MM 21: Phase Transformations II

Time: Wednesday 10:15–13:00 Location: SCH/A215

MM 21.1 Wed 10:15 SCH/A215

On the nature of solutal melting in Cu-Pd — •Nagarjuna Remalli[1], Huai Zhang[1,2], Nisha Singh[1], Nuria Navarrete[1], Julien Zollinger[3], and Florian Kargl[1,4] — [1]Institute for Frontier Materials on Earth and in Space, German Aerospace Center (DLR), 51147 Cologne, Germany — [2]Department of Mechanical Engineering, University of Alberta, AB T6G 2G8 Alberta, Canada — [3]Université de Lorraine, Institut Jean Lamour, 54000 Nancy, France — [4]Foundry Institute, Fundamentals of Solidification, RWTH Aachen University, 52072 Aachen, Germany

We report on the kinetics of the solid-liquid (s-l) interface during solutal melting of isomorphous Cu-Pd melting couples. Using X-ray radiography (XRR) with sub-second time resolution the solutal melting dynamics along with the evolution of solute concentration fields was investigated. To this end circular melting couples of different thicknesses (220 μm and 460 μm) were in-situ monitored in an isothermal field at 1090°C slightly above the melting point of copper (1085°C) and well below the one of palladium (1555°C).

Sample thickness dependent differences in dissolution speed were observed which are suggested to be related with buoyancy-driven convective flow. By comparing SEM analysis results of the re-solidified Cu-Pd alloys with the in-situ results good agreement was found. Persistent non-equilibrium conditions were found at the s-l interface at the end of melting, independent of sample thickness or melting mechanism.

MM 21.2 Wed 10:30 SCH/A215

Chemoelastic effects, phase equilibria, and uphill diffusion in Cu-Pd nanoparticles — •Idan Klein, Feitao Li, and Eugen Rabkin — Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa 3200003, Israel

We fabricated nanoparticles (NPs) of Cu-40 at.% Pd alloy via solid state dewetting and subsequent slow-cooling of Cu-Pd bilayers deposited on a sapphire substrate. We observed that some nanoparticles which experienced partial transformation from a disordered A1 FCC phase to the ordered B2 β-CuPd exhibited compositional discontinuity, with the ordered phase being richer in Pd. This compositional discontinuity was associated with fully or partially coherent interphase boundary. At the same time the FCC particles that did not experience any transformation, the fully transformed β-CuPd particles, and partially transformed particles with incoherent interphase boundary exhibited homogeneous distribution of the components. We developed a thermodynamic model which demonstrated that misfit-strain from the coherent interface influences the thermodynamics of the system, depressing the transformation temperature. Re-distribution of the components causes changes to the lattice parameter of each of the phases, mitigating the misfit between them, reducing free energy and encouraging the phase transformation.

MM 21.3 Wed 10:45 SCH/A215

Mechanism of structure formation during electrochemical dealloying — •Gideon Henkelmann[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

During electrochemical dealloying of a solid solution, atoms of the more noble species rearrange by surface diffusion to form a connected nanoporous structure with a characteristic length scale. Details of the underlying nanoscale self-organization process, specifically the criteria that select this characteristic length scale, remain to be understood. Here, we study this issue by kinetic Monte Carlo simulations. While previous studies started out with corroding a planar single-crystal surface, our approach starts by forming an internal cavity and follows the evolution of the surface of the growing void. This allows us to focus on passivation or bifurcation of the corrosion front in a realistic scenario with curved and rough surfaces. We find that passivation is governed by simple geometric criteria related to the enrichment of the more noble species on the pore surface. Furthermore, the variation of the resulting structure size with the overpotential may be rationalized by a Gibbs-Thomson-type scaling law.

MM 21.4 Wed 11:00 SCH/A215

ab-initio investigation of short-range order in Fe-Si-Al alloys — •Daniil Khodachenko[1], Franco Moitzi[1,2], Andrei Ruban[2], Oleg Peil[2], and Vsevolod Razumovskiy[1,2] — [1]Christian Doppler Laboratory for digital materials design guidelines for mitigation of alloy embrittlement, Leoben Austria — [2]Materials Center Leoben Forschung GmbH, Leoben Austria

Unique electromagnetic properties of steels with silicon and aluminum make them an excellent choice for the production of transformers and electric motors. These so-called electrical steels have enhanced energy efficiency due to reduced core losses and enhanced magnetic permeability. However, increasing the concentration of silicon and aluminum beyond a critical amount leads to significantly reduced ductility, which makes production very challenging.

