Phase-field modeling of microstructure evolution: Recent applications, perspectives and challenges

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Abstract

We briefly review the state-of-the-art in phase-field modeling of microstructure evolution. The focus is placed on recent applications of phase-field simulations of solid-state microstructure evolution and solidification that have been compared and/or validated with experiments. They show the potential of phase-field modeling to make quantitative predictions of the link between processing and microstructure. Finally, some current challenges in extending the application of phase-field models within the context of integrated computational materials engineering are mentioned.

Keywords: Phase-field, Microstructure evolution, Solid state transformations, Solidification

1. Introduction

The processing-microstructure-properties linking is the central paradigm of Materials Science, indicating that the arrangement and properties of the different phases at the microscopic level determines to large extent the macroscopic behavior of materials. The main building block of most materials are crystalline regions whose properties are determined by the presence of defects

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in the lattice (such as solute atoms, dislocations, secondary phases, precipitates, etc.) as well as by the lattice boundaries (dendrites, grain and twin boundaries, etc.). It was understood early that numerical simulations at the “mesoscale” (encompassing the interaction of the homogeneous crystalline lattice with defects) were necessary to understand the complex processing-structure-properties relationships as well as to guide the design of materials with outstanding properties. Most of the effort in linking microstructure to properties has relied on the finite element method (and similar approaches, such as using fast Fourier transforms) in which the mesoscopic domain is divided in homogeneous regions limited by boundaries and the response of each domain is controlled by the appropriate partial differential equations. The overall response of the material is determined by solving the boundary value problem in which the solution to the differential equations also satisfies the boundary conditions [1, 2]. This strategy has been extremely successful for analyzing the microstructure-properties links as long as the topology of the boundaries between different homogeneous regions do not change. However, this is usually not the case during processing as the evolution of the boundaries is precisely part of the solution of the problem.

Since the early 90’s, the phase-field (PF) method has emerged as an outstanding tool for simulating the formation and evolution of microstructures during processing [3–14]. The key idea of the PF approach is the description of interfaces using continuous fields. Discontinuities of properties across interfaces as well as specific boundary conditions at the interface (found in models that consider sharp interfaces) are smeared out and represented by a smooth variation of one or several auxiliary fields (the phase fields) across a diffuse interface. In this way, the problem is solved by integrating a unique set of partial differential equations in the whole domain, and the evolution of the different interfaces comes out naturally as part of the solution. Hence, the PF method provides a powerful tool to handle notoriously challenging free-boundary problems for arbitrarily complex interfaces. Moreover, its generality and flexibility make the PF approach convenient to apply to a broad range of phenomena across materials science, and beyond, including fracture [15–18], liquid metal dealloying [19, 20], sintering [21–23], and many other applications [24].

In this short and far-from-exhaustive review, we first highlight a few recent applications of the PF method to phase transformations and microstructural evolution, which demonstrate its current potential to make quantitative predictions of the link between processing and microstructure. Particular
emphasis is given to microstructure evolution in metals, alloys, and relevant model systems subjected to either solidification or solid-state transformations. In the second part, we briefly review some of the current challenges to extend the application of PF within the framework of integrated computational materials engineering.

2. Phase-Field Modeling Fundamentals

The cornerstone of nearly every PF model is the formulation of the free energy $F$ as a functional

$$ F = \int f(\phi_1, \phi_2, \ldots, \phi_n, c_1, c_2, \ldots, c_n, \nabla \phi_1, \nabla \phi_2, \ldots, \nabla \phi_n, \nabla c_1, \nabla c_2, \ldots, \nabla c_n, p, T, \ldots) \, dV $$

(1)

containing a set of non-conserved fields $\phi_i$ (for instance, order parameters describing crystalline symmetries) and conserved fields $c_i$ (for instance, species concentration). The energy density $f$ typically includes (1) a potential with local minima in the two (or more) coexisting phases (for instance “double-well” or “double-obstacle” potentials [11]), (2) gradient terms of $\nabla \phi_i$ and $\nabla c_i$ that relate to the energetic cost of interfaces and (3) bulk energy density terms as a function of the local fields $\phi_i$ and $c_i$, local state variables (e.g. temperature $T$, pressure $p$, stress/strain), and/or external stimuli. The evolution of conserved fields, $c_i$, and non-conserved fields, $\phi_i$, are thus given by a set of equations that guarantees a decrease in total free energy with time according to

$$ \frac{\partial c_i}{\partial t} = \nabla \cdot \left( M_{c_i} \nabla \frac{\delta F}{\delta c_i} \right) = \nabla \cdot \left( M_{c_i} \nabla \left( \frac{\partial f}{\partial c_i} - \nabla \cdot \frac{\partial f}{\partial \nabla c_i} \right) \right) $$

(2)

$$ \frac{\partial \phi_i}{\partial t} = -M_{\phi_i} \frac{\delta F}{\delta \phi_i} = -M_{\phi_i} \left[ \frac{\partial f}{\partial \phi_i} - \nabla \cdot \frac{\partial f}{\partial \nabla \phi_i} \right] $$

(3)

respectively referred to as Cahn-Hilliard [25, 27] and Allen-Cahn [28, 29] (or time-dependent Ginzburg-Landau) equations. Parameters $M_{c_i}$ and $M_{\phi_i}$ are positive mobilities, e.g. linked to atomic ($c_i$) or interfacial ($\phi_i$) mobilities, and may depend on local state variables and interface orientation.

The main differences between a given phase-field model and another reside primarily in the set of conserved and non-conserved fields chosen to
describe the problem at hand, the resulting formulation of the various contributions to the total free energy, and the choice of interpolation of the different variables across interfaces. Microstructural evolution is driven by a reduction of the system free energy — namely a reduction of bulk free energy for phase transformations, a reduction of interfacial energy for coarsening or grain growth, and often a subtle combination of both. The general form of the energy functional is a decisive advantage of the method, permitting to couple a broad range of distinct phenomena in a consistent framework.

3. Phase-Field modeling of Solid-State Microstructure Evolution

3.1. Fundamental concepts

Phase-field models for solid-state microstructural evolution commonly derive from the microscopic elasticity theory of structural transformations by Khachaturyan [30–33]. Such models involve actual order parameters, \( \phi_i \), representing long-range atomic ordering as well as symmetry and orientation relationships between coexisting phases, which naturally arise for many solid-solid transformations. Different transformations may be represented by a different number of non-conserved order parameters, \( \phi_i \), which may be coupled to conserved parameters, \( c_i \) [3–5].

The fields \( \phi_i \) thus provide a valuable description of the crystalline structure of the different phases, and the anisotropy of interfacial properties (e.g. free energy) derives naturally from the gradient terms in the free energy. On the other hand, beyond a few relatively simple cases (e.g. anti-phase boundaries), the energetics of phase transformations need to be described phenomenologically, thus introducing unknown parameters that may require identification through dedicated experiments or theories. In most models, conserved and non-conserved fields are coupled in a way that prevents changing the interface width and its energy independently, hence limiting the upscaling of the diffuse interface width for computational purposes [3–5].

Previous detailed reviews of the PF method oriented toward solid-state microstructure evolution can be found in [3–5].

3.2. Highlighted applications

The phase-field method has been applied to a broad range of solid-state microstructural evolution phenomena. In this review, we highlight recent studies of four mechanisms, including a diffusive transformation (precipitation), a displacive transformation (martensitic), a coarsening mechanism
(grain growth), and a deformation mechanism (twinning). Other notable applications include, for instance, the modeling of dislocations and their interaction with microstructure evolution \cite{35,40} and the introduction of plastic and viscoplastic effects \cite{41,46}.

3.2.1. Precipitation

Precipitation is a solid-state diffusive phase transformation used in a broad range of metallic alloys due to the strengthening effect of precipitates. If precipitates form homogeneously in the matrix, they have a random spatial distribution. However, interactions among nearby precipitates and/or pre-existing lattice defects, such as dislocations and grain boundaries, may result in non-random distributions. For example, the transformation strain from precipitation may result in an increase of nucleation energy barrier adjacent to the precipitate. The precipitate may interact with neighboring ones and/or form on pre-existing lattice defects to decrease this barrier.

