Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

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On this conference the Metals and Materials Division sets a topical focus on interface-dominated phenomena: segregation, nucleation and phase transformations.

The overall properties of modern nano-structured metals and alloys are to a large extent determined by the mechanical and kinetic behavior of the interfaces in their microstructure. Therefore, a precise characterization and understanding of the processes at interfaces is a key to effective alloy development. In this symposium, we want to review the state of the art in theoretical and experimental analysis, as well as in modeling of interface structure and evolution as a response to annealing, segregation, irradiation, and mechanical deformation, as well as the coupling between these processes. In particular, we focus on contributions on atomistic, micro- and multiscale simulations of interface dominated microstructures, on the experimental characterization and mechanical testing of such structures, as well as on the development of thermodynamic and micromechanical models of interfacial effects.

Overview of Invited Talks and Sessions

(Lecture halls H2 and H8; Poster P)

Invited Talks

MM 1.1	Mon	10:00–10:30	H8	**Using mobile interfaces to rapidly move atoms and create sharp chemical boundaries in Fe-C-Mn alloys** — •Sybrand van der Zwaag
MM 4.1	Mon	15:15–15:45	H2	**Investigation of the early stage of reactive interdiffusion in the Cu-Al system by in-situ transmission electron microscopy** — Florent Moisy, •Xavier Sauvage, Eric Hug
MM 6.1	Wed	10:00–10:30	H8	**CALPHAD-informed density-based grain boundary thermodynamics** — •Reza Darvishi Kamachali, Lei Wang, Linlin Li, Anna Manzoni, Birgit Skrotzki, Gregory Thompson
MM 7.1	Wed	11:15–11:45	H8	**Computational methods for grain boundary segregation in metallic alloys** — •Lorenz Romaner, Daniel Scheiber, Vsevolod Razumovskiy, Oleg Peil, Christoph Dösinger, Alexander Reichmann

Plenary Talk

PV VIII	Tue	16:30–17:15	Audimax 1	**The Structural Origins of Wood Cell Wall Toughness** — •Cynthia Volkert

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert

SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Potentials for NVs sensing magnetic phases, textures and excitations (SYNV)

See SYNV for the full program of the symposium.

SYNV 1.1	Mon	13:30–14:00	Audimax 2	**Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology** — •Chunhui Du
SYNV 1.2	Mon	14:00–14:30	Audimax 2	**Nanoscale imaging of spin textures with single spins in diamond** — •Patrick Maletinsky
SYNV 1.3	Mon	14:30–15:00	Audimax 2	**Spin-based microscopy of 2D magnetic systems** — •Jörg Wrachtrup
SYNV 1.4	Mon	15:15–15:45	Audimax 2	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques
SYNV 1.5	Mon	15:45–16:15	Audimax 2	**Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors** — •Dominik Bucher

Invited talks of the joint symposium Amorphous materials: structure, dynamics, properties (SYAM)

See SYAM for the full program of the symposium.

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)

See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Invited talks of the joint symposium The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects (SYPQ)

See SYPQ for the full program of the symposium.

SYPQ 1.1	Fri	10:00–10:30	Audimax 2	**Quantum dots operating at telecom wavelengths for photonic quantum technology** — •Simone Luca Portalupi
SYPQ 1.2	Fri	10:30–11:00	Audimax 2	**Photonic graph states for quantum communication and quantum computing** — •Stefanie Barz
SYPQ 1.3	Fri	11:00–11:30	Audimax 2	**Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects** — •Pavel Bushev
SYPQ 1.4	Fri	11:45–12:15	Audimax 2	**Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure** — •Brian Gerardot
SYPQ 1.5	Fri	12:15–12:45	Audimax 2	**Quantum communication in fibers and free-space** — •Rupert Ursin

Sessions

MM 1.1–1.3	Mon	10:00–11:00	H8	**Topical Session Interface-Dominated Phenomena - Moving Interfaces**
MM 2.1–2.6	Mon	11:15–12:45	H8	**Topical Session Interface-Dominated Phemomena - Moving Interfaces / Functional Properties**
MM 3.1–3.6	Mon	13:30–15:00	H2	**Topical Session Interface-Dominated Phenomena - Defect Structures and Mechanical Properties**
MM 4.1–4.3	Mon	15:15–16:15	H2	**Topical Session Interface-Dominated Phenomena - Diffusion**
MM 5.1–5.13	Tue	10:00–12:45	P	**Topical Session Interface Dominated Phenomena - Poster**
MM 6.1–6.3	Wed	10:00–11:00	H8	**Topical Session Interface-Dominated Phenomena - Thermodynamics**
MM 7.1–7.5	Wed	11:15–12:45	H8	**Topical Session Interface-Dominated Phenomena - Segregation and Embrittlement**
MM 8	Wed	18:00–19:00	MVMM	**Annual General Meeting**

Annual General Meeting of the Metal and Material Physics Division

Wednesday 18:00–19:00 Online Session (session link will be announced in time)

MM 1: Topical Session Interface-Dominated Phenomena - Moving Interfaces

Time: Monday 10:00–11:00 Location: H8

Invited Talk MM 1.1 Mon 10:00 H8

Using mobile interfaces to rapidly move atoms and create sharp chemical boundaries in Fe-C-Mn alloys — •Sybrand van der Zwaag — TU Delft, Delft, the Netherlands

In this presentation we will show how cyclic partial phase transformations in Fe-X alloys and low alloyed steels can be used to rapidly displace substitutional solute atoms and to leave behind ridges of solute atoms upon reversal of the interface migration. These enriched regions locally retard the passing interfaces during a subsequent transformation and this causes a macroscopically detectable halting of the rate of transformation and/or a change in resulting microstructure.

The concept works not only for diffusional and bainitic phase transformations but can (under well-selected conditions) also be used to manipulate the austenite to martensite transformation and to create nano-structured medium Mn steels with exceptional mechanical properties such as a strength above 2 GPa and a uniform elongation in excess of 20%.

The experimental observations are linked to 1D and 3D transformation models and in-situ TEM observations of the moving interface.

MM 1.2 Mon 10:30 H8

Abnormal grain growth in nanocrystalline PdAu: The Case of the Fractal Fingerprint — Raphael A. Zeller[1], Christian Braun[2], Markus Fischer[1], Jörg Schmauch[2], Christian Kübel[3], Rainer Birringer[2], and •Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Ulm, Germany — [2]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [3]Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

In most polycrystalline materials, coarsening tends to be a civilized affair, with adjacent grains taking pains to exchange atoms so as to maintain a smooth boundary. The grains that grow in nanocrystalline PdAu, however, behave like uncouth neighbors crashing a fancy dinner party: once they get revved up, all hell breaks loose! Before you know it, a few nanometer-sized grains have grown four orders of magnitude in diameter, and the resulting interfaces are so convoluted that they resemble fractal objects. Our usual notion of curvature-driven grain boundary migration fails to explain the persistence of these interfacial fluctuations, but recent experiments find the onset of fractality to depend on the Au concentration as well as on a characteristic length scale. We consider this evidence to be a kind of "fractal fingerprint" that, ultimately, incriminates a specific mechanism as being responsible for the system's abnormal grain growth.

