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Editorial: Phase field method and integrated computing materials engineering

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Editorial on the Research Topic
Phase field method and integrated computing materials engineering

Nano- and meso-scale phase-field methods (PFM) have increasingly been used in a wide range of metallic materials, in addition to both inorganic and organic non-metallic materials. In the context of integrated computing materials and engineering (ICME), phase-field methods, together with other physical modeling or machine learning (ML) technologies, have become powerful tools for designing corresponding experiments and understanding material processes when dealing with the design and manufacturing of metals, alloys, or non-metallic materials. Solidification, precipitation, and deformation correspond to the casting, aging, forging, or additive manufacturing processes, etc., and controlling the microstructures in these processes is key for preparing high-performance materials or manufacturing components. The coupling of microscopic and mesoscale modeling during the design and manufacturing processes of materials or casting within the ICME framework is shown in Figure 1.

In this Research Topic of "PFM-ICME," the research work is unexpectedly included in this framework, showing the potential of PFM-ICME in the application of a variety of materials processes.

- H atom diffusion and void defects. Using the phase-field model, the grain structures and irradiated void defects of hydrogen (H) atoms in porous polycrystalline tungsten (W) are generated (Li et al., DOI: 10.3389/fmats.2022.935129). The effects of grain morphology and porosity on the effective diffusion coefficient of H in W alloy are investigated, providing a good way to understand the influence of complex microstructures on H diffusion and assisting in the design of W-based materials for the fusion reactor.
- Solid-state phase transformation (precipitation PFM). A macroscopic constituent redistribution phase-field model is developed by introducing the effect of irradiation on atom mobility and the effect of temperature on interface mobility (Wen et al.), and an expression of phase boundary width is proposed that applies to both microscopic and macroscopic scenarios. The interfacial parameters and Zr concentration distribution near the fuel surface in U-10wt% Zr metallic fuels are discussed. PFM combined with COSMAP software is used to investigate the precipitation of carbide $M_{23}C_6$ by surface quenching on GCr15 (Fe-Cr-C) alloy-bearing rings (Liu et al.).
- Additive manufacturing (solidification and precipitation PFM). A two-relaxation-time lattice Boltzmann model is proposed to simulate melt flows and free surface dynamics of Ti-6Al-4V alloy in an electron beam selective melting additive manufacturing process (Chen et al.). The model describes the dynamics of solid-liquid phase change and heat transfer and is employed

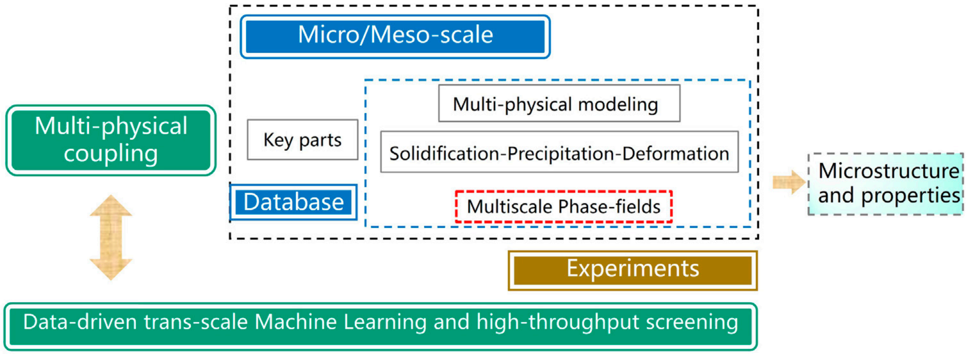

FIGURE 1
The design schematic of metallic materials processes in the PFM-ICME framework.

to simulate the influence of process parameters on single and multiple tracks of electron beam selective melting on a single layer of the powder bed. Another example (Chen et al.) is simulating the micro-structure evolution of Inconel 718 alloy homogenization during laser powder bed fusion (L-PBF).

- Precipitation of zirconium hydride blisters (corrosion PFM). The natural growth of hydride blisters and structural evolution after applying radial stress are investigated using a phase-field model coupled with anisotropic elastic, and the corrosion kinetics, stress distribution, and displacement changes are discussed (Wu et al.).
- Columnar to equiaxed transition (CET) (directional solidification PFM) (Zeng et al.) The transformation of columnar dendrites to equiaxed crystals during directional solidification of Al alloy in the convective environment of the actual roll casting process is investigated with the Kim-Kim-Suzuki (KKS) PFM, considering the microflow field and the roll casting experiment.
- Grain boundary dislocations in plastic deformation (phase field crystal, PFC). The dislocation arrangement and decomposition at grain-boundaries (GB) during constant-volume plastic deformation of the FCC bi-crystal system are studied by using the two-mode phase-field crystal (2PFC) method (Li et al.). The effects of different GB misorientations (GBMs) and tensile deformation directions are analyzed in terms of dislocation arrangement and decomposition. The atomic density profile changed periodically at equilibrium in three different symmetrical tilt GBs, but the initial GB dislocation arrangement remains almost the same when tensile deformation is applied in the x- or y-direction and is symmetrically arranged in a "bowknot" structure. Stress at GB is more concentrated with the increase in strain, and dislocation decomposition can reduce stress concentration.
- Coating growth (PFM in Materials Genome Engineering). Within the framework of Materials Genome Engineering (MGE), high-throughput 3D phase-field simulations for TiN coating growth during physical vapor deposition (PVD) combined with the multi-objective optimization strategy and the corresponding experiments are performed to screen the optimal coating properties (Dai et al.).

This Research Topic also includes a molecular dynamics simulation of the nano-crack closure mechanism and interface behaviors of polycrystalline austenitic steel (Chen et al.), demonstrating the modeling variety of ICME. Phase field methods, first principles, molecular dynamic simulations, machine learning technologies, macroscopic multi-physical field simulations, numerical algorithms, and corresponding experiments are often coupled together to solve many materials processes. As a result, the "Integrated phase-field methods (IPFM)", rather than a single PFM, will have greater application potential in the future design of high-performance metallic or non-metallic materials, and in the manufacturing of castings and other components. IPFM is becoming one of the most important and promising core parts within the scope of ICME.

Author contributions

The author confirms being the sole contributor of this work and has approved it for publication.

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Conflict of interest

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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