The phase-field method has been used extensively to simulate precipitation in a wide range of metallic alloys, such as Ni \cite{42,47,67}, Ti \cite{68,75}, Al \cite{76,85}, and Mg \cite{86,96} alloys. Research studies have covered a series of aspects related to the growth and coarsening of precipitates, such as the shape and distribution of precipitates \cite{47,80,88}, the interactions between precipitations and external stress fields, such as the stress fields caused by other precipitates \cite{89,94} or lattice defects \cite{88,92}, and the directional coarsening (rafting) and stability of cuboidal matrix/precipitate microstructures in superalloys \cite{55,63}. Here we illustrate the application of the PF method to study the formation of $\theta'$ (Al$_2$Cu) precipitates in Al-Cu alloys.

The $\theta'$ is a key strengthening phase in Al-Cu alloys widely used in automobile and aerospace industries over the past century \cite{97}. To accurately predict the shape and formation mechanism of $\theta'$ precipitates, input parameters are needed that include transformation strains, elastic constants, free energy curves of both $\theta'$ precipitates and $\alpha$-Al matrix, and interfacial energy between $\theta'$ precipitates and $\alpha$-Al matrix. These parameters can be calculated by atomistic approaches, such as first principles and molecular dynamics/statics, and/or collected from available databases (see e.g. \cite{76,78,80,83}). Simulation results have revealed that both the anisotropic interfacial energy and elastic strain energy favor the precipitate growth along the same habit plane, and that shear strain plays a dominant role on the equilibrium shape of $\theta'$ precipitates (see, e.g., Fig. 1 \cite{80}). It was also shown that pre-existing lattice defects, such as dislocations, can facilitate the nucleation
and growth of precipitates, in Al [80, 84] (Fig. 1) but also in other alloys [42, 47, 70, 71, 86, 92].

Figure 1: Precipitation of $\theta'$ in an Al-Cu alloy [80]: TEM images showing (a) random and (b) orientation-correlated $\theta'$ precipitates in an Al-4 wt.% Cu alloy aged at 180°C for 66 hours, and phase-field simulation of (c) the homogeneous nucleation of $\theta'$ precipitates, leading to a random precipitate distribution, and (d) precipitates formed under the stress field of mixed dislocations, leading to correlated orientations.

3.2.2. Martensitic transformation

Diffusionless (or displacive) phase transformations occur when a change in crystal structure is induced by a cooperative movement of large groups of atoms. A common, and likely the most studied, displacive transformation is the martensitic transformation, in which the driving forces can come from either Gibbs free energy differences between the matrix and the secondary phases, or from the external applied stress. Due to lattice changes from
the matrix to the product phase, this transformation is accompanied by the generation of transformation strain, which is a hindrance for transformation.

To date, Landau theory and phase-field models have been extensively used to model for martensitic transformations [98–127]. Simulations have allowed identifying important mechanisms for martensitic microstructure formation, for instance focusing on the shape and distribution of phases in martensitic microstructures [104–111], nucleation mechanisms [113–116], or the effect of plasticity [123–126] on transformation kinetics and resulting microstructures.

From an industrial perspective, the martensitic transformation in steels is of the utmost importance, as it confers martensitic steels higher strength and hardness than most other steel grades. Yet, rapid transformation kinetics makes it challenging to observe in situ, hence making simulations all the more useful. A recent application of the PF method to the martensitic transformation is illustrated in Fig. 2 where the experimental microstructures observed in low-carbon steels and the simulated microstructures accounting for 24 orientation variants in a finite strain framework are compared [122]. Beyond steels, notable recent PF studies on martensitic transformations have focused on Ni-Ti-based shape memory alloys [110, 121, 128] and tetragonal-to-monoclinic transformation in Zr alloys [129–131].

![Experimental EBSD map of lath martensite](image1.png) ![Simulated martensite microstructure](image2.png)

Figure 2: Martensitic microstructures in low-carbon steels [122]: (left) EBSD orientation maps of a steel containing 0.3 wt%C and (right) phase-field simulated microstructure with color map showing the 24 Kurdjumov-Sachs orientation variants. Reproduced with permission from [122].
3.2.3. Grain Growth

Most technological materials are polycrystalline. Their grain size is critical to determine their properties, and it can be modified through annealing (i.e., heating), which leads to the coarsening of the microstructure \[132, 133\]. This phenomenon is referred to as grain growth, and its main underlying mechanism is clear: the reduction in free energy through a decrease of grain boundary (GB) area. GB energies are known to depend on the misorientation of the grains and on the inclination of the GB plane \[134, 135\]. Their mobilities are also assumed to depend mostly on the five degrees of freedom representing the GB misorientation and inclination \[136–138\]. PF models provide a compelling tool to investigate grain growth, as they allow the integration of anisotropic GB properties, and their dependence upon GB misorientation and inclination.

A broad variety of PF models have been developed to simulate grain growth \[139–186\]. They were used to study coarsening mechanisms in single-phase \[139–152\], two-phase \[153–157\], and three-phase microstructures \[158–169\], and to explore a variety of phenomena, including the evolution toward a characteristic grain size distribution \[146–152\], the effect of anisotropic GB properties \[160–168\], the effect secondary particles, e.g., Zener pinning \[169–177\], abnormal grain growth \[178–180\], and recrystallization \[181–186\], among other applications.

A recent PF study of grain growth \[187\] is illustrated in Figure 3. Simulations are compared with time-resolved X-ray 3D tomography data recorded during annealing of an iron sample. By fitting simulations and experiments (Fig. 3a,b) \[187, 188\], the authors extract the mobilities of several hundreds of grain boundaries. Remarkably, reduced GB mobilities do not show any correlation with the GB macroscopic degrees of freedom (see, e.g., misorientation in Fig. 3c) and some even seem to be time-dependent. These results, which appear to agree with results from atomistic simulations \[189, 190\], challenge the conventional assumption that GB mobilities are primarily governed by the GB misorientation and inclination.

3.2.4. Deformation twinning

Twining is one of the major deformation modes in metallic materials \[191–192\], in particular for hcp crystals or in nanocrystalline metals \[193–197\]. The formability, yield strength, and tension-compression yield asymmetry of some metallic materials, such as wrought Mg alloys, are all closely related with deformation twinning.
In a PF framework, twin crystals are essentially assimilated to martensite plates and the applied stress/strain provides the driving force. The evolution of twin crystals is thus equivalent to the gliding of twinning dislocations. The PF method has been applied to study twinning and detwinning in both cubic [198, 201] and hexagonal materials [202, 205], including under finite strain, e.g. coupling with crystal plasticity theory (see, e.g. [206, 207]) or extending Khachaturyan’s classical theory (e.g. [208]).

A recent application of the PF method [205] to the study of the formation and autocatalytic nucleation of \{10\bar{1}2\} twins in a polycrystalline Mg
microstructure is depicted in Fig. 4. Under the effect of an applied strain (Fig. 4a), a twin crystal nucleates at a triple-junction (Fig. 4b), grows and triggers the formation of other twin crystals in the neighboring grains, which ultimately form a twin chain (Fig. 4c,d) that thickens until a steady state microstructure is reached (Fig. 4e). In particular, this study has shed light on the links existing between twin nucleation and residual shear stresses, stress-free transformation strain of the emerging twins, grain orientations, and stress concentrated at grain boundaries.

Figure 4: Phase-field simulation of the formation and autocatalytic nucleation of \{10\overline{1}2\} deformation twins in Mg [205]: (a) Polycrystalline sample, grain orientations, and applied strain along Y and Z directions, and (b-e) time evolution of the nucleation and growth of twins under an applied strain with \(\varepsilon_{YY} = -0.0005\) and \(\varepsilon_{YY} = 0.0005\).

4. Phase-Field modeling of Solidification

4.1. Fundamental concepts

Solidification has been a particularly successful application field of the PF method. Models for solidification mostly rely on the approach proposed by Langer [209], which considers a diffuse interface at an arbitrary scale below that of the microstructure of interest. The phase field \(\phi\) is thus a global
measure of order between solid and liquid phases [8]. By using a unique phase field, rather than several order parameters, the intrinsic crystalline anisotropy is not naturally rendered, but anisotropic interfacial properties (e.g., excess free energy and kinetic coefficient) can be introduced ad hoc through an orientation dependence of the gradient energy coefficients [8, 210–215].

