Special Issue

Multiscale Modeling for the Optimization of the Microstructures and Properties of Intermetallic Alloys

Message from the Guest Editors

We invite numerical research work that is purely computational or combined with experiments, which advances our understanding of the interrelationships among the macroscopic and mesoscopic behaviors and the microscopic processes of intermetallic compounds, as well as other advanced complex metallic alloys, such as metallic glasses and high-entropy alloys. We welcome contributions focusing on, but not restricted to, the following topics:

- Modeling and simulation of the thermomechanical behaviors of microstructures in intermetallic systems;
- Simulations of microstructure evolution and phase stability;
- Numerical simulations which address the relationship between mechanical and functional properties and the microstructure at all length scales;
- Numerical modeling that provides a deeper understanding of experimental observations;
- Time- and/or length-scale-bridging modeling which explicitly connects processes on different scales and thereby promotes the formulation of effective theories;
- Simulation approaches deploying machine-learningand data-driven methods to explore microstructureproperty relationships

Guest Editors

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Deadline for manuscript submissions

closed (31 December 2023)



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About the Journal

Message from the Editorial Board

Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

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