MSE 2024

24 - 26 Sep 2024 (Darmstadt)

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Topic M: Modelling and Simulation

M02: Computational and experimental thermodynamics and kinetics of materials

The symposium provides a platform for discussing the thermodynamics and kinetics of materials. The focus is on the constitution of materials and the modelling of phase transformations, aiming to provide fundamental understanding of microstructure formation and offer new information for materials design and applications in the perspective of material scientists, metallurgists, physicists and engineers.

Specifically encouraged are computational contributions on CALPHAD-type kinetic and thermodynamic databases (incl. 3rd generation) using classical expert evaluation, first-principle, Monte-Carlo and data-driven methods that allow the derivation of stable, metastable, kinetic and defect phase diagrams as well as contributions on modelling approaches with sharp and diffuse interface at the micro- and meso-scale considering solution phase thermodynamics, near-equilibrium and non-equilibrium states at the interface (rapid transformations).

Microstructural investigation of phase equilibria and pattern formation employing, e.g., X-ray diffraction, high-resolution microscopy as well as experimental results using dilatometry and calorimetry are highly welcome.

Materials of interest are metals and ceramics, respectively. However, applications related to composites, soft matter and biological materials are welcome to explore synergetic approaches. Theory and applications of thermodynamics and kinetics to describe “materials behavior in engineering systems”, e.g., for energy storage and conversion or for circular economy are also in the scope of this symposium.

Symposium Organizer


Prof. Dr. Ernst Gamsjäger
Montanuniversität Leoben


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