An important feature of these models is the existence of well-defined free-boundary equations, which have analytical solutions in both sharp and diffuse interface formulations [11]. On the one hand, the existence of these solutions imposes severe constraints on the model formulation — for instance, it may be challenging to ensure that the driving force for the phase transformation be constant across the interface [11,13]. On the other hand, spurious effects arising from the use of an arbitrarily wide interface can be quantitatively corrected, since the deviation from a known solution can be quantified. Quantitative formulations have thus been developed for “mesoscopic” interface widths, e.g., using matched asymptotic analysis [212, 216, 217] and solute “antitrapping” terms [217, 218], which allow increasing the interface width for numerical convenience, as long as it remains small enough to accurately resolve the interface curvature [11, 219, 220].

PF models for solidification are built on fundamental concepts of thermodynamics [8, 11, 13]. General formulations may use an entropy [221] or a grand-potential [222, 223] functional, but the majority of models are based on the construction of a free energy functional [5, 13]. The thermodynamic foundations of such models allow (1) a natural integration of some fundamental physics, such as interface curvature (Gibbs-Thomson) effects and (2) a clear correlation of all model parameters to physical properties, e.g., mobility terms $M_\phi$ and $M_c$ naturally relating to the interface kinetic coefficient and solute diffusion coefficient, respectively.

4.2. Highlighted applications

Details and equations of PF models for solidification were already reviewed in details in several articles [7–14]. Here, we focus on a few recent examples of application of the method to quantitatively simulate and explain the formation of complex microstructures from the liquid state.

Early PF simulations of solidification (e.g., [210]) were qualitative by nature, in spite of striking morphological similarities between computed patterns and actual microstructures. Simulations became more quantitative
around the turn of the century with the development of quantitative models for “upscaled” interface widths [212, 216–218], which opened the way to three-dimensional simulations at experimentally relevant length and time scales, with the support of high-performance computing [224–235].

A major success of the PF method has been to provide a quantitative simulation tool to discuss classical theories and address long-standing questions in the field of dendritic growth. PF simulations have, for instance, permitted to validate microscopic solvability theory [236–240], and to investigate the morphology of three-dimensional dendritic tips [241, 242].

Progressively, PF results have been compared to experimental measurements on a more quantitative basis. Comparisons were made on microstructural length scales measured on solidified samples, e.g. scaling laws for secondary dendrite arm spacings in cast Al-Cu ingots [243, 244], or from in situ imaging of solidification experiments on transparent organic systems [245–247] or more recently using X-ray imaging of metallic alloys [248, 249]. Looking at kinetic effects, the dependence of dendrite growth velocity with undercooling was predicted by a quantitative model [250] using MD-calculated parameters for interface energy [251, 252] and kinetic coefficient [253] and exhibited a remarkable agreement with experimental data measured in highly undercooled Ni [254, 255].

The examples above represent a small — and by no means exhaustive — sample of efforts to quantitatively compare PF results with solidification experiments and theories. Below, we highlight in further details two outstanding applications of PF simulations that have lead to quantitative predictions and explanations of experimentally observed phenomena in solidification.

4.2.1. Growth orientation transitions in metallic alloys

Unconventional “feathery” dendrites have been reported for decades [256]. More recently, on the basis of electron backscatter diffraction (EBSD) analysis, it was suggested that a change of solid-liquid free energy due to solute addition might be at the origin of morphological transitions in Al alloys [257, 258]. This assumption was validated for Al-Zn alloys by a combination of solidification experiments and quantitative phase-field simulations [214, 259] (Fig. 5). Solidification experiments had revealed a continuous transition from ⟨100⟩ to ⟨110⟩ preferred dendritic growth orientation as the alloy Zn content was increased [214, 259] (Fig. 5a). The transition was consistent across different setups and different cooling rates, thus pointing at an effect of interfacial energy rather than kinetics. This interpretation was
validated by quantitative PF simulations [214]. After extending the expression of the solid-liquid interface free energy anisotropy, PF simulations revealed that small changes in the anisotropy parameters were sufficient to trigger this orientation transition in both equiaxed [214] and columnar [215] (Fig. 5b) growth. Independently, molecular dynamics (MD) simulations on a model Lennard-Jones system revealed that alloying may give rise to sufficient changes in interface free energy anisotropy [260].

In the past few years, several other dendrite orientation transitions (DOT) were reported, mostly in Al and Mg alloys — two elements with weak solid-liquid interfacial anisotropy [261–263]. In Al-Ge, a transition was observed as a function of the Ge content, by combining X-ray in situ imaging, EBSD analysis, and PF modeling [264]. Another recent study has discussed the underlying mechanisms of a DOT in Al-Sm alloys, combining experiments, phase-field, and atomistic simulations [265]. The authors suggest that the mismatch of lattice constants between Al and Sm (rather than liquid order-

Figure 5: Transition of preferred dendritic growth direction in Al-Zn alloys: (a) experimentally observed continuous transitions from (100) to (110) growth direction as a function of Zn content [214] and (b) corresponding phase-field simulation showing the influence of solid-liquid free energy anisotropy parameters [215]. Reproduced with permission from (a) [214] and (b) [215].
ing) is the reason for the transition, and they report unexpected dependence of interface energy and its anisotropy upon Sm content and temperature. Other examples of observed orientation transitions include several Mg alloys \cite{266,269}, as well as another type of transition from a \langle 100 \rangle to a \langle 111 \rangle growth direction in Al-Cu droplets as a function of their cooling rate \cite{270}. 

4.2.2. Solidification experiments in microgravity

Classical theories of solidification have focused on the interplay of interface capillarity with diffusive transport of heat and/or species \cite{238,240,271}. However, in the vast majority of solidification processes, the release of heat and solute at the solid-liquid interface induces density inhomogeneities in the liquid that, under the effect of gravity, lead to buoyant convection. This phenomenon, acknowledged for decades \cite{272–274}, has prevented the solidification of bulk samples in homogeneous conditions \cite{275}. Hence, most of solidification theory was discussed in light of thin-sample quasi-2D experiments, in which convection is limited (however often not completely suppressed \cite{248,276}) by confinement. These limitations have provided a strong motivation to develop solidification experiments in platforms offering lower gravity levels — e.g. space shuttles \cite{277,278}, parabolic flights \cite{279}, or the International Space Station (ISS) \cite{280,281}. Hence, after decades of sustained efforts from both modeling and experimental communities, solidification simulations and experiments of bulk samples under homogeneous conditions can now be compared on a quantitative basis at the scale of entire three-dimensional cellular or dendritic arrays.

A recent example of study combining microgravity solidification with phase-field simulations focused on experiments performed in the DEvice for the study of Critical LIquids and Crystallization (DECLIC) installed aboard the ISS \cite{280,281}. This setup allows directional solidification of transparent organic alloys (widely used as model systems for metals \cite{240,282}), with \textit{in situ} imaging of the solid-liquid interface pattern formation. Experiments on dilute succinonitrile-camphor alloys revealed an unexpected oscillatory behavior of cellular arrays, which was explained using phase-field simulations (Fig. 6) \cite{283–285}. For several experiments within a narrow range of control parameters (namely temperature gradient and growth velocity), oscillations of the individual cell areas were observed across entire arrays, with an oscillation period between about 25 and 125 minutes. The oscillations did not exhibit the long-range spatial coherence that had been observed in thin-sample experiments performed on Earth \cite{280}. However, small regions with local
spatial order showed coherent oscillations of subgroups of cells. Quantitative phase-field simulations (Fig. 6b) were capable of reproducing the overall array behavior (Fig. 6a) with a remarkable agreement on the oscillation period (Fig. 6c,d). By allowing to scan a broad range of parameters, simulations allowed to identify the link between this oscillatory behavior and a gap in the array stable spacing range, occurring within a narrow range of temper-

Figure 6: Oscillations in three-dimensional cellular patterns [283, 284]: (a) experimental in situ observation and (b) phase-field simulation of the solid-liquid interface, seen from the liquid side facing the growth direction, with tagged numbers of neighboring cells. Locally ordered regions of the array exhibit coherent breathing-mode oscillations. In hexagonal ordered regions, both experiment (c) and simulation (d) exhibit three sublattices oscillating $2\pi/3$ out-of-phase with one another at a period $\tau \approx 45$ min.
ature gradients. The lack of overall oscillation coherency was attributed to frequent tip-splitting events (Fig. 6a-b) promoting the global disorder of the array. Later quantitative analyses of DECLIC experiments with quantitative phase-field simulations have explored the evolution of the three-dimensional cell tip shape (reconstructed through interferometry) during this oscillatory regime \[287\], the effect of sample size and grain orientation on the appearance of the oscillations \[288\], and the importance of accounting for heat transport kinetics in order to quantitatively predict initial transient dynamics of the planar interface destabilization and cell/dendrite spacing selection \[289, 290\]. Ongoing and future investigations along that research line shall shed light on the formation and stability of three-dimensional grain boundaries \[291\], as well as the effect of the array ordering on microstructure selection in cellular and dendritic arrays \[292, 293\].