MM 1.3 Mon 10:45 H8

Dislocation path and long-range strain associated with interface migration — •Jin-yu Zhang, Zhi-peng Sun, Fu-zhi Dai, and Wen-zheng Zhang — School of Materials Science and Engineering, Tsinghua University, Beijing

Major interphase interfaces generated from phase transformations in steels or Ti alloys are semicoherent. The knowledge of dislocation motion and long-range strain accompanying the interface migration is fundamental to the understanding of phase transformations. In this study, we performed a molecular dynamics simulation on the migration of various α/β interfaces in pure Ti. The simulation results explicitly demonstrated that the interfacial dislocation path can deviate significantly from the slip planes of individual dislocations due to the dislocation interaction when the interface contains multiple sets of dislocations. For these complex situations, previous theories based on conventional slip planes would lead to either non-atom-conservation or slip-sequence-dependent results. We developed a new geometric model, which is capable to generate self-consistent descriptions on the dislocation path and the shear displacement during migration of a general semicoherent interface, in the condition that atoms are conserved during interface migration. This model is validated by the simulations and it covers the simple cases applicable by previous theories. The present study offers new insight into the dislocation path during interface migration and provides a general framework for evaluating the long-range strain caused by interface migration during a phase transformation process, such as precipitation and martensite transformation.

MM 2: Topical Session Interface-Dominated Phemomena - Moving Interfaces / Functional Properties

Time: Monday 11:15–12:45 Location: H8

MM 2.1 Mon 11:15 H8

Theory and modeling of the austenite-martensite interface structure and glissile transformation in steels — •Francesco Maresca[1] and William Curtin[2] — [1]University of Groningen, Groningen, Netherlands — [2]EPFL, Lausanne, Switzerland

The austenite-martensite (fcc-bcc) transformation controls the formation of microstructures in a wide range of high strength steels. Recent progress in the physical metallurgy of steels has shown that nanolaminate austenite/martensite microstructures contribute to high material toughness and resistance to hydrogen-embrittlement. Despite its relevance for applications, there is no established theory for the transformation capable to predict the contribution of the austenite-martensite phase transformation to ductility. To clarify the mechanism of transformation, we have performed atomistic simulations of the interface reproducing the major experimental TEM and HRTEM observations in Fe alloys. The atomistic model reveals for the first time the structure and motion of the athermal and glissile fcc austenite/bcc martensite interface in steels. The interface structure consists of [-101](111)fcc screws, as envisioned by previous theories, and [1-11](-101)bcc screws with kinks, which was not envisioned before. The atomistic findings have guided the formulation of a new, parameter-free double-shear predictive theory of martensite crystallography. Theory predictions show that the fcc/bcc lattice parameter ratio is the key factor controlling the shape deformation (i.e. the in-situ transformation strain), which can achieve more than 90%, namely three times the existing experimental estimates. The theory can be used to guide design of tougher AHSS.

MM 2.2 Mon 11:30 H8

Atomistic simulation of grain boundary phases and transitions in fcc metals — •Tobias Brink and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries (GBs) can be treated as interface phases (also called "complexions") with different thermodynamic excess properties. Congruent phase transitions in pure metals—where the macroscopic GB parameters remain constant—are hard to observe experimentally, but GB phases with distinct atomic structures could recently be identified in a copper tilt GB (Meiners et al., Nature 579, 2020). It remains an open question if such phases are specific to this copper GB or a more general feature of fcc metals. Using molecular dynamics computer simulations, we investigated both Cu and Al ⟨111⟩ tilt GBs with different misorientations to verify if the copper GB phases can indeed be generalized. We furthermore used simulations with Lennard-Jones pair potentials to determine how much materials physics needs to be included in the model to recover the phases of the more realistic potentials. Recurring structural motifs appeared in all of these systems, but we found that the actual material strongly influences which phases occur and their stability. This probably excludes the possibility of deriving simple rules for the atomic structure of GB phases.

Acknowledgment: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446; GB-CORRELATE).

MM 2.3 Mon 11:45 H8

Simulations of a fs laser induced A7 to sc transition in antimony — •Bernd Bauerhenne[1,2], Felipe Valencia[3], and Martin E. Garcia[1,2] — [1]Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany — [2]Center for Interdisci-

plinary Nanostructure Science and Technology (CINSaT), Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany — [3]Physics Department, Universidad Nacional de Colombia, Edificio 404, Ciudad Universitaria, Bogota, Colombia

We simulated the fs laser excitation of a 50 nm thick free standing antimony film using more than 4 million atoms. In our simulations, we condidered the laser-induced changes of the potential energy surface and the effects of the incoherent electron-phonon collisions - the electron-phonon coupling - into account. To do so, we derived an electronic temperature (Te) dependent interatomic potential for antimony. For this, we fitted forces and energies obtained from ab-initio MD simulations of a thin antimony film at increased Te. Furthermore, we calculated the Te-depend electron-phonon coupling constant for antimony ab-initio. In our large-scale MD simulations, we observed a laser induced A7 to sc like transition at moderate intensities. If the excitation intensity is further reduced, the transition starts at the surface and moves to the center of the film. In addtion, we analyzed the influeces of the laser-induced changes of the potential energy surface and of the electron-phonon coupling on the transition.

MM 2.4 Mon 12:00 H8

Nanoscale Friction Under Active Control in Systems With Tailored Degrees of Freedom — •Niklas A. Weber[1], Miru Lee[2], Richard L.C. Vink[1], Matthias Krüger[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

In this project, we use lateral force microscopy to investigate how friction of manganite films can be controlled by the properties of the surrounding materials. Specifically, we use phase transformations [1,2] and superlattice thin film samples [3] to actively control the film properties while keeping the surfaces unchanged.
We observed an increase in friction during resistive switching of a $La_{0.55}Ca_{0.45}MnO_3$ film [1] and during heating of a $La_xSr_{1-x}MnO_3$ thin film through the metal-insulator phase transformation [2]. Careful consideration of the different contributions and comparison with literature lead to the conclusion that the electronic contributions are not sufficient to account for our observations and make phononic contributions a promising candidate.
To test our hypothesis, we have started to perform measurements on $LaMnO_3/SrMnO_3$ superlattice systems in which the propagation of phonons can be actively manipulated by the layer spacing [3], while the morphology of the surface layer remains unchanged.
[1] H. Schmidt et.al., Phys. Rev. Mater. 2020, 4, 113610.
[2] N. A. Weber et.al., Adv. Sci. 2021, 2003524.
[3] D. Meyer et al., arXiv:2009.14532v3.