The theoretical origin of these embrittlement effects is still not fully understood, as ab initio modeling based on Density Functional Theory (DFT) is rather challenging, due to requiring large supercells and complex magnetic interactions. Such first-principles simulations frequently use approximations that assume a fully random distribution of the alloying elements. However, real systems are not perfectly random, due to atomic interactions, which result in short-range ordering (SRO) of the atomic sites. We investigate atomic SRO phenomena using accurate DFT- and Green's function-based methods to study effective cluster interactions and their magnetic state dependence. Finally, we perform Monte-Carlo simulations to investigate phase transitions and the effect of SRO in these materials.

MM 21.5 Wed 11:15 SCH/A215

Ordering in Mo-Cr-Ti-Al refractory high-entropy alloys via machine learned interatomic potential — •Jiyao Zhang[1], Klemens Lechner[1], Markus Masswohl[2], Petra Spörk-Erdely[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Institute of Materials Science, Joining and Forming, Graz University of Technology, Kopernikusgasse 24/I, 8010 Graz, Austria

Refractory high-entropy alloys (RHEAs) offer exceptional mechanical and thermal properties, such as excellent high-temperature strength, making them favorable competitors to nickel-based superalloys. Origin of the superior high-temperature performance of the Mo-Cr-Ti-Al RHEA can be tracked to its two-phase microstructure of disordered BCC and ordered B2 phases. Modeling RHEAs poses significant challenges, as accurate density functional theory (DFT) calculations are extremely time-consuming, a difficulty worsened by the alloys' complex compositions. Universal machine learning interatomic potentials (UMLIPs) have recently emerged as a promising solution. Trained on vast DFT datasets, UMLIPs enable near-DFT accuracy for large-scale simulations of thousands of atoms. In this work, we utilize UMLIPs in mixed Monte Carlo/Molecular Dynamics simulations to evaluate the thermal stability of ordered versus disordered states in Mo-Cr-Ti-Al system as a function of the Al contents. Furthermore, we analyze the impact of composition on order/disorder transition temperature and elastic properties. We validate our findings against experimental data.

15 min. break

MM 21.6 Wed 11:45 SCH/A215

Shear-stress dependent formation of Si-polymorphs during saw dicing analyzed by raman spectroscopy — •Zainab Zainab[1,2], Jörg Debus[2], and Hannes Kurtze[1] — [1]Bernburger street 55, 06366 Köthen (Anhalt) — [2]August-Schmidt-Str. 4, 44227 Dortmund

Raman spectroscopic analysis of diced silicon wafers reveals that the saw cutting process generates considerable amounts of metastable silicon polymorphs (BC8/R8) along with the original diamond-cubic structure (DC-Si). We demonstrate that the formation of these phases exhibits a distinct spatial distribution that correlates with the shear stress profile imposed by the rotating blade. The DC-Si signal is strongest near the bottom of the cut (wafer tape side), while BC8 and R8 phases are most concentrated near the top surface at the blade entry point. This gradient arises from differences in the mechanical stress state: at the top, the steeper blade angle generates substantial shear stress in addition to normal compressive stress, facilitating shear-induced phase transformation at locally applied pressures. At the bottom, the nearly parallel blade trajectory produces predominantly normal stress with minimal shear, suppressing the formation of metastable phases. Additionally, we find that specific feed rates enhance phase transformations and intensify the spatial gradient. These findings confirm that shear stress is the critical enabling factor for polymorph formation during mechanical processing of silicon, consistent with recent studies showing dramatic reduction in transformation pressures under non-hydrostatic conditions.

MM 21.7 Wed 12:00 SCH/A215

Investigating the temperature-driven structural phase transition in α-In2Se3: A Raman study — •Saswata Talukdar, Mitanshi Gupta, Devesh Negi, Suvodeep Paul, Shalini Badola, Shivani Tripathi, Ravi Shankar Singh, and Surajit Saha — Indian Institute of Science Education and Research Bhopal, Bhopal, 462066, India

In recent years, the complex characteristics and polymorphic nature of indium selenide (In2Se3) have distinguished it as a prominent candidate among 2D semiconductors for memory and nano-electronic applications. Despite comprehensive research on its thermal, electrical, and optical properties, the structural dynamics, especially the phase transitions over temperature, remain elusive. In this work, temperature-dependent Raman spectroscopy of bulk α-In2Se3 reveals well-defined spectral signatures corresponding to its multiple polymorphic phases, providing direct evidence of its structural transitions. Our results also show that the phase transition is governed not solely by temperature, but it is further influenced by the local strain, which forms wrinkles on the surface of the material, playing a crucial role in directing the transition pathway. Moreover, comparative Raman measurements on exfoliated flakes highlight a pronounced thickness-dependent modulation of the transition behavior, underscoring the critical role of dimensionality in governing phase stability and evolution. Altogether, this work presents a comprehensive picture of the phase transitions in In2Se3, offering valuable insights for its integration into future high-performance phase-change memory applications.