5. Perspectives and Challenges

The examples presented above demonstrate that PF models are at the core of future developments within the framework of Integrated Computational Materials Engineering (ICME) \[294–296\], whose goal is to integrate available modeling tools into a multiscale strategy capable of linking processing, structure, properties, and performance of engineering materials \[297\]. By providing a consistent thermodynamic framework with a natural integration of interfaces and kinetics at the scale of microstructures, PF occupies a central role into this ICME paradigm. This leads to a number of novel approaches and challenges for future developments, some of which are briefly outlined below.

5.1. Identification of parameters for quantitative simulations

The energy functional at the core of PF models depends on a large number of parameters that control the different energy contributions (e.g. chemical, interface, elastic deformation) as well as the atomic and interfacial mobilities in Cahn-Hilliard and Allen-Cahn equations. Quantitative predictions of the microstructure evolution requires a careful identification of parameters and constitutive relations, from experiments when possible, but often from other simulation methods.

A natural link exists between PF and CalPhaD methods, since both rely on a free energy description, and the two methods have been coupled successfully in various applications \[298, 300\]. However, the CalPhaD method
depends upon databases of experimental, theoretical, and/or computational data, which may be missing for new alloys, or inexistent for interfacial properties, hence requiring atomistic and/or first principles simulations [301].

For instance, cluster expansion strategies in combination with statistical mechanics can be used to predict the phase diagrams and the Gibbs free energies of different phases (including metastable phases) for alloys [302–304]. The interface energies between matrix and precipitates for different crystallographic orientations can be computed using density functional theory [78–82, 87–91], and grain boundary energy and mobility can be determined by means of MD simulations [134–136]. For solidification, MD simulations can also be used to determine the solid-liquid interface energy [252, 261, 262, 305–310] as well as its kinetic coefficient [253, 305, 311–316]. However, for such simulations to be predictive, one must pay special attention to selecting interatomic potentials that remain accurate up to the melting temperature (see e.g. [307–310]).

5.2. Computational cost and acceleration strategies

5.2.1. Algorithms and parallelization

An important limitation of the PF method is its computational cost, which restricts the length and time scales of applications. This limitation can be addressed, to some extent, by numerical techniques (e.g. parallelization [224–228], adaptive meshing [229–232], explicit time stepping [233–235], or spectral methods [317–319]), but the development of new formulations that remain accurate while using wider diffuse interfaces (or coarser numerical grids) is still actively pursued.

5.2.2. New model formulations

Among newly proposed formulations, a remarkable new method was recently proposed that relies on an intrinsically discrete formulation, and remains accurate (rotational invariance, no grid pinning) with coarser spatial discretization than usually required [320]. This new method was recently applied to grain growth, taking advantage of its computational advantage to perform simulations on a statistically significant number of grains leading to a scale-invariant regime [321].

In solidification, the thin interface limit [212, 216, 217] has demonstrated its computational benefits, and even as it remains to be performed for the majority of published models, this type of analysis has now been performed for a range of models (e.g. [223, 322, 323]). Unequal finite phase diffusivities
complicates the thin-interface asymptotic matching \[324\]. For alloys, the phenomenological solute anti-trapping concept has been extended to arbitrary diffusivity ratio \[325\]-\[327\]. An interesting new formulation was recently proposed that introduces a kinetic cross coupling between non-conserved and conserved fields, due to non-diagonal terms in force-flux Onsager relations \[328\]-\[330\], opening a way to quantitatively simulations of phase transformations with finite diffusivities in all phases.

5.2.3. Integration with machine learning

Recent promising examples of code acceleration or innovative use of PF simulations have involved machine learning (ML). Materials science applications of ML have seen an exponential growth over the past years \[331\], and they have an extremely wide range of applications, from text mining to solving partial differential equations (PDEs) \[331\]-\[333\]. In this framework, PF simulations can be used as a tool for generating high-throughput synthetic training data \[334\]-\[336\], or as a model in which to plug in machine-learned functions or parameters (e.g. free energies, mobilities) \[336\]-\[338\]. Alternatively, ML can also be used to directly solve PDEs in a fast and approximate manner \[339\]-\[340\]. Recent examples of PF-ML integration include: ML of free energy landscapes to predict the shape and composition of precipitates \[337\], PF-trained ML identification of growth rate constants for electromigration in microelectronics solder joints \[336\], or high-throughput PF generation of synthetic microstructure for ML based on two-point correlation and principal component analysis applied to spinodal decomposition \[334\]. Further than microstructure evolution, ML was also used in combination with a range of PF models, for instance for fracture mechanics simulations \[338\] or to predict the breakdown strength of polymer-based dielectrics \[335\]. Beyond a direct integration with PF, the potential of ML to improve PF simulations is tremendous, for instance providing alternate routes for predictions of phase diagrams, development of accurate interatomic potentials, or automated multidimensional microstructure analysis \[331\]-\[332\]. Importantly, statistically-based methods provide a convenient tool to analyze uncertainty propagation in ICME model chains (see e.g. \[341\]). In turn, ML also comes with outstanding challenges, related for instance to the size and uncertainty of the training data, or the selection of appropriate training metrics.
5.3. Nucleation

Nucleation is of paramount importance to microstructure selection, but still challenging to address quantitatively and predictively with PF. Mesoscale descriptions of nucleation have to rely on approximations. For instance, random noise can be used that satisfies the fluctuation-dissipation theorem [48, 105, 342–346], but in general unphysically strong noise is required to prompt nucleation events. Other methods rely upon explicitly seeding supercritical nuclei, either from a statistical distribution of inoculants, or explicitly made to match classical nucleation theory while respecting conservation balances [85, 347–350]. In the context of solidification, some of the challenges related to nucleation in PF models have notably been discussed in Refs [351] and [352].

5.4. Rapid solidification

The emergence of fusion-based additive manufacturing of metals has revived the interest in quantitative modeling of rapid solidification, when the solid-liquid interface is far from equilibrium [353–355]. An important consequence of rapid solidification in alloys is solute trapping, which stems from a jump in the chemical potential across the interface [356–360]. Using a realistic interface width, solute trapping is well predicted by conventional PF simulations through solute gradient terms in the free energy functional [34, 361], or alternatively introducing a relaxation condition for the solute flux though the interface [362]. However, since the amount of solute trapped depends on the interface thickness, modeling the departure from equilibrium and the resulting solute trapping using an upscaled interface width has remained a challenge.

In the finite interface dissipation model, separate compositions profiles for solid and liquid phases are linked by a kinetic equation describing the exchange of components between phases [363–365]. The model introduces an effective interface permeability, an important parameter [366], which can be calibrated, for instance, by matching with calculations at smaller scale with physical interface width [367]. Alternative methods include using a relaxation equation for the partition coefficient [368], or prescribing interface conditions through thermodynamic extremal principle [369]. Recently, a pragmatic approach was also proposed that consists in modifying the conventional anti-trapping current term [218], performing a thin-interface asymptotic analysis on the resulting equations, and calibrating the parame-
ters of the modified anti-trapping term to an analytical rapid solidification model, typically using the classical continuous growth model [370, 371].

5.5. Coupling microstructure evolution with micromechanics

Another important area of development is the application of PF models to simulate the microstructural changes associated with thermo-mechanical processing, such as grain fragmentation and recrystallization taking place by the combination of temperature and mechanical stresses. Coupling of PF models of microstructure evolution with finite element of FFT solvers for the mechanical deformation appears as a most promising route to allow the “virtual processing” and “virtual design” of novel microstructures with optimized properties for specific applications. This coupling requires a careful analysis of the differences in the time scales associated with the microstructure evolution and the application of the mechanical stresses. Particularly interesting approaches to achieve these goals have been developed by coupling crystal plasticity and PF models [185, 186, 206, 208, 372, 375].