MM 2.5 Mon 12:15 H8

Interplay of domain structure and phase transitions in ferroelectric $BaTiO_3$ — Madhura Marathe, Ruben Khachaturyan, Yijing Yang, and •Anna Grünebohm — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Domain walls and phase boundaries are fundamental ingredients of ferroelectrics and strongly influence their functional properties. Although both interfaces have been studied for decades, often only a phenomenological macroscopic understanding has been established and it is now timely to revisit nucleation and the coupling of domains and phase transitions on an atomistic level [1]. We study domain walls in $BaTiO_3$ by means of molecular dynamics simulations based on the effective Hamiltonian approach [2]. We show that domain walls may promote the tetragonal to orthorhombic phase transition [3] and can act as nucleation centers.

[1] A. Grünebohm et al., Interplay of domain structure and phase transitions: theory, experiments and functionality, (2021).
[2] Nishimatsu et al., Phys. Rev. B 78, 104104 (2008).
[3] A. Grünebohm and M. Marathe, Phys. Rev. Mater. 4, 114417 (2020).

MM 2.6 Mon 12:30 H8

Optical properties of 3D nanosponge models created by phase-field simulations — •Malte Grunert[1], Sebastian Bohm[1], Hauke Lars Honig[1], Dong Wang[1], Jinhui Zhong[2], Peter Schaaf[1], Christoph Lienau[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Germany — [2]University of Oldenburg, Germany

We present an efficient method for the numerical creation of three-dimensional nanoporous sponge models with specified geometric properties. Such nanoporous structures can be manufactured with different geometric properties and exhibit fascinating optical properties [1,2]. We show how phase-field simulations can be used to obtain nanoporous structures with predefined optical and structural characteristics. The sponge geometries generated in this way show excellent similarity to experimentally produced sponges and the averaged geometric properties are comparable. In addition, the optical properties such as the absorption and scattering cross sections are similar. The computer-generated sponges also exhibit experimentally confirmed optical properties such as strong spatial localization of fields and the associated strong local field enhancement.

[1] G. Hergert, J. Vogelsang, F. Schwarz, D.Wang, H. Kollmann, P. Groß, C. Lienau, E. Runge and P. Schaaf, *Long-lived electron emission reveals localized plasmon modes in disordered nanosponge antennas*, Light: Science & Applications **6**, e17075 (2017).
[2] J. Zhong et al., *Nonlinear plasmon-exciton coupling enhances sum-frequency generation from a hybrid metal/semiconductor nanostructure*, Nature Communications **11**, 1464 (2020)

MM 3: Topical Session Interface-Dominated Phenomena - Defect Structures and Mechanical Properties

Time: Monday 13:30–15:00 Location: H2

MM 3.1 Mon 13:30 H2

Imaging the Deformation-Induced Accumulation of Defects in Nanoporous Gold — •Maowen Liu[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Hereon

Nanoporous gold (NPG) provides a model material for studying small-scale deformation and the mechanical behavior of network solids. While studies of nanopillars indicate dislocation starvation, the strain hardening of NPG suggests dislocation accumulation. Yet, the approach to confirm that latter process by direct experimental observation, namely transmission electron microscopy (TEM), is impaired by the need to distinguish native defects in the microstructure from artifacts due to sample slicing or thinning. Here, we report a TEM study of the defect structure in electron-transparent NPG leaf deformed by rolling. The results confirm that plastic deformation significantly enhances the defect density. Specifically, twins are formed on several crystallographic planes, and their interaction forms Lomer-Cottrell locks. This inhibits dislocation escaping from NPG, thus avoiding the dislocation starvation scenario that is often considered in the "smaller is stronger" context of small-scale plasticity. Instead, strain-hardening is apparently linked to accumulation and interaction of twins.

MM 3.2 Mon 13:45 H2

How the interface type manipulates the thermomechanical response of nanostructured metals: A case study on nickel — •Oliver Renk[1], Verena Maier-Kiener[2], Christian Motz[3], Daniel Kiener[2], Jürgen Eckert[1], and Reinhard Pippan[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria — [2]Montanuniversität Leoben — [3]Saarland University, Germany

The presence of interfaces with nanoscale spacing significantly enhances the strength of materials, but also changes the rate controlling processes of plastic flow. Due to the confined grain volumes, intragranular dislocation-dislocation interactions are replaced by emission and absorption of dislocations from and at the interfaces. Both processes not only depend on the interfacial spacing, but also on the interface structure. The present study attempts to rationalize this effect by investigating the thermomechanical behavior of samples consisting of three different interfaces. Nickel samples with predominant fractions of

low- and high-angle as well as twin boundaries with a similar average spacing of 150 nm are investigated using high temperature nanoindentation strain rate jump tests. Depending on the interface structure, hardness, strain rate sensitivity and apparent activation volumes evolve different with temperature. While in case of high-angle boundaries for all quantities a pronounced thermal dependence is found, the other two interface types behave almost athermal. These differences can be rationalized based on the different interfacial diffusivity, affecting the predominant process of interfacial stress relaxation.

MM 3.3 Mon 14:00 H2

Atomistic simulation study of grain boundary migration for different complexions in copper — •Swetha Pemma[1], Rebecca Janisch[2], Gerhard Dehm[1], and Tobias Brink[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Interdisciplinary Centre of Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, 44780 Bochum, Germany

Grain boundary (GB) migration is significant to study the microstructural evolution which determines the properties of polycrystalline materials. Previous studies showed that the coupling between applied shear and GB migration differed for different complexions on the same GB. In this work, shear coupled grain boundary migration (SCGBM) of two complexions ("pearl" and "domino") observed experimentally in Σ19b $\langle 111 \rangle$ tilt GBs in copper was investigated by molecular dynamics simulations. Effects of these complexions on the shear-coupling factor, critical shear stress for GB motion, and elementary GB migration mechanism were analysed. The coupling factors of the complexions were observed to be of same magnitude and sign for several temperatures and shear velocities. However, the critical shear stress differs by 31 % between pearl and domino, indicating a difference in activation barriers. Additionally, the precise atomistic mechanisms of SCGBM were examined using nudged elastic band calculations.

Acknowledgment: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446; GB-CORRELATE).

MM 3.4 Mon 14:15 H2

Prismatic slip in pure Magnesium with a Neural Network Potential — •Markus Stricker[1] and William A. Curtin[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]LAMMM, EPFL, Lausanne, Switzerland

Studying fundamental mechanisms of deformation in metals and alloys requires dependable interatomic potentials because dislocations and cracks are above scales accessible with first-principles calculations. While classical potential forms like the modified embedded atom method (MEAM) have been successfully employed in many cases, non-fcc metals and almost all alloys are not modeled sufficiently quantitative. As a first step towards Mg-alloys we present a broadly applicable machine learned potential for pure Magnesium in the Behler-Parrinello neural-network framework trained on first-principles density-functional theory. We show that the potential predicts dislocation and crack structures very well and subsequently apply it to cross-slip of prismatic screw dislocations, which is not accessible to first-principles approaches. Prismatic slip is achieved by double-cross-slip of stable basal dislocations in steps of c/2 driven by a shear stress on the prismatic plane. The geometry of the observed process compares very well with the process deduced from experiments, the enthalpy barrier not. This mimics the stress-driven double-kink nucleation in bcc elements: the geometry of the mechanism is predicted well, but stress and activation barriers are overestimated by first-principles predictions.

