MM 23: Phase Transformations

Time: Wednesday 17:15–18:30 Location: H23

MM 23.1 Wed 17:15 H23

study on solid/liquid interfacial energy of Al-Cu alloys and its anisotropy under a static magnetic fields — •Chenglin Huang[1], Peter Galenko[2], Rainer Backofen[3], Ken Elder[4], Sansan Shuai[1], Jiang Wang[1], and Zhongming Ren[1] — [1]State Key Laboratory of Advanced Special Steel, School of Materials Science and Engineering, Shanghai University, 200444, P. R. C — [2]Department of Physics and Astronomy, Friedrich Schiller University of Jena, 07743, Germany — [3]Institute of Scientific Computing, Technische Universität Dresden, 01062 , Germany — [4]Department of Physics, Oakland University, Rochester, MI, 48309-4487, USA

In recent decades, external magnetic fields have been widely used in materials processing to control microstructure and optimize properties. Key phenomena include magnetic levitation, crystallographic orientation changes, magnetically induced phase transitions, and TEMHD. External magnetic fields also impact thermophysical properties such as phase transition temperatures, resistivity, viscosity, diffusion, and surface tension. These effects are closely linked to interface changes, where properties differ from the bulk. Despite their importance, quantitative studies on solid/liquid interfaces under magnetic fields remain limited. Accurately measuring interfacial energy and anisotropy, and exploring atomic-scale behavior under magnetic fields, are key challenges. This research systematically investigates the effects of external magnetic fields on interfacial energy and its anisotropy in Al-Cu alloys, offering theoretical and practical insights for controlling solidification under such fields.

MM 23.2 Wed 17:30 H23

From electronic structure to thermodynamic phase diagrams with automated workflows — •Sarath Menon[1], Marvin Poul[1], Tilmann Hickel[2], Ralf Drautz[3], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]Ruhr University Bochum

Phase diagrams are useful for understanding coexistence lines, phase stability, and phase transitions under varying thermodynamic conditions. Calculating phase diagrams involves determining the Helmholtz and Gibbs free energies of different phases and their dependence on thermodynamic state variables - a task that is both intricate and computationally demanding.

In this work, we introduce automated workflows for the calculation of Helmholtz and Gibbs free energies, incorporating configurational entropy, and provide accompanying computational tools. A key component of our approach is the alchemical transformation method, where atomic species are systematically altered along a thermodynamic path to evaluate free energy changes with composition.

We demonstrate the effectiveness of this methodology using an Atomic Cluster Expansion (ACE) machine-learning interatomic potential, parametrized using the ASSYST method, to generate unbiased *ab initio* structure datasets, and compute the phase diagram of the Au-Cu system. Our workflows are independent of the interatomic potential and the material system, making them readily transferable and paving the way for making the computation of thermodynamic phase diagrams a routine task in the field of atomistic simulations.

MM 23.3 Wed 17:45 H23

Phase formation at an interface between Ni and Sn layers during a soldering process — •Sandra Gaertner, Sergiy V. Divinski, Harald Rösner, and Gehard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

Soldering is a method for creating permanent bonds between metal parts, often resulting in the formation of intermetallic compounds. The transition to lead-free solder, driven by environmental regulations, has increased the interest in Sn-based solder alloys. However, the soldering process for interconnects involves complex processes related to material transport, phase stability, phase formation, and kinetic aspects of phase transformation. In this study, we investigated the interdiffusion and diffusion-controlled phase formation in a SnSb-solder alloy between a Ni-based layer with a small amount of Si and a Cu substrate, employing SEM and TEM. Analysis of the untreated states revealed a lamellar-type structure of the Ni-based layer, characterized by a uniform distribution of elements, while the solder alloy exhibited a β-Sn matrix and a SbSn phase. Following the soldering process, we observed the formation of various intermetallic compounds like CuSnNi and SnCu, encased within the β-Sn matrix. The SbSn phase remained as small inclusions. Moreover, the Ni-based layer initially shrank, resulting in a residual thin film that displayed an increased Si content compared to its untreated counterpart. This study highlights the intricate mechanisms involved in Cu transport from the substrate through the solder material. Alongside Sn, Cu drives the transformation of the Ni-based layer, ultimately leading to its complete consumption.

MM 23.4 Wed 18:00 H23

Temperature-modulated dilatometry as a tool for studying precipitation kinetics in alloys — •Marcel Simhofer[1], Philipp Brunner[1], Jiehua Li[2], Wolfgang Sprengel[1], and Roland Würschum[1] — [1]Inst. of Mater. Phys., NAWI Graz, Graz Univ. of Technol., Graz 8010, Austria — [2]Inst. of Casting Res., Montanuniv. Leoben, Leoben 8700, Austria

Temperature-modulated dilatometry is implemented as a tool for studying phase equilibration processes in alloys. As a case example, the phase equilibration between the saturated solid solution Al(Mg) and intermetallic Al_3Mg_2 in the Al(Mg) binary alloy is studied. The varying solubility of Mg in Al upon temperature modulation causes a modulation of the relative fractions of the two phases, which can be in-situ monitored by dilatometry owing to their different atomic volumes. The phase shift between the length change caused by phase equilibration and the applied sinusoidal temperature variation yields access to equilibration kinetics. The observed variation of the phase shift with the modulation frequency is quantitatively analyzed in the framework of a simple kinetic model, revealing that the equilibration process is controlled by the diffusion of Mg in Al.

M. Simhofer et al., J.Alloys&Comp. 1010 (2025) 176984

MM 23.5 Wed 18:15 H23

Formation mechanism of bicontinuous structure during peritectic melting of TiAg — •Zhongyang Li[1], Lukas Lührs[1], Tobias Krekeler[2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Electron Microscopy Unit, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Reverse peritectic reactions, and specifically the peritectic melting of TiAg, have been proposed as dealloying-like processes that produce quite similar microstructures but avoid the restrictions on sample size inherent in liquid-metal dealloying (LMD). Here, studies of the microstructure evolution during peritectic melting of TiAg suggest a formation mechanism that is not LMD-like but rather relies on liquid film migration. The process starts with wetting of the TiAg grain boundaries by the alloy melt. Successively, both Ti and Ag continue to dissolve from one side of, while β-Ti deposits on the other side and the liquid film sweeps the pristine TiAg crystal. TiAg-Ti interfaces with well-defined orientation relationship and with concentration gradients support this picture, as does the phase morphology in partly decomposed samples. The process generates a bicontinuous structure with a solid Ti skeleton, interpenetrated by the Ag-rich melt, which is conserved even after coarsening. This study clarifies the mechanism of peritectic melting in TiAg, and it may provide a basis for identifying other alloy systems suitable for producing bicontinuous microstructures by that process.