5.6. Multiscale strategies and “upscaling”

From the mesoscale upwards, the PF method operates at the ideal length scale to simulate microstructural representative volume elements (RVE) for bridging with models at higher length scales. Upscaling strategies include, for instance: direct calculation of physical parameters (e.g. specific interface areas [376] and permeability [377, 378] of dendritic arrays); benchmarking to calibrate numerical parameters for coarse-scale models (e.g. applied to columnar growth competition with a cellular automaton [379]); and RVE sampling and statistical analysis (e.g. applied to the precipitation and growth of δ′ precipitates in Al-Li alloys [380]).

5.7. Computational benchmarks

The development of standard benchmark problems has emerged as a pressing matter throughout the PF community as PF modeling has become a standard computational engineering tool. This is important in order to not only test computational efficiency, but also guarantee the accuracy and reproducibility of simulations [381, 385].
5.8. Perspectives and novel applications

The generality and ease of implementation of the phase-field method makes it an ideal tool for simulations of microstructure formation and evolution at the “mesoscale”. Its applications go much further than those highlighted in this short review. It is expected that the PF method will play an important role into linking length and time scales in the simulation of advanced manufacturing, such as in additive manufacturing processes of metals (e.g. [21, 22, 386–388]), or microstructure evolution in new classes of materials (e.g. metallic foams [389, 390]). The PF method also provides an outstanding tool to predict and control the development of micro-/nano-patterned materials, such as nano-templated eutectics [391] or ice-templated structures [392] for instance used in biomedical applications [393] or manufacturing of magnetic composites [394]. Furthermore, phase-field simulations can help understanding the formation of complex hierarchical biomaterials with outstanding properties [395] (e.g. mollusk shells [396, 397]). In conclusion, in spite of intrinsic scale limitations and remaining fundamental challenges, phase-field models should most certainly play a central role in future discovery and design of innovative materials with outstanding properties for both structural and functional applications.

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References

[1] S. Nemat-Nasser, M. Hori, Micromechanics: Overall Properties of Heterogeneous Materials, North-Holland, 1999.

[2] J. Segurado, R. A. Lebensohn, J. LLorca, Computational homogenization of polycrystals, Advances in Applied Mechanics 51 (2018) 1 – 114.
[3] L.-Q. Chen, Y. Wang, The continuum field approach to modeling microstructural evolution, Jom 48 (12) (1996) 13–18.

[4] L.-Q. Chen, Phase-field models for microstructure evolution, Annual review of materials research 32 (1) (2002) 113–140.

[5] N. Moelans, B. Blanpain, P. Wollants, An introduction to phase-field modeling of microstructure evolution, Calphad 32 (2) (2008) 268–294.

[6] R. Qin, H. Bhadeshia, Phase field method, Materials science and technology 26 (7) (2010) 803–811.

[7] M. Ode, S. G. Kim, T. Suzuki, Recent advances in the phase-field model for solidification, ISIJ international 41 (10) (2001) 1076–1082.

[8] W. J. Boettinger, J. A. Warren, C. Beckermann, A. Karma, Phase-field simulation of solidification, Annual review of materials research 32 (1) (2002) 163–194.

[9] A. Karma, Phase-field models of microstructural pattern formation, Thermodyn. Microstruct. Plast. NATO Sci. Ser. II Math. Phys. Chem 108 (2003) 65–89.

[10] I. Singer-Loginova, H. Singer, The phase field technique for modeling multiphase materials, Reports on progress in physics 71 (10) (2008) 106501.

[11] I. Steinbach, Phase-field models in materials science, Modelling and simulation in materials science and engineering 17 (7) (2009) 073001.

[12] I. Steinbach, Phase-field model for microstructure evolution at the mesoscopic scale, Annual Review of Materials Research 43 (2013) 89–107.

[13] M. Plapp, Phase-field modelling of solidification microstructures, Journal of the Indian Institute of Science 96 (3) (2016) 179–198.

[14] N. Provatas, K. Elder, Phase-field methods in materials science and engineering, John Wiley & Sons, 2011.
[15] C.-H. Chen, E. Bouchbinder, A. Karma, Instability in dynamic fracture and the failure of the classical theory of cracks, Nature Physics 13 (12) (2017) 1186–1190.

[16] Y. Lubomirsky, C.-H. Chen, A. Karma, E. Bouchbinder, Universality and stability phase diagram of two-dimensional brittle fracture, Physical review letters 121 (13) (2018) 134301.

[17] A. Mesgarnejad, A. Karma, Vulnerable window of yield strength for swelling-driven fracture of phase-transforming battery materials, npj Computational Materials 6 (1) (2020) 1–10.

[18] A. Emdadi, M. A. Zaeem, Phase-field modeling of crack propagation in polycrystalline materials, Computational Materials Science 186 (2021) 110057.

[19] P.-A. Geslin, I. McCue, B. Gaskey, J. Erlebacher, A. Karma, Topology-generating interfacial pattern formation during liquid metal dealloying, Nature communications 6 (1) (2015) 1–8.

[20] I. McCue, B. Gaskey, P.-A. Geslin, A. Karma, J. Erlebacher, Kinetics and morphological evolution of liquid metal dealloying, Acta Materialia 115 (2016) 10–23.

[21] F. Abdeljawad, D. S. Bolintineanu, A. Cook, H. Brown-Shaklee, C. DiAntonio, D. Kammler, A. Roach, Sintering processes in direct ink write additive manufacturing: A mesoscopic modeling approach, Acta Materialia 169 (2019) 60–75.

[22] Y. Yang, O. Ragnvaldsen, Y. Bai, M. Yi, B.-X. Xu, 3d non-isothermal phase-field simulation of microstructure evolution during selective laser sintering, npj Computational Materials 5 (1) (2019) 1–12.

[23] Y. Yang, T. D. Oyedeji, P. Kühn, B.-X. Xu, Investigation on temperature-gradient-driven effects in unconventional sintering via non-isothermal phase-field simulation, Scripta Materialia 186 (2020) 152–157.

[24] M. R. Tonks, L. K. Aagesen, The phase field method: Mesoscale simulation aiding material discovery, Annual Review of Materials Research 49 (2019) 79–102.
[25] J. W. Cahn, J. E. Hilliard, Free energy of a nonuniform system. i. interfacial free energy, The Journal of chemical physics 28 (2) (1958) 258–267.

[26] J. W. Cahn, J. E. Hilliard, Free energy of a nonuniform system. iii. nucleation in a two-component incompressible fluid, The Journal of chemical physics 31 (3) (1959) 688–699.

[27] J. W. Cahn, On spinodal decomposition, Acta metallurgica 9 (9) (1961) 795–801.

[28] J. Cahn, S. Allen, A microscopic theory for domain wall motion and its experimental verification in fe-al alloy domain growth kinetics, Le Journal de Physique Colloques 38 (C7) (1977) C7–51.

[29] S. M. Allen, J. W. Cahn, A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening, Acta metallurgica 27 (6) (1979) 1085–1095.

[30] A. Khachaturyan, Microscopic theory of diffusion in crystalline solid solutions and time evolution of diffuse scattering of x-rays and thermal neutrons, Soviet Physics Solid State, USSR 9 (9) (1968) 2040.

[31] A. G. Khachaturyan, Theory of structural transformations in solids, Wiley, 1983.

[32] L.-Q. Chen, A. Khachaturyan, Computer simulation of structural transformations during precipitation of an ordered intermetallic phase, Acta metallurgica et materialia 39 (11) (1991) 2533–2551.

[33] Y. Wang, L.-Q. Chen, A. Khachaturyan, Kinetics of strain-induced morphological transformation in cubic alloys with a miscibility gap, Acta Metallurgica et Materialia 41 (1) (1993) 279–296.

[34] A. A. Wheeler, W. J. Boettinger, G. B. McFadden, Phase-field model of solute trapping during solidification, Physical Review E 47 (3) (1993) 1893.

[35] S. Hu, L. Chen, Solute segregation and coherent nucleation and growth near a dislocation—a phase-field model integrating defect and phase microstructures, Acta materialia 49 (3) (2001) 463–472.
[36] Y. Wang, Y. Jin, A. Cuitino, A. Khachaturyan, Phase field microelasticity theory and modeling of multiple dislocation dynamics, Applied Physics Letters 78 (2001) 2324–2326.