MM 3.5 Mon 14:30 H2

Ab-initio study of the Mo/SiC interfacial adhesion — •David Sebastian Kasdorf and Karsten Albe — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, TU Darmstadt, Otto-Berndt-Str. 3, Darmstadt D-64287, Germany

Mo-Si-based alloys are a potential alternative to commercially available Ni-based superalloys for high-temperature applications. While the optimization of corrosion, oxidation and creep behavior of Mo-Si-based alloys are the object of current research efforts, also materials that could act as a thermal barrier coating (and possibly bond coats) need to be identified in order to maximize the temperature capabilities. Failure modes like delamination and fractures often happen at the interfaces between the metallic substrate and ceramic top coats as the interfacial adhesion presents the limiting factor of the fracture toughness in the materials system.

We performed first-principles calculations to study the ideal work of separation and theoretical strength of Mo/SiC interfaces. In those calculations, bcc Molybdenum acts as a representative for Mo-Si-based alloys as a Mo solid solution phase is common in those alloys. Similarly, β-SiC was chosen as the second part of the interface since it is a typical high-temperature crystallization product of Si-based ceramic coatings.

MM 3.6 Mon 14:45 H2

Unravelling the lamellar size-dependent fracture behavior of fully lamellar intermetallic γ-TiAl — •Anupam Neogi and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Strengthening of metals by incorporating nano-scale coherent twin boundaries is one of the important breakthroughs in overcoming the strength-ductility trade-off in recent years. Also, nano-scale twin boundaries in the nano-lamellar in lightweight Ti-Al alloys promise great potential, but their contribution to the deformation and fracture behavior needs to be better understood for designing optimum microstructures. To this end, we carry out linear elastic fracture mechanics informed, large-scale atomistic simulations of fully lamellar γ-TiAl, and find, that nano-scale lamellae are not only effective in improving the fracture toughness and crack growth resistance, but the lamellar size possesses a significant controlling role on the crack tip mechanisms. The fracture initiation toughness exhibits an increasing trend with decreasing lamellar size until $\sim$3 nm. In this regime, the crack tip events are mostly dislocation-based plasticity. Below the critical lamellar size of $\sim$3 nm, the crack advances via a quasi-brittle manner, i.e., the cleavage of atomic bonds at the crack tip accompanied by some plasticity events, such as twin-boundary migration and dislocation nucleation. A layer-wise stacking fault energy-based analysis, including the quantitative analysis of dislocation barrier energy, elucidates the nano-scale lamellar size-dependent fracture behavior of γ-TiAl.

MM 4: Topical Session Interface-Dominated Phenomena - Diffusion

Time: Monday 15:15–16:15 Location: H2

Invited Talk MM 4.1 Mon 15:15 H2

Investigation of the early stage of reactive interdiffusion in the Cu-Al system by in-situ transmission electron microscopy — Florent Moisy[1], •Xavier Sauvage[2], and Eric Hug[1] — [1]CRISMAT Ensicaen, Caen, France — [2]GPM University Rouen Normandy, Rouen, France

The early stage of the reactive interdiffusion in the Al/Cu system was investigated by in-situ TEM at 350°C and 300°C. Original Al/Cu interfaces were created by a purely mechanical process using co-deformation at room temperature by drawing. During the reactive interdiffusion three IMCs were detected: Al2Cu and AlCu grew in the Al side and the Al4Cu9 in the Cu side. Systematic comparisons with ex-situ annealed samples and with regions out of the electron beam proved that there was no significant artefact (thin foil or beam effect). Although GBs may act as fast diffusion path, no preferential growth of IMC along these defects could be observed. The mean growth rates of all IMCs follow a classical parabolic law indicating that the kinetic of the transformation is controlled by diffusion mechanisms. A strong deviation was observed however in the early stage of the reaction. Nanoscaled Mg2Si particles located in the Al phase strongly interact with the transformation front. It leads to large fluctuations of the velocity of interphase boundaries at the nanoscale. The pinning effect in connection with change in local concentration gradients and driving forces will be discussed.

MM 4.2 Mon 15:45 H2

Silver-rich clusters reveal the initial ligament size dur-

ing nanoporous gold dealloying via kinetic Monte Carlo simulation — •Yong Li[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

When nanoporous gold is made by dealloying Ag-Au, residual silver forms clusters that impact the material's functional properties. We point out that the clusters carry information on the geometry of the initial nanoscale network. Using atomistic kinetic Monte Carlo simulation, we studied the evolution of silver-rich clusters and ligament size for dealloying at various potentials. Our simulations demonstrate that dealloying involves two distinct stages. Primary dealloying generates the initial ligament network, while secondary dealloying brings coarsening of the ligaments and further dissolution. During primary dealloying, the sizes of clusters and ligaments are constant over time and they decrease with increasing dealloying potential with a Gibbs-Thompson type relation. At this stage, the ratio between ligament size and clusters size is 1.30±0.07 and independent of the potential. During secondary dealloying, the ligament size (L) for dealloying with various potentials converge to a common coarsening law, $L \propto t^{1/4}$. By contrast, the silver-clusters size still remains constant. That observation establishes that the surviving clusters provide a way to measure the initial ligament size.

MM 4.3 Mon 16:00 H2

Theoretical aspects of the reactive element effect — Andy Chen[1], Arthur Heuer[1], Matthew Foulkes[2], and •Michael Finnis[2] — [1]CWRU, Cleveland OH, U.S.A — [2]Imperial College London, UK

We are interested in the mechanism of growth of alumina scales on aluminium-containing alloys, and how the presence of certain elements such as Hf, Zr and Y operates to retard the growth of such scales, thereby improving their adherence and protective quality. These questions have been open for several decades, and are still not completely resolved [1]. We report here some recent results of experiments and theory, and in-sights that we have obtained. From tracer diffusion experiments, followed by Time of Flight - Secondary Ion Mass Spectroscopy (TOF-SIMS), diffusion coefficients of O and Al through alumina scales have been estimated and compared with measurements of weight-gain. Noting that grain boundaries are now believed to be the route for ion and electron diffusion, both of which are necessary for oxidation, we have applied Density Functional Theory to calculate the segregation energy of these reactive elements to a range of sites on grain boundaries in α-Al2O3,using our previous models of grain boundary structure [2]. Segregation of Hf and Zr and oxygen vacancies to the grain boundaries is favoured, with a spread of energies that we assess, and our calculations suggest how this may indirectly reduce the mobility of ions or electrons. Shortcomings of the classical theory of oxidation [3], originally due to Wagner, are discussed. The evidence is now overwhelming that the conventional hopping of cation and anion vacancies is not a relevant process.

