MSE 2024

24 - 26 Sep 2024 (Darmstadt)

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Topic M: Modelling and Simulation

M05: Interfaces in Advanced Materials: from atomistic – to meso-scale

Grain boundaries and other interfaces exert a significant influence on the mechanical, physical, and chemical properties of polycrystalline materials. For better understanding of the complex structures and phenomena occurring at interfaces in materials during their manufacturing and service, it is essential to combine atomistic simulations with meso-scale and continuum modelling, as well as to employ machine learning approaches for uncovering the composition-structure property relationships.

The purpose of this symposium is to explore and discuss state-of-the-art applications of theoretical and computational tools that enable reliable simulations of grain boundaries and other interfaces in realistically complex materials and their properties. Multi-scale and gap-bridging approaches that seek to bring together theoretical and experimental results are of particular importance. Also of significance is the application of physics-informed machine learning (ML) techniques as well as CALPHAD-integrated studies that can capture the underlying physics and make high-fidelity predictions on interface energetics and other quantities of interest. The focus areas of computational studies include the broad microstructure evolution phenomena as in segregation phenomena, precipitate-matrix interactions, intermetallic compounds and generalized stacking fault energies, embrittlement phenomena, grain growth and recrystallization.

We warmly invite all contributions on the structure, dynamics, and thermodynamics of interfaces, as well as on their role in the property formation and evolution in metals, alloys, ceramics, multi-layered and composite materials. Symposium contributions on the implementation of ML schemes and automated or high-throughput approaches to address fundamental questions in interface properties are also welcomed.

Symposium Organizer


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