[37] D. Rodney, Y. Le Bouar, A. Finel, Phase field methods and dislocations, Acta materialia 51 (1) (2003) 17–30.

[38] Y. Wang, J. Li, Phase field modeling of defects and deformation, Acta Materialia 58 (4) (2010) 1212–1235.

[39] I. Beyerlein, A. Hunter, Understanding dislocation mechanics at the mesoscale using phase field dislocation dynamics, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 374 (2066) (2016) 20150166.

[40] A. Hunter, B. Leu, I. J. Beyerlein, A review of slip transfer: applications of mesoscale techniques, Journal of materials science 53 (8) (2018) 5584–5603.

[41] X. Guo, S.-Q. Shi, X. Ma, Elastoplastic phase field model for microstructure evolution, Applied Physics Letters 87 (22) (2005) 221910.

[42] N. Zhou, C. Shen, M. Mills, Y. Wang, Contributions from elastic inhomogeneity and from plasticity to $\gamma'$ rafting in single-crystal ni–al, Acta Materialia 56 (20) (2008) 6156–6173.

[43] K. Ammar, B. Appolaire, G. Cailletaud, S. Forest, Combining phase field approach and homogenization methods for modelling phase transformation in elastoplastic media, European Journal of Computational Mechanics/Revue Européenne de Mécanique Numérique 18 (5-6) (2009) 485–523.

[44] A. Gaubert, Y. Le Bouar, A. Finel, Coupling phase field and viscoplasticity to study rafting in ni-based superalloys, Philosophical Magazine 90 (1-4) (2010) 375–404.

[45] K. Ammar, B. Appolaire, G. Cailletaud, S. Forest, Phase field modeling of elasto-plastic deformation induced by diffusion controlled growth of a misfitting spherical precipitate, Philosophical magazine letters 91 (3) (2011) 164–172.
[46] P. Shanthraj, L. Sharma, B. Svendsen, F. Roters, D. Raabe, A phase field model for damage in elasto-viscoplastic materials, Computer Methods in Applied Mechanics and Engineering 312 (2016) 167–185.

[47] D. Li, L. Chen, Shape of a rhombohedral coherent ti11ni14 precipitate in a cubic matrix and its growth and dissolution during constrained aging, Acta materialia 45 (6) (1997) 2435–2442.

[48] Y. Wang, D. Banerjee, C. Su, A. Khachaturyan, Field kinetic model and computer simulation of precipitation of l12 ordered intermetallics from fcc solid solution, Acta materialia 46 (9) (1998) 2983–3001.

[49] J. Zhu, T. Wang, A. Ardell, S. Zhou, Z. Liu, L. Chen, Three-dimensional phase-field simulations of coarsening kinetics of $\gamma'$ particles in binary ni–al alloys, Acta materialia 52 (9) (2004) 2837–2845.

[50] T. Wang, G. Sheng, Z.-K. Liu, L.-Q. Chen, Coarsening kinetics of $\gamma'$ precipitates in the ni–al–mo system, Acta Materialia 56 (19) (2008) 5544–5551.

[51] B. S. Fromm, K. Chang, D. L. McDowell, L.-Q. Chen, H. Garmestani, Linking phase-field and finite-element modeling for process–structure–property relations of a ni-base superalloy, Acta materialia 60 (17) (2012) 5984–5999.

[52] Y. Wen, B. Wang, J. Simmons, Y. Wang, A phase-field model for heat treatment applications in ni-based alloys, Acta materialia 54 (8) (2006) 2087–2099.

[53] V. Vorontsov, C. Shen, Y. Wang, D. Dye, C. Rae, Shearing of $\gamma'$ precipitates by a $\{112\}c$ dislocation ribbons in ni-base superalloys: A phase field approach, Acta Materialia 58 (12) (2010) 4110–4119.

[54] N. Zhou, C. Shen, M. J. Mills, J. Li, Y. Wang, Modeling displacive–diffusional coupled dislocation shearing of $\gamma'$ precipitates in ni-base superalloys, Acta Materialia 59 (9) (2011) 3484–3497.

[55] N. Zhou, C. Shen, M. Mills, Y. Wang, Phase field modeling of channel dislocation activity and $\gamma'$ rafting in single crystal ni–al, Acta Materialia 55 (16) (2007) 5369–5381.
[56] N. Zhou, C. Shen, M. Mills, Y. Wang, Large-scale three-dimensional phase field simulation of γ’-rafting and creep deformation, Philosophical Magazine 90 (1-4) (2010) 405–436.

[57] G. Boussinot, A. Finel, Y. Le Bouar, Phase-field modeling of bimodal microstructures in nickel-based superalloys, Acta Materialia 57 (3) (2009) 921–931.

[58] M. Cottura, Y. Le Bouar, A. Finel, B. Appolaire, K. Ammar, S. Forest, A phase field model incorporating strain gradient viscoplasticity: application to rafting in ni-base superalloys, Journal of the Mechanics and Physics of Solids 60 (7) (2012) 1243–1256.

[59] M. Cottura, B. Appolaire, A. Finel, Y. Le Bouar, Coupling the phase field method for diffusive transformations with dislocation density-based crystal plasticity: Application to ni-based superalloys, Journal of the Mechanics and Physics of Solids 94 (2016) 473–489.

[60] M. Degeiter, Y. Le Bouar, B. Appolaire, M. Perrut, A. Finel, Instabilities in the periodic arrangement of elastically interacting precipitates in nickel-base superalloys, Acta Materialia 187 (2020) 41–50.

[61] J. Boisse, N. Lecoq, R. Patte, H. Zapolsky, Phase-field simulation of coarsening of γ precipitates in an ordered γ’ matrix, Acta Materialia 55 (18) (2007) 6151–6158.

[62] M. A. Ali, J. V. Görler, I. Steinbach, Role of coherency loss on rafting behavior of ni-based superalloys, Computational Materials Science 171 (2020) 109279.

[63] M. A. Ali, W. Amin, O. Shchyglo, I. Steinbach, 45-degree rafting in ni-based superalloys: A combined phase-field and strain gradient crystal plasticity study, International Journal of Plasticity (2020) 102659.

[64] R. Mohanty, A. Leon, Y. Sohn, Phase-field simulation of interdiffusion microstructure containing fcc-γ and l12-γ’ phases in ni–al diffusion couples, Computational materials science 43 (2) (2008) 301–308.

[65] T. Kitashima, H. Harada, A new phase-field method for simulating γ’ precipitation in multicomponent nickel-base superalloys, Acta Materialia 57 (6) (2009) 2020–2028.
[66] V. Vorontsov, R. Voskoboinikov, C. Rae, Shearing of $\gamma'$ precipitates in ni-base superalloys: a phase field study incorporating the effective $\gamma$-surface, Philosophical Magazine 92 (5) (2012) 608–634.

[67] J. Kundin, L. Mushongera, T. Goehler, H. Emmerich, Phase-field modeling of the $\gamma'$-coarsening behavior in ni-based superalloys, Acta materialia 60 (9) (2012) 3758–3772.

[68] R. Shi, Y. Wang, Variant selection during $\alpha$ precipitation in ti–6al–4v under the influence of local stress—a simulation study, Acta materialia 61 (16) (2013) 6006–6024.

[69] A. Boyne, D. Wang, R. Shi, Y. Zheng, A. Behera, S. Nag, J. Tiley, H. Fraser, R. Banerjee, Y. Wang, Pseudospinodal mechanism for fine $\alpha/\beta$ microstructures in $\beta$-ti alloys, Acta materialia 64 (2014) 188–197.

[70] R. Shi, N. Zhou, S. Niezgoda, Y. Wang, Microstructure and transformation texture evolution during $\alpha$ precipitation in polycrystalline $\alpha/\beta$ titanium alloys—a simulation study, Acta Materialia 94 (2015) 224–243.

[71] D. Qiu, R. Shi, D. Zhang, W. Lu, Y. Wang, Variant selection by dislocations during $\alpha$ precipitation in $\alpha/\beta$ titanium alloys, Acta Materialia 88 (2015) 218–231.

[72] D. Qiu, R. Shi, P. Zhao, D. Zhang, W. Lu, Y. Wang, Effect of low-angle grain boundaries on morphology and variant selection of grain boundary allotriomorphs and widmanstätten side-plates, Acta Materialia 112 (2016) 347–360.