[1] W. T. Chen, B. Gleeson, and A. Heuer. Oxidation of Metals, 92(3-4):137-150, 2019. [2] Hannes Guhl, Hak-Sung Lee, Paul Tangney, W. M. C. Foulkes, Arthur H. Heuer, Tsubasa Nakagawa, Yuichi Ikuhara, and Michael W. Finnis. Acta Materialia, 99:16-28, 2015. [3] A. Atkinson. Reviews of Modern Physics, 57:437-470, 1985.

MM 5: Topical Session Interface Dominated Phenomena - Poster

Time: Tuesday 10:00–12:45 Location: P

MM 5.1 Tue 10:00 P

Temperature and chemical bonding effects on the brittle-to-ductile transition in metal-metalloid glasses — •Daniel Şopu[1,2], Franco Moitzi[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences, Leoben, Austria — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Montanuniversität Leoben, Leoben, Austria

The relationship between the deformation behavior of metal-metalloid glasses and their intrinsic properties is studied using large-scale molecular dynamics simulations. The influence of composition and temperature on the tensile deformation behavior of amorphous PdSi alloys is investigated. A transition from cracking perpendicular to the loading direction to shear banding can be achieved by increasing the temperature or decreasing the amount of silicon. A decrease in silicon content leads to fewer covalent bonds and, therefore, lower activation barriers for shear transformation zones and, consecutively, a high probability for shear band formation. On the other hand, at low temperatures these barrier cannot be overcome and cracking will dominate over shear banding. In this case, high activation barriers for local relaxation impedes stress redistribution into the glassy structure and, finally, cracking occurs. Additionally, the cracking path also depends on the degree of homogeneity. A corrugated fracture surface similar to experiment can be formed due to crack defection and cavitation ahead of the crack tip in chemically inhomogeneous samples. In contrast, a sharp cleavage-like fracture occurs for more homogeneous samples.

MM 5.2 Tue 10:00 P

Enabling materials design of ionic systems with automated corrections: AFLOW-CCE — •Rico Friedrich[1,2], Marco Esters[1], Corey Oses[1], Stuart Ki[1], Maxwell J. Brenner[1], David Hicks[1], Michael J. Mehl[1], Mahdi Ghorbani-Asl[2], Arkady Krasheninnikov[2], Cormac Toher[1], and Stefano Curtarolo[1,3] — [1]Center for Autonomous Materials Design, Duke University, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, USA

Materials databases such as AFLOW [1] leverage *ab initio* calculations for autonomous materials design. The predictive power critically relies on accurate formation enthalpies - quantifying the thermodynamic stability of a system. For ionic materials such as oxides and nitrides, standard DFT leads to errors of several hundred meV/atom [2,3].

We have recently developed the "coordination corrected enthalpies" (CCE) method yielding highly accurate room temperature formation enthalpies with mean absolute errors down to 27 meV/atom [3]. Here, we introduce AFLOW-CCE [4]: a tool where users can input a structure file and receive the CCE corrections, or even the CCE formation enthalpies if pre-calculated LDA, PBE or SCAN values are provided. The results can be used for the design of *e.g.* 2D materials.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).
[3] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).
[4] R. Friedrich *et al.*, Phys. Rev. Mater. **5**, 043803 (2021).

MM 5.3 Tue 10:00 P

Molecular Dynamics study of the influence of microstructure on reaction front propagation in Al-Ni multilayers — •Fabian Schwarz and Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

Reactive multilayers can be used for energy storage as well as releasing large amounts of heat in a short time. We use Molecular Dynamics (MD) simulations to study the influence of the crystal structure on the reaction front propagation in Al-Ni multilayers. Different microstructures, namely amorphous, single crystal, columnar grains and randomly oriented grains of varying size are investigated. The effect of the microstructure on the propagation speed is studied and compared to existing experimental results. Furthermore, MD simulations allow to study the inter-diffusion of the Al and Ni layers. We found that crystallinity has a significant impact on the front propagation speed, which is likely related to different diffusion mechanisms. The more disordered the individual layers become, e.g. by increasing the grain boundary density, the higher is the resulting propagation speed.

MM 5.4 Tue 10:00 P

Grain boundary segregation and precipitation in an Al-Zn-Mg-Cu alloy — •Huan Zhao[1], Baptiste Gault[1,2], Liam Huber[1], Wenjun Lu[1], Nicolas Peter[1], Dirk Ponge[1], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Department of Materials, Royal School of Mines, Imperial College London, London, United Kingdom

High-strength Al-Zn-Mg-Cu alloys are highly susceptible to intergranular embrittlement, which severely limits their lifetime. In this talk, I

will present our recent work on the effect of solute segregation in the precipitation behavior at grain boundaries (GBs) compared to grain interiors. Solute segregation could accelerate the precipitation behavior at GBs, which causes the formation of coarse precipitates and precipitate free zones along GBs. Furthermore, the interplay of solute segregation and the local structure at GBs has been considered. We show that faceting occurs at GBs and that the distinct segregation and precipitation behavior occurs within the same GB. Investigations on the solute distribution inside the precipitates, matrix, and at GBs related to SCC resistance in Al-Zn-Mg-Cu alloys will also be discussed.

MM 5.5 Tue 10:00 P

On the role of rotational twin boundaries in lamellar TiAl on the deformation behavior — •Ashish Chauniyal and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Twin boundaries in lamellar TiAl alloys have a determining influence on their mechanical properties. During deformation, the twin boundaries prevent easy glide of dislocations, thereby contributing to strengthening. In nano-scale lamellae, twin boundaries can cause considerable dislocation pileups which contribute to strengthening, but compromise ductility. To maintain deformability, it is desirable to have movement of dislocations and sufficient dislocation sources to nucleate new dislocations. In this regard, the twin boundaries in lamellar TiAl are special as the tetragonality of the γ phase ($L1_0$) leads to several variants of rotational twin boundaries by rotating in steps of 60° around the [111] axis. While a $\gamma/\gamma_{180°}$ boundary is fully coherent, $\gamma/\gamma_{60°}$ and $\gamma/\gamma_{120°}$ boundaries exhibit a lattice misfit at the interface, which can result in coherency or semi-coherency. For a coherent interface a residual coherency stress is generated within the lamallae which can have a profound influence during deformation. For a semi-coherent interface, misfit dislocations at the interface can act as nucleation sources. In this work we model these interfaces atomistically and compare their deformation behavior by carrying out large scale atomistic simulations. Our simulations reveal the mechanisms of dislocation nucleation and propagation in lamellar layers with rotational twin boundaries.

