FLAIR Colloquium

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High-performance phase-field simulations for microstructure prediction and multi-physics modeling toward material DX

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Abstract

Achieving material digital transformation (DX) at the microstructural level is essential for accelerating the development of advanced materials and the improvement of existing ones. This necessitates highly accurate prediction of microstructure evolution through numerical simulations, with the phase-field (PF) method widely recognized as the most powerful numerical model for this purpose. However, fully harnessing the potential of the PF method involves overcoming several key challenges, including the lack of reliable material property data, limited multi-physics modeling capabilities, and high computational cost. In this talk, I will present our recent efforts to address these challenges, structured around the following four topics:

Topic 1: Data assimilation for estimating unknown material properties
We are developing a data assimilation framework that integrates PF simulations with in situ X-ray observations of dendrite growth during alloy solidification. This approach is expected to enable the simultaneous estimation of material parameters and the four-dimensional reconstruction of dendrite evolution. Our recent progress on this topic will be presented [Acta Mater. 281 (2024) 120356].

Topic 2: Multi-physics modeling and high-performance simulations of semi-solid deformation
Solidification and casting involve complex multi-physics phenomena, including solid–liquid phase transformation, liquid flow, grain motion, and intergranular interactions. To accurately capture these effects, we have developed a coupled PF–lattice Boltzmann (PF–LB) model for simulating semi-solid deformation. I will introduce the model and present simulation results for simple shear deformation [Materialia 38 (2024) 102295].

Topic 3: High-performance simulations of melt pool dynamics and grain growth in AM
Powder bed fusion (PBF) in metal additive manufacturing (AM) is a highly complex multi-physics process involving rapid solidification, intense fluid flow, keyhole and pore formation, and evaporation. To accurately simulate melt pool dynamics in PBF, we are developing a PF–LB model together with a high-performance computing framework. We also aim to efficiently simulate grain growth using the PF method under various scanning strategies in PBF [Mater. Trans. 64 (2023) 1150].

Topic 4: Large-scale sintering simulations of alumina with massive particles

Unlike conventional grain growth, sintering requires modeling the rigid-body motion of individual particles, which significantly increases computational cost. We have conducted the largest PF simulations of alumina sintering to date using a GPU supercomputer [J. Mater. Res. Tech. 34 (2025) 1803]. I will also present our recent implementation of periodic boundary conditions in PF sintering simulations.