[73] R. Shi, D. P. McAllister, N. Zhou, A. J. Detor, R. DiDomizio, M. J. Mills, Y. Wang, Growth behavior of $\gamma'/\gamma''$ coprecipitates in ni-base superalloys, Acta Materialia 164 (2019) 220–236.

[74] J. D. C. Teixeira, B. Appolaire, E. Aeby-Gautier, S. Denis, F. Bruneau, Modeling of the effect of the $\beta$ phase deformation on the $\alpha$ phase precipitation in near-$\beta$ titanium alloys, Acta materialia 54 (16) (2006) 4261–4271.

[75] J. D. C. Teixeira, B. Appolaire, E. Aeby-Gautier, S. Denis, G. Cailletaud, N. Späth, Transformation kinetics and microstructures of ti17
titanium alloy during continuous cooling, Materials Science and Engineering: A 448 (1-2) (2007) 135–145.

[76] D. Li, L. Chen, Computer simulation of stress-oriented nucleation and growth of $\theta'$ precipitates in Al–Cu alloys, Acta Materialia 46 (8) (1998) 2573–2585.

[77] V. Vaithyanathan, C. Wolverton, L. Chen, Multiscale modeling of precipitate microstructure evolution, Physical review letters 88 (12) (2002) 125503.

[78] V. Vaithyanathan, C. Wolverton, L. Chen, Multiscale modeling of $\theta'$ precipitation in Al–Cu binary alloys, Acta Materialia 52 (10) (2004) 2973–2987.

[79] Y. Ji, B. Ghaffari, M. Li, L.-Q. Chen, Phase-field modeling of $\theta'$ precipitation kinetics in 319 aluminum alloys, Computational Materials Science 151 (2018) 84–94.

[80] H. Liu, B. Bellón, J. Llorca, Multiscale modelling of the morphology and spatial distribution of $\theta'$ precipitates in Al–Cu alloys, Acta Materialia 132 (2017) 611–626.

[81] A. Rodríguez-Veiga, B. Bellón, I. Papadimitriou, G. Esteban-Manzanares, I. Sabirov, J. Llorca, A multidisciplinary approach to study precipitation kinetics and hardening in an Al-4Cu (wt.%) alloy, Journal of Alloys and Compounds 757 (2018) 504–519.

[82] G. Esteban-Manzanares, A. Ma, I. Papadimitriou, E. Martínez, J. Llorca, Basal dislocation/precipitate interactions in Mg-Al alloys: an atomistic investigation, Modelling and Simulation in Materials Science and Engineering 27 (2019) 075003.

[83] K. Kim, A. Roy, M. Gururajan, C. Wolverton, P. W. Voorhees, First-principles/phase-field modeling of $\theta'$ precipitation in Al-Cu alloys, Acta Materialia 140 (2017) 344–354.

[84] H. Liu, Y. Gao, L. Qi, Y. Wang, J.-F. Nie, Phase-field simulation of Orowan strengthening by coherent precipitate plates in an aluminum alloy, Metallurgical and Materials Transactions A 46 (7) (2015) 3287–3301.
[85] H. Liu, I. Papadimitriou, F. Lin, J. LLorca, Precipitation during high temperature aging of al- cu alloys: A multiscale analysis based on first principles calculations, Acta Materialia 167 (2019) 121–135.

[86] Y. Gao, H. Liu, R. Shi, N. Zhou, Z. Xu, Y. Zhu, J. Nie, Y. Wang, Simulation study of precipitation in an mg–y–nd alloy, Acta Materialia 60 (12) (2012) 4819 – 4832.

[87] Y. Ji, A. Issa, T. Heo, J. Saal, C. Wolverton, L.-Q. Chen, Predicting $\beta'$ precipitate morphology and evolution in mg–re alloys using a combination of first-principles calculations and phase-field modeling, Acta materialia 76 (2014) 259–271.

[88] H. Liu, Y. Gao, J. Liu, Y. Zhu, Y. Wang, J. Nie, A simulation study of the shape of $\beta'$ precipitates in mg–y and mg–gd alloys, Acta Materialia 61 (2) (2013) 453 – 466.

[89] H. Liu, Y. Zhu, N. Wilson, J. Nie, On the structure and role of $\beta'_f$ in $\beta_1$ precipitation in mg–nd alloys, Acta Materialia 133 (2017) 408–426.

[90] H. Liu, W. Xu, N. Wilson, L. Peng, J. Nie, Formation of and interaction between $\beta'_f$ and $\beta'$ phases in a mg–gd alloy, Journal of Alloys and Compounds 712 (2017) 334–344.

[91] S. DeWitt, E. L. Solomon, A. R. Natarajan, V. Araullo-Peters, S. Rudraraju, L. K. Aagesen, B. Puchala, E. A. Marquis, A. Van Der Ven, K. Thornton, et al., Misfit-driven $\beta''''$ precipitate composition and morphology in mg-nd alloys, Acta Materialia 136 (2017) 378–389.

[92] H. Liu, Y. Gao, Z. Xu, Y. Zhu, Y. Wang, J. Nie, Guided self-assembly of nano-precipitates into mesocrystals, Scientific reports 5 (2015) 16530.

[93] H. Liu, W. Xu, L. Peng, W. Ding, J. Nie, A simulation study of the distribution of $\beta'$ precipitates in a crept mg-gd-zr alloy, Computational Materials Science 130 (2017) 152–164.

[94] G. Han, Z. Han, A. A. Luo, A. K. Sachdev, B. Liu, A phase field model for simulating the precipitation of multi-variant $\beta$-mg17al12 in mg–al-based alloys, Scripta Materialia 68 (9) (2013) 691–694.
[95] G. Han, Z. Han, A. A. Luo, B. Liu, Three-dimensional phase-field simulation and experimental validation of $\beta$-mg 17 al 12 phase precipitation in mg-al-based alloys, Metallurgical and Materials Transactions A 46 (2) (2015) 948–962.

[96] Z. Han, G. Han, A. A. Luo, B. Liu, Large-scale three-dimensional phase-field simulation of multi-variant $\beta$-mg17al12 in mg–al-based alloys, Computational Materials Science 101 (2015) 248–254.

[97] I. Polmear, D. StJohn, J.-F. Nie, M. Qian, Light alloys: metallurgy of the light metals, Butterworth-Heinemann, 2017.

[98] G. Barsch, J. Krumhansl, Twin boundaries in ferroelastic media without interface dislocations, Physical Review Letters 53 (11) (1984) 1069.

[99] A. Saxena, Y. Wu, T. Lookman, S. Shenoy, A. Bishop, Hierarchical pattern formation in elastic materials, Physica A: Statistical Mechanics and its Applications 239 (1-3) (1997) 18–34.

[100] S. Shenoy, T. Lookman, A. Saxena, A. Bishop, Martensitic textures: Multiscale consequences of elastic compatibility, Physical Review B 60 (18) (1999) R12537.

[101] R. Ahluwalia, T. Lookman, A. Saxena, Elastic deformation of polycrystals, Physical review letters 91 (5) (2003) 055501.

[102] T. Lookman, S. Shenoy, K. Rasmussen, A. Saxena, A. Bishop, Ferroelastic dynamics and strain compatibility, Physical Review B 67 (2) (2003) 024114.

[103] R. Ahluwalia, T. Lookman, A. Saxena, R. C. Albers, Landau theory for shape memory polycrystals, Acta Materialia 52 (1) (2004) 209–218.

[104] Y. Wang, A. Khachaturyan, Three-dimensional field model and computer modeling of martensitic transformations, Acta materialia 45 (2) (1997) 759–773.

[105] A. Artemev, Y. Jin, A. Khachaturyan, Three-dimensional phase field model of proper martensitic transformation, Acta materialia 49 (7) (2001) 1165–1177.
[106] A. Artemev, Y. Jin, A. Khachaturyan, Three-dimensional phase field model and simulation of cubic$\rightarrow$tetragonal martensitic transformation in polycrystals, Philosophical Magazine A 82 (6) (2002) 1249–1270.

[107] Y. U. Wang, Y. M. Jin, A. G. Khachaturyan, The effects of free surfaces on martensite microstructures: 3d phase field microelasticity simulation study, Acta Materialia 52 (4) (2004) 1039–1050.