MM 5.6 Tue 10:00 P

High hydrogen mobility in an amide-borohydride compound studied by quasielastic neutron scattering — •Neslihan Aslan[1], Sebastian Busch[1], Wiebke Lohstroh[2], Claudio Pistidda[3], and Martin Müller[1,4] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University Munich (TUM), Garching, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [4]Institute of Materials Physics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

The hydrogen storage performance of reactive hydride composites Mg(NH2)2 + 2 LiH can be significantly improved by the addition of LiBH4 and the subsequent formation of the amide-borohydride compound Li4(BH4)(NH2)3 during hydrogen release. To understand the chemical behaviour and atomic motions of Li4(BH4)(NH2)3, we present an in situ phase analysis with X-ray synchrotron diffraction and quasielastic neutron scattering (QENS) during heating.

Li4(BH4)(NH2)3 melts at 494 K and the crystallization of a second phase is detected and identified as LiNH2. In molten phase, the neutron measurements confirm a long-range diffusive motion of hydrogen-containing species with the diffusion coefficient $D \sim 10^{-6}\,\frac{\mathrm{cm}^2}{\mathrm{s}}$. In solid phase, localized rotational motions are observed that have been attributed to (BH4)- tetrahedra units mainly undergoing rotations around C_3 axes.

MM 5.7 Tue 10:00 P

Substrate-Induced Anisotropic Superconductivity in Layered Materials: the role of Nonlocal Coulomb Interactions and Band Hybridisation — •Manuel Simonato[1], Anand Kamlapure[1], Emil Sierda[1], Manuel Steinbrecher[1], Umut Kamber[1], Elze. J. Knol[1], Peter Krogstrop[2,3], Mikhail I. Katsnelson[1], Alexander Khajetoorians[1], and Malte Rösner[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen 6525AJ, Netherlands — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — [3]Microsoft Quantum Materials Lab Copenhagen, 2800 Lyngby, Denmark

We investigate how anisotropic substrate materials, such as black-phosphorus (BP), can affect the properties of layered superconductors (SC), both via dielectric screening of the Coulomb interaction and via band hybridization. We employ generic lattice models to describe the SC in BCS theory and utilize Thomas-Fermi screening theory for the Coulomb interactions. The SC-substrate hybridization is studied by means of an effective two-band model, which yields an extension of conventional BCS theory in the Nambu-Gorkov formalism. We derive a new gap equation, from which the effective gap and other SC properties are evaluated. Our predictions for the spectral density function show great qualitative agreement with experimental data for thin Pb films on BP substrates.

MM 5.8 Tue 10:00 P

Sampling the parameter space of grain boundaries with a sequential sampling technique - Atomistics meets statistics — •Timo Schmalofski[1], Martin Kroll[2], Holger Dette[2], and Rebecca Janisch[1] — [1]ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Department of Mathematics, Ruhr-University Bochum, 44780 Bochum, Germany

The grain boundary energy is a function of five degrees of freedom (DOF). Two DOF describe the inclination of the grain boundary plane and the remaining three DOF the misorientation between both grains (one for the misorientation angle and two for the rotation axis). The sampling of this grain boundary energy space or even subspaces of it has been shown to be very challenging due to the so-called "cusps", steep energy minima at special misorientations and/or inclinations. Several approaches have been tried to sample energy subspaces, but they mostly need a large amount of datapoints for sufficient accuracy, and in addition an a-priori knowledge of the positions of the energy cusps. Therefore, in this work, statistical methods are combined with atomistic simulations and a sequential sampling technique is designed. In this presentation this technique will be introduced and compared to a regular sampling technique, to prove its advantages when sampling a whole subspace with a minimal amount of datapoints and discovering unknown cusps automatically. The presentation will focus on the sampling of only one dimensional subspaces of symmetrical tilt grain boundaries to prove the concept, but the application can be generalized towards multidimensional subspaces.

MM 5.9 Tue 10:00 P

The methods of neutron diffraction intensity calculation — •Anastasiia Kuznetsova[1], Jie Luo[2], Hareesh Chavana[3], Veronika Reich[1], Sebastian Busch[1], and Martin Müller[4] — [1]GEMS at MLZ, Hereon, Lichtenbergstr. 1, 85748 Garching b. München, Germany — [2]ILL, 71 avenue des Martyrs, 38000 Grenoble, France — [3]ICG Place Eugene Bataillon, Bat. 15, 34095 Montpellier, France — [4]Hereon, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Neutron diffraction intensity on a crystal is commonly calculated as crystal's structure factor squared. The SASSENA program, suitable for atomic movement modeling, and the Debye formula, applicable for any material, not obligatory a periodic one, were tested for calculation of diffraction on crystalline powders. Mono- and biatomic structures of cP, bcc, and fcc crystal lattices of two different sizes each were used as model crystals. Furthermore, for Po, which data on scattering length were not listed, it was set artificially and also varied. The first method sums up reflections from all crystalline planes for the same Q-vector; the second one takes into account both crystalline structure and atomic motions; the third one spherically averages all possible orientations of the system. The resulting curves were juxtaposed and for Debye formula, the intensities were also correlated with structure factors squared and plotted against Q to obtain some kind of dependence. Given their results' difference, one has to choose a proper calculation method and to justify their choice. Due to some Q-dependence of intensities ratios the presence of some explanation for the divergence among the results of both formulas was assumed.

MM 5.10 Tue 10:00 P

Broadband coupling of fast electrons with high-Q whispering gallery mode resonators — •Niklas Müller, Vincent Hock, Christopher Rathje, Nora Bach, Holger Koch, and Sascha Schäfer — Institute of Physics, University of Oldenburg, 26129 Oldenburg, Germany

The inelastic interaction of fast electrons with spatially confined intense light fields has recently enabled new techniques in ultrafast transmission electron microscopy (UTEM), enabling the coherent control of free-electron states. Advanced quantum control scenarios, including

electron-light entanglement and non-trivial electron/photon counting statistics, become accessible if non-classical light states are applied. However, to mitigate the reduced coupling strength when considering few-photon-states, novel concepts for coupling electrons to high-Q optical resonators are required. Here, we demonstrate the excitation of high-Q whispering gallery modes in a silica microfiber taper in a transmission electron microscope by relativistic electrons (200 keV) passing close to the fiber surface. The evanescent electric field of the passing electron induces a femtosecond electric polarization in the silica, which can be decomposed into optical whispering gallery modes (WGM). The dtected coherent cathodoluminescence spectra consist of octave-spanning frequency combs with narrow-bandwidth peaks. By probing the WGM resonances for different distances from the taper apex, we demonstrate that the peaks within the comb exhibit a frequency spacing inversely scaling with the local fiber circumference. Q-factors up to 700 a measured, depending on the local taper angle.

MM 5.11 Tue 10:00 P

Large scale process for adjustable resonances as a versatile platform for SERS — •Marcel Below and Jörg Schilling — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06108 Halle, Germany

Samples on cm^2-scale with hexagonal lattices of gold nanoscatterers were created with different controlled periods by using three-beam interference lithography. The resulting nanoscatterers have an elliptical shape and the size of their semi-axes is linked to the period of the lattice.