MM 21.8 Wed 12:15 SCH/A215

Transforming martensite in Ni-Mn-Ga within picoseconds — •Klara Lünser[1,2], Yuru Ge[3,4], Fabian Ganss[3], Daniel Schmidt[5,6], Daniel Hensel[5], Mike J. Bruckhoff[7], Bruno Neumann[3,4], Mariana Brede[5], Sakshath Sadashivaiah[8,9], Markus E. Gruner[7], Peter Gaal[5,6], and Sebastian Fähler[3] — [1]University Duisburg-Essen — [2]RCFEMS, Bochum — [3]HZDR, Dresden — [4]TU Dresden — [5]Leibniz IKZ, Berlin — [6]TXproducts, Hamburg — [7]CENIDE, University of Duisburg-Essen — [8]Helmholtz-Institut Jena — [9]GSI Darmstadt

Martensitic transformations are driving a wide range of emerging applications, including high-stroke actuation, mechanocaloric refrigeration, and thermoelastic energy harvesting. However, systematic investigations of the fast dynamics and fundamental speed limits of martensitic transformations are scarce. In this study, we employed a synchrotron-based time-resolved diffraction technique to investigate the martensitic transformation induced by 200 fs laser pulses. Our results show that the transformation from martensite to austenite occurs within 100 ps, limited by the synchrotron probe pulse duration. We also demonstrated that an appropriate laser fluence and undercooling can complete a full transformation cycle within 5 ns, the fastest value reported for martensitic transformation. Our study highlights the importance of analyzing the lattice temperature during martensitic transformations and discusses the need for and limits of this approach. Furthermore, we found that stress must be considered as a competing influence on the martensitic transformation, in addition to temperature.

MM 21.9 Wed 12:30 SCH/A215

In-situ view on contact and solutal melting of Al-Cu — •Florian Kargl[1,2], Matthias Kolbe[1], and Nagarjuna Remalli[1] — [1]Institute for Frontier Materials on Earth and in Space, German Aerospace Center, Cologne, Germany — [2]Foundry Institute, Fundamentals of Solidification, RWTH Aachen University, Aachen, Germany

Melting plays an important role in many technical processes such as casting, additive manufacturing, etc. but is far less understood than solidification. We report on the kinetics of the solid-liquid interface during contact and solutal melting of Al-Cu melting couples. Al-Cu melting couples consisting of an Al-annulus and a Cu-disc in close contact were processed in an isothermal temperature field. The melting process was in-situ monitored with X-radiography with a sub-second time resolution determining interface kinetics and liquid composition changes. For contact melting a temperature below the melting points of Al and Cu but above the eutectic temperature was chosen. For solutal melting the sample was processed above the melting point of Al. We observed contact melting to be initiated along Cu-grain boundaries with intermetallic layers representing the entire phase diagram forming between the liquid and the still solid Cu. The layer structure has been verified post-mortem by optical imaging and quantified by SEM-EDX. Solutal melting was found to be dependent on sample thickness with buoyancy convection increasing the reaction speed in thicker samples. Further, asymmetric reaction patterns were observed to arise due to Al2O3-layer build-up and/or initial Al2O3-presence at the Al-Cu interface and/or partial Al-detachment during melting.

MM 21.10 Wed 12:45 SCH/A215

Forming bicontinuous microstructures by distributed internal melting at the Ni3Sn4 peritectic — •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 Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

A recent study on peritectic melting of TiAg suggests that a bicontinuous structure can be obtained through liquid film migration (LFM) during annealing. Without the requirement of mass exchange with the environment, peritectic melting is free of the restrictions on sample size. To date, application of this method is limited to TiAg. In this work, the intermetallic compound Ni3Sn4 is selected as the new parent system for peritectic melting. After annealing and quenching, spherical clusters are obtained, consisting of crystallographically aligned Ni3Sn2 ligaments and interpenetrating Sn phase. The phase decomposition proceeds via the LFM mechanism, i.e. complete melting of Ni3Sn4 and growth of Ni3Sn2 across the melt layer. Constitutional supercooling, induced by a composition gradient within the melt, promotes cellular growth of Ni3Sn2 nuclei, resulting in a ligament structure. Based on previous studies on peritectic and partial melting, we propose the concept of distributed internal melting, which utilizes the internal premelting sites (vacancies, dislocations and grain boundaries) to initiate LFM and generates bicontinuous structures through heat treatment.