[108] D. Fan, L.-Q. Chen, Computer simulation of twin formation during the displacive $c \rightarrow t'$ phase transformation in the zirconia-yttria system, Journal of the American Ceramic Society 78 (3) (1995) 769–773.

[109] Y. Wen, Y. Wang, L.-Q. Chen, Effect of elastic interaction on the formation of a complex multi-domain microstructural pattern during a coherent hexagonal to orthorhombic transformation, Acta materialia 47 (17) (1999) 4375–4386.

[110] Y. Gao, N. Zhou, F. Yang, Y. Cui, L. Kovarik, N. Hatcher, R. Noebe, M. Mills, Y. Wang, P-phase precipitation and its effect on martensitic transformation in (ni, pt) ti shape memory alloys, Acta Materialia 60 (4) (2012) 1514–1527.

[111] Y. Gao, N. Zhou, D. Wang, Y. Wang, Pattern formation during cubic to orthorhombic martensitic transformations in shape memory alloys, Acta materialia 68 (2014) 93–105.

[112] J. Zhu, Y. Gao, D. Wang, T.-Y. Zhang, Y. Wang, Taming martensitic transformation via concentration modulation at nanoscale, Acta Materialia 130 (2017) 196–207.

[113] Y. Wang, A. G. Khachaturyan, Multi-scale phase field approach to martensitic transformations, Materials Science and Engineering: A 438 (2006) 55–63.

[114] P. Zhao, C. Shen, J. Li, Y. Wang, Effect of nonlinear and noncollinear transformation strain pathways in phase-field modeling of nucleation and growth during martensite transformation, npj Computational Materials 3 (1) (2017) 1–10.
[115] G. Xu, C. Wang, J. I. Beltrán, J. LLorca, Y. Cui, Landau modeling of dynamical nucleation of martensite at grain boundaries under local stress, Computational Materials Science 118 (2016) 103–111.

[116] W. Zhang, Y. Jin, A. Khachaturyan, Modelling of dislocation-induced martensitic transformation in anisotropic crystals, Philosophical Magazine 87 (10) (2007) 1545–1563.

[117] J. Zhu, H. Wu, D. Wang, Y. Gao, H. Wang, Y. Hao, R. Yang, T.-Y. Zhang, Y. Wang, Crystallographic analysis and phase field simulation of transformation plasticity in a multifunctional $\beta$-ti alloy, International Journal of Plasticity 89 (2017) 110–129.

[118] V. I. Levitas, D. L. Preston, Three-dimensional landau theory for multivariant stress-induced martensitic phase transformations. ii. multivariant phase transformations and stress space analysis, Physical review B 66 (13) (2002) 134207.

[119] V. I. Levitas, M. Javanbakht, Surface-induced phase transformations: multiple scale and mechanics effects and morphological transitions, Physical review letters 107 (17) (2011) 175701.

[120] Y.-W. Cui, T. Koyama, I. Ohnuma, K. Oikawa, R. Kainuma, K. Ishida, Simulation of hexagonal–orthorhombic phase transformation in polycrystals, Acta materialia 55 (1) (2007) 233–241.

[121] O. Shchyglo, U. Salman, A. Finel, Martensitic phase transformations in $\text{Ni}-\text{Ti}$-based shape memory alloys: The landau theory, Acta materialia 60 (19) (2012) 6784–6792.

[122] O. Shchyglo, G. Du, J. K. Engels, I. Steinbach, Phase-field simulation of martensite microstructure in low-carbon steel, Acta Materialia 175 (2019) 415–425.

[123] A. Yamanaka, T. Takaki, Y. Tomita, Elastoplastic phase-field simulation of self-and plastic accommodations in cubic→tetragonal martensitic transformation, Materials Science and Engineering: A 491 (1-2) (2008) 378–384.
[124] A. Yamanaka, T. Takaki, Y. Tomita, Elastoplastic phase-field simulation of martensitic transformation with plastic deformation in polycrystal, International journal of mechanical sciences 52 (2) (2010) 245–250.

[125] H. K. Yeddu, A. Malik, J. Ågren, G. Amberg, A. Borgenstam, Three-dimensional phase-field modeling of martensitic microstructure evolution in steels, Acta materialia 60 (4) (2012) 1538–1547.

[126] A. Malik, H. K. Yeddu, G. Amberg, A. Borgenstam, J. Ågren, Three dimensional elasto-plastic phase field simulation of martensitic transformation in polycrystal, Materials Science and Engineering: A 556 (2012) 221–232.

[127] M. Mamivand, M. A. Zaeem, H. El Kadiri, A review on phase field modeling of martensitic phase transformation, Computational Materials Science 77 (2013) 304–311.

[128] D. Wang, Q. Liang, S. Zhao, P. Zhao, T. Zhang, L. Cui, Y. Wang, Phase field simulation of martensitic transformation in pre-strained nanocomposite shape memory alloys, Acta Materialia 164 (2019) 99–109.

[129] M. Mamivand, M. A. Zaeem, H. El Kadiri, L.-Q. Chen, Phase field modeling of the tetragonal-to-monoclinic phase transformation in zirconia, Acta Materialia 61 (14) (2013) 5223–5235.

[130] M. Mamivand, M. A. Zaeem, H. El Kadiri, Phase field modeling of stress-induced tetragonal-to-monoclinic transformation in zirconia and its effect on transformation toughening, Acta materialia 64 (2014) 208–219.

[131] C. Cissé, M. A. Zaeem, A phase-field model for non-isothermal phase transformation and plasticity in polycrystalline yttria-stabilized tetragonal zirconia, Acta Materialia 191 (2020) 111 – 123.

[132] H. Atkinson, Overview no. 65: Theories of normal grain growth in pure single phase systems, Acta Metallurgica 36 (3) (1988) 469–491.

[133] F. J. Humphreys, M. Hatherly, Recrystallization and related annealing phenomena, Elsevier, 2012.
[134] G. S. Rohrer, Grain boundary energy anisotropy: a review, Journal of materials science 46 (18) (2011) 5881–5895.

[135] S. Ratanaphan, D. L. Olmsted, V. V. Bulatov, E. A. Holm, A. D. Rollett, G. S. Rohrer, Grain boundary energies in body-centered cubic metals, Acta Materialia 88 (2015) 346–354.

[136] A. Rollett, G. Gottstein, L. Shvindlerman, D. Molodov, Grain boundary mobility—a brief review, Zeitschrift für Metallkunde 95 (4) (2004) 226–229.

[137] G. Gottstein, D. Molodov, L. Shvindlerman, D. Srolovitz, M. Winning, Grain boundary migration: misorientation dependence, Current opinion in solid state and materials science 5 (1) (2001) 9–14.

[138] G. Gottstein, L. S. Shvindlerman, Grain boundary migration in metals: thermodynamics, kinetics, applications, CRC press, 2009.

[139] L.-Q. Chen, W. Yang, Computer simulation of the domain dynamics of a quenched system with a large number of nonconserved order parameters: The grain-growth kinetics, Physical Review B 50 (21) (1994) 15752.

[140] D. Fan, L.-Q. Chen, Computer simulation of grain growth using a continuum field model, Acta Materialia 45 (2) (1997) 611–622.

[141] D. Fan, C. Geng, L.-Q. Chen, Computer simulation of topological evolution in 2-d grain growth using a continuum diffuse-interface field model, Acta materialia 45 (3) (1997) 1115–1126.

[142] C. Krill iii, L.-Q. Chen, Computer simulation of 3-d grain growth using a phase-field model, Acta materialia 50 (12) (2002) 3059–3075.

[143] I. Steinbach, F. Pezzolla, B. Nestler, M. Seeßelberg, R. Prieler, G. J. Schmitz, J. L. Rezende, A phase field concept for multiphase systems, Physica D: Nonlinear Phenomena 94 (3) (1996) 135–147.

[144] R. Kobayashi, J. A. Warren, W. C. Carter, Vector-valued phase field model for crystallization and grain boundary formation, Physica D: Nonlinear Phenomena 119 (3-4) (1998) 415–423.
[145] M. T. Lusk, A phase–field paradigm for grain growth and recrystallization, Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences 455 (1982) (1999) 677–700.

[146] S. G. Kim, D. I. Kim, W. T. Kim