Spectral transmission measurements show two broad drops of transmission at different wavelengths depending on the polarization of the light. These are identified as single particle plasmonic resonances and can be shifted from the visible to the mid-IR with increasing size of the nanoscatterers. FEM simulations reveal that both plasmonic resonances are caused by the shape of the individual nanoscatterers.

Additionally, considerably sharper and asymmetric drops of transmission, known as Fano resonances, were observed. These Fano resonances are caused by an overlap of the single particle plasmonic resonance of each nanoscatterer and the collective response of the lattice.

When a sample is immersed in a solution of 4-MBA molecules, the molecules bond to the surface of the gold nanoscatterers. Subsequent Raman measurements show a clear SERS signal and a strong dependency on the polarization of the excitation laser. These results present a possible route for large area SERS substrates with tunable plasmonic resonances.

MM 5.12 Tue 10:00 P

Influence of oxygen on the development of facets on the ligaments of nanoporous gold — •Ulrike Dette[1], Stefan A. Berger[1], Ling-Zhi Liu[2], Jürgen Markmann[1,3], and Jörg Weissmüller[3,1] — [1]Institut für Werkstoffmechanik, Helmholtz-Zentrum Hereon — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg

Even at comparably low temperatures, gold atoms diffuse on the surface of ligaments in nanoporous gold and create facets. Defects and residual silver act as pinning points for the diffusion and thus the facets. For a better understanding of the faceting mechanism and the role of oxygen in it, we annealed nanoporous gold in argon atmosphere at 500°C for 3 h with different oxygen partial pressures controlled by an electrolyzer. We used samples with and without residual silver on the surface. The results show that the higher the oxygen level the stronger the faceting and bigger the ligament size. Therefore, oxygen does support the faceting of nanoporous gold and the coarsening of the ligaments during annealing. We additionally found that the more residual silver on the surface the more silver clusters are formed during annealing and the smaller the facets become. It confirms that residual silver does act as a pinning point for the facets.

MM 5.13 Tue 10:00 P

Revealing highly stable copper based alloys using active learning — •Angel Diaz Carral[1], Azade Yazdan Yar[1], Siegfried Schmauder[2], and Maria Fyta[1] — [1]Institute for Computational Physics (ICP), Universität Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — [2]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Pfaffenwaldring 32 70569, Stuttgart, Germany

Copper based alloys, due to their high electrical conductivity and high strength, are of great importance for electric and electronic applications such as connectors or lead frames. To this end, we investigate the stability of Cu-Ni-Si-Cr alloys, that is copper alloys with nickel, silicon and chromium impurities. Through computational means, we scan a large number of impurities' concentration and configurations. A relaxation-on-the-fly active learning algorithm is applied in order to investigate the influence of this scanning and reveal the alloys of higher stability. The latter are used at a next step in larger scale simulations in order assist the design of alloys with pre-selected properties. Here, we mainly focus on the first part, the learning process and the stable alloy structures. We discuss the efficiency of this approach, the predictions that can be made and the impact in designing alloys.

MM 6: Topical Session Interface-Dominated Phenomena - Thermodynamics

Time: Wednesday 10:00–11:00 Location: H8

Invited Talk MM 6.1 Wed 10:00 H8

CALPHAD-informed density-based grain boundary thermodynamics — •Reza Darvishi Kamachali[1], Lei Wang[1], Linlin Li[2], Anna Manzoni[1], Birgit Skrotzki[1], and Gregory Thompson[3] — [1]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin — [2]State Key Laboratory of Rolling and Automation, Northeastern University, Shenyang 110819, PR China — [3]University of Alabama, Department of Metallurgical Materials Engineering, 35487 Tuscaloosa, AL, USA

The Gibbs free energy of a grain boundary is a complex thermodynamic function of temperature, pressure, and composition. These complexities add to the intrinsic crystallographic and chemical constraints imposed by the adjacent bulk phase. Recently we have proposed a density-based model for assessing grain boundary thermodynamics that enables a CALPHAD-informed description of the grain boundary. As such, the Gibbs free energy of the grain boundary is directly linked to available CALPHAD thermodynamic data. In this talk, new aspects of interfacial segregation and phase transformation are revealed by benchmarking the current model for various experimental cases, including several steels, high-entropy alloys and aluminum alloys. The effects of elastic interactions on the grain boundary segregation and the application of the model to a nanocrystalline Pt-Au alloy, with numerous grain boundaries of various characters, will be discussed.

MM 6.2 Wed 10:30 H8

Methods for Gibbs triple junction excess determination: Ti segregation in CoSi2 thin film — •Hannes Zschiesche, Ahmed Charai, Claude Alfonso, and Dominique Mangelinck — CNRS, IM2NP, Faculté de Saint-Jérôme, Aix-Marseille Université, Marseille, France

Triple junctions (TJs) are present in poly crystalline material where three grain boundaries join together. They influence directly the thermodynamics and kinetics of the material and thereby its properties. Thus, their description by geometric and thermodynamic parameters is of great interest. One of these parameters is the Gibbs TJ segregation excess. Eich et al., Acta Mater, 2018 predicted TJ excess in a Fe-Cr alloy based on simulations. However, to compare such predictions on experimentally acquired TJs methods are needed for the determination of Gibbs TJ segregation excess.

We propose methods to determine Gibbs TJ segregation excess in an atomically resolved 3D volume where single atom counting is possible, as provided by atom probe tomography (APT). Firstly, we test the methods on a simulated model volume in which the excess value is known. Further, we investigate an APT volume of CoSi2 thin film that contains three grain boundaries and a TJ which show segregation of Ti. CoSi2 is well known as contact material in microelectronics and can grow in epitaxy on Si by the introduction of a Ti interlayer. The developed methods allow to quantify the Ti excess at the CoSi2 TJ.

This work offers new possibilities for fundamental characterization

of materials and an example of its application.

MM 6.3 Wed 10:45 H8

A quantum-mechanical study of impact of vibrational entropy on the segregation of Cu to antiphase boundaries in Fe_3Al — •Martin Friák[1,2], Miroslav Černý[2,3], and Mojmír Šob[4,1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Central European Institute of Technology (CEITEC), Brno University of Technology, Brno, Czech Republic — [3]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We have performed an *ab initio* study of segregation of Cu atoms towards antiphase boundaries (APBs) in Fe_3Al. The Cu atoms are predicted to segregate towards the studied APBs (the APB energy is then equal to 84 mJ/m^2) but the related energy gain is only 4 meV per Cu atom. Both Cu atoms (as point defects) and APBs (as extended defects) have their specific impact on local magnetic moments of Fe atoms (and they non-linearly combine when both types of defects are present). We have also performed phonon calculations and found all studied states mechanically stable. The band gap in phonon frequencies of Fe_3Al is barely affected by Cu substituents but reduced by APBs. The phonon contributions into segregation-related energy changes are significant, ranging from a decrease by 16 % at T = 0 K to an increase by 17 % at T = 400 K (changes with respect to the segregation-related energy difference between static lattices). Further, we have found non-linear trends in changes induced by the Cu segregation in the phonon entropy and phonon energy.

MM 7: Topical Session Interface-Dominated Phenomena - Segregation and Embrittlement

Time: Wednesday 11:15–12:45 Location: H8

Invited Talk MM 7.1 Wed 11:15 H8

Computational methods for grain boundary segregation in metallic alloys — •Lorenz Romaner[1], Daniel Scheiber[2], Vsevolod Razumovskiy[2], Oleg Peil[2], Christoph Dösinger[1], and Alexander Reichmann[1] — [1]Department Materials Science, Montanuniversität Leoben, A-8700 Leoben — [2]Materials Center Leoben Forschung GmbH, A 8700 Leoben

Modeling of grain boundary segregation phenomena is an important discipline of integrated computational materials design. Several computational methods, including in particular atomistic, thermokinetic or mechanical models are available to model grain boundary excess and to assess the associated material properties. Segregation energies plays a central role in this connection and large databases are being created to get a comprehensive overview over materials. With the availability of such databases, machine learning approaches can be used to learn the trends in the periodic table and get segregation energies even for alloys for which no data exist at present. We present an investigation on machine learning segregation energies obtained from density functional theory simulations. We will discuss the critical role of feature engineering and analyze different physical parameters including cohesive energies, solution energies, geometry of the segregation site and many more. Furthermore, we show results for a variety of metallic alloys focusing on the class of transition metals and on comparison with experiment. Finally, the challenges of machine learning of segregation energies and grain boundary engineering in general will be discussed.

MM 7.2 Wed 11:45 H8

Revealing in-plane grain boundary composition features through machine learning from atom probe tomography data — •Xuyang Zhou[1,2], Ye Wei[1], Markus Kühbach[1,3], Huan Zhao[1], Florian Vogel[4], Reza Darvishi Kamachali[5], Gregory B. Thompson[2], Dierk Raabe[1], and Baptiste Gault[1,6] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Department of Metallurgical & Materials Engineering, The University of Alabama, Tuscaloosa, USA — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]Institute of Advanced Wear & Corrosion Resistant and Functional Materials, Jinan University, Guangzhou, China — [5]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany — [6]Department of Materials, Royal School of Mines, Imperial College London, London, UK

The structures of grain boundaries (GBs) have been investigated in great detail. However, much less is known about their chemical features, owing to the experimental difficulties to probe these features at the atomic length scale inside bulk material specimens. Atom probe tomography (APT) is a tool capable of accomplishing this task, with an ability to quantify chemical characteristics at near-atomic scale. Using APT data sets, we present here a machine-learning-based approach for the automated quantification of chemical features of GBs. This machine-learning-based approach provides quantitative, unbiased, and automated access to GB chemical analyses, serving as an enabling tool for new discoveries related to interface thermodynamics, kinetics, and the associated chemistry-structure-property relations.

MM 7.3 Wed 12:00 H8

How grain boundary doping affects the mechanical properties in ultra-fine grained tungsten and nanocrystalline tungsten composites — •Michael Wurmshuber[1], Simon Doppermann[1], Stefan Wurster[2], Severin Jakob[1], Markus Alfreider[1], Klemens Schmuck[1], Rishi Bodlos[3], Lorenz Romaner[1], Verena Maier-Kiener[1], Helmut Clemens[1], and Daniel Kiener[1] — [1]Department Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700 Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700 Leoben, Austria — [3]Materials Center Leoben GmbH, Roseggerstraße 12, 8700 Leoben, Austria

Brittle intercrystalline fracture due to weak grain boundaries is a major problem in both refractory metals as well as nanostructured metals. Naturally, it is therefore also the preferred failure mode in ultra-fine grained tungsten, which is a prime candidate for the divertor material in nuclear fusion. In this work, ultra-fine grained tungsten samples doped with various ab-initio informed elements are fabricated and characterized. A clear improvement of mechanical properties could be observed for samples doped with boron and hafnium. Furthermore, nanocrystalline W-Cu samples were fabricated and doped with the same elements. While boron and hafnium also have a positive effect on the mechanical properties in these samples, the addition of rhenium leads to an even more pronounced improvement, pushing the boundaries set by the strength-ductility paradigm.

MM 7.4 Wed 12:15 H8

Atomistic Insight into Hydrogen Trapping at MC/BCC-Fe Phase Boundaries: The Role of Local Atomic Environment — •Boning Zhang[1,2], Jie Su[2], Maoqiu Wang[2], Zhenbao Liu[2], Zhigang Yang[1], Matthias Militzer[3], and Hao Chen[1] — [1]Tsinghua University, Beijing, China — [2]Central Iron and Steel Research Institute, Beijing, China — [3]The University of British Columbia, Vancouver, Canada

A physical understanding of hydrogen trapping at microstructural defects such as grain boundaries (GBs) and phase boundaries (PBs) is vitally important for the design of hydrogen embrittlement (HE) resistant metals. As compared with GBs, the mechanism of hydrogen trapping at PBs is rather unclear due to the complex atomic environment. We perform systematic density functional theory (DFT) calculations to reveal the origin of hydrogen trapping at PBs between body centered cubic (BCC)-Fe and NaCl-type carbides (MCs). We found hydrogen trapping energetics at MC/BCC-Fe PBs depend not only on local volume dilation of the trapping sites, but also on the local atomic environment. An array of descriptors such as lattice strain, geometric volume, and charge density, which have been proven to effectively predict hydrogen trapping at GBs, fail to quantify hydrogen trapping at MC/BCC-Fe PBs. We analyzed the electronic interactions at PBs and found that they are closely related to hydrogen binding energies, and the Bader volume of hydrogen is a universal descriptor for assessing trapping energetics at PBs. This study provides a new insight into hydrogen trapping at microstructural defects.

MM 7.5 Wed 12:30 H8

Ab initio study of hydrogen segregation and embrittlement at grain boundaries in bcc Fe — •Abril Azócar Guzmán, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Hydrogen embrittlement is a fundamental problem in materials science that affects structural materials such as steel. Grain boundaries in ferritic microstructures play a dual role in the context of hydrogen embrittlement: they could act as H traps and thus reduce the amount of mobile H in the system. Alternatively, this trapping could promote hydrogen enhanced decohesion (HEDE) at the grain boundaries. Understanding the relationship between strain, hydrogen solubility, and cohesive strength can help elucidate the HEDE mechanism and influence the segregation process. We present the results of *ab initio* studies of the effect of H, as well as C, on Fe at $\Sigma5$ and $\Sigma3$ symmetrical tilt grain boundaries. The calculated results show that the presence of H significantly reduces both the work of separation and the intergranular cohesive strength; these quantities can aid to derive traction-separation laws for cohesive zone models in mesoscale simulations. Additionally, we analyse the solubility of H under mechanical load, which allows us to predict H distribution in microstructures with residual stresses, or under applied load.

MM 8: Annual General Meeting

Time: Wednesday 18:00–19:00 Location: MVMM

Annual General Meeting