22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

Phase-field Model of Diffusional Processes Involving Both Stochiometric and Solution Phases

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The ability to predict the microstructures of multiphase solids and their evolution is critical to manipulating their properties. One of long-standing challenges is to model diffusional and phase transformation processes leading to the formation and temporal evolution of three-dimensional multiphase microstructures containing a mixture of ordered stoichiometric compounds with fixed compositions and disordered solid solutions with variable chemical compositions. Although phase-field method has been extensively employed to predict mesoscale structural evolution, almost all existing phase-field models treat ordered stoichiometric compounds as disordered solid solutions with parabolic compositional dependences of their chemical potentials assuming a rather arbitrary curvature, leading to possibly orders of exaggerated non-stoichiometries, thermodynamic inconsistencies, and numerical instabilities. In this presentation, we discuss a phase-field model of stoichiometric and solution phases involving simultaneous diffusion and reaction processes [1]. The model avoids the use of thermodynamically inconsistent parabolic approximations of the chemical potentials of the stoichiometric compounds and offers a straightforward connection to existing thermodynamic databases containing a combination of multiple stoichiometric and solution phases. We illustrate its application using a well-known example of precipitation of stoichiometric θ' precipitates in a solid solution matrix in which the elastic strain energy contribution also plays an important role in the resulting precipitate morphology. The proposed phase-field model can be extended to modeling other common diffusion and reaction processes such as crystallization of stoichiometric compounds from a liquid solution, vapor-phase deposition of stoichiometric thin films or two-dimensional materials on a substrate, oxidation of alloys, electrochemical deposition, interfacial reactions between two solution phases, etc.

[1] Y.Z. Ji and L.Q. Chen, Phase-field model of stoichiometric compounds and solution phases. Acta Materialia, 2022. 234: 118007, 10.1016/j.actamat.2022.118007.