energy of the system. When the average grain size increases monotonically with time but the grain size distribution remains self-similar, the process is called normal grain growth (NGG). In contrast, abnormal grain growth (AGG) is characterized by the much faster growth of a few grains at the expense of neighbors, resulting in a bimodal size distribution. Analytic models and computer simulations do a good job of describing NGG, but they generally fail at predicting AGG in real systems–owing to insufficient knowledge of the underlying mechanism(s). If one could observe sequential microstructural changes during AGG, then one might gain a deeper understanding of the phenomenon. To that end, we have investigated grain growth in the aluminum alloy AA5252, which is known to manifest AGG. Time-resolved electron backscatter diffraction (EBSD) measurements reveal abnormal microstructural evolution in 2D, from which we extract clues regarding the underlying mechanism for AGG.

MM 23.31 Tue 18:15 P2/OG1+2

Resistometric and dilatometric determination of GP-zone formation and growth — •Fabian Miller, Nikolai Riedmiller, Johannes Berlin, Tobias Stegmüller, and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

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. Both resistometry and dilatometry are simple online methods to monitor changes in the microstructure of a metallic alloy. In this work we focused on natural and artificial aging of Al-Cu system with samples containing 2 - 4 wt.% of Cu. Natural aging depends on quenched in vacancies, so on the quenching conditions. Samples were homogenized at various temperatures and rapidly quenched to ambient temperature. Afterwards measurements with both techniques 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 for samples with ternary trace alloying metals than Cu. Dilatometry shows a clear contraction of the samples during GP-zone formation and an expansion, if θ' phase forms.

MM 23.32 Tue 18:15 P2/OG1+2

Circularity: a microstructural clue to the origin of extreme abnormal grain growth in nanocrystalline Pd-Au — •Fabian Andorfer[1], Jules M. Dake[1], Johannes Wild[2], Torben Boll[2], Dorothée Vinga Szabó[2], Stefan Wagner[2], Astrid Pundt[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University — [2]Karlsruhe Institute of Technology KIT

Heat treatment causes polycrystalline materials to manifest either normal or abnormal grain growth. During normal growth, the average grain size increases monotonically, but the grain size distribution remains unimodal. In contrast, when abnormal grain growth occurs,

some grains acquire a significant growth advantage compared to the remaining matrix grains, resulting in a bimodal distribution of grain sizes. Inert-gas condensed nanocrystalline Pd-Au alloys undergo an extreme form of such abnormal grain growth: While the grain boundaries separating the abnormal and matrix grains in conventional samples tend to be rather smooth, in nanocrystalline Pd-Au the same boundaries take on rough and highly convoluted shapes - similar to a jagged coastline! In such cases, the measurement and calculation of grain circularity has proven to be a promising tool for classifying the nature of a given grain's abnormality. We have determined the circularity of abnormal grains emerging in nanocrystalline Pd-Au samples, and we have compared the results to values reported in the literature or obtained from simulations. From this information, we hope to gain a deeper understanding of the mechanism(s) responsible for the extreme growth mode observed in nanocrystalline Pd-Au.

MM 23.33 Tue 18:15 P2/OG1+2

Manipulating microstructures by means of magnetic fields — •Thomas Brede[1], Fernando Maccari[2], and Rainer Backofen[3] — [1]Institut für Materialphysik, Universität Göttingen, Deutschland — [2]Institut für Materialwissenschaften, Technische Universität Darmstadt, Darmstadt — [3]Institut für wissenschaftliches Rechnen, Technische Universität Dresden, Dresden

In this project, the isolated influence of strong magnetic fields on the development of the microstructure of ferromagnetic thin films during annealing processes is investigated. For this purpose, thin films out of Iron, Nickel and Cobalt are prepared and characterized, then heat treated in the same heater with and without magnetic field and subsequently characterized. The experiments are accompanied by phase field crystal modeling to separate the different possible influences on the microstructure.
Through the parallel approach of experimental and modeling work, the effect of external magnetic fields on the development of microstructure and grain orientation will be investigated to understand the direct effect of the magnetic field. Through a deeper understanding of the isolated influence of a magnetic field, additional conclusions should be possible about the influence of induced magnetic fields in the case of sample treatment with high currents.

MM 23.34 Tue 18:15 P2/OG1+2

Anharmonicity of the antiferrodistortive soft mode in barium zirconate $BaZrO_3$ — •Petter Rosander[1], Erik Fransson[1], Cosme Milesi-Brault[2,3,4], Constance Toulouse[2], Frédéric Bourdarot[5], Andrea Piovano[5], Alexei Bossak[6], Mael Guennou[2], and Göran Wahnström[1] — [1]Chalmers University of Technology, Göteborg, Sweden — [2]University of Luxembourg, Belvaux, Luxembourg — [3]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg — [4]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [5]Institut Laue-Langevin, Grenoble, France — [6]European Synchrotron Radiation Facility, Grenoble, France

Few perovskites adopt the ideal cubic phase at low temperatures. However, a promising candidate to, on average, remain cubic, even at 0K, is barium zirconate. The competing phase is a structure with sequentially tilted oxygen octahedra. This distortion is driven by the soft tilt mode at the R-point of the cubic Brillouin zone.

We report data from inelastic neutron scattering (INS) on a single crystal of barium zirconate. This reveals that the tilt mode softens substantially from 9.4 meV at room temperature to 5.6 meV at 2K. Additionally, the INS measurement unveils that the acoustic phonon mode at the same point in the Brillouin zone is almost temperature independent, which is in stark contrast to the tilt mode. The theoretical calculations show that it is critical to account for quantum fluctuations in order to correctly reproduce the experimental temperature dependence.

MM 23.35 Tue 18:15 P2/OG1+2

Terahertz third harmonic generation from a correlated metal — •Gulloo Lal Prajapati[1], Sergey Kovalev[1], Jan-Christoph Deinert[1], Alexey Ponomaryov[1], Atiqa Arshad[1], Gaurav Dubey[2], and Dhanvir Singh Rana[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal, India

High harmonic generation, a result of intense nonlinear light-matter interaction, has exciting prospects for probing fundamental ultrafast dynamics in matter and it is the basis for attosecond photonics [1, 2]. Here, we present an experimental study on terahertz (THz) third harmonic generation (THG) on a correlated metal, LaNiO3 which exhibits non-Fermi liquid type of metallic state [3]. We observe an intense THG signal, which is usually not expected in metals, upon pumping it by 0.3 THz pulses with peak fields of about 100 kV/cm. Decreasing temperature or increasing fluence increases the intensity of this THG signal. We speculate the origin of such THG emission could be due to the anharmonic nature of LaNiO3 conduction band caused by electronic correlation or directional nature of Ni-3d orbitals. Further investigations are under way to pinpoint the exact mechanism of the observed THG. Our study paves the way for THz THG emission from strongly correlated systems, and enables tracking of their properties on ultrafast timescales. References: 1. Nature Photon 12, 266, 270 (2018). 2. Nature 561, 507, 511 (2018). 3. Annu. Rev. Mater. Res. 46, 305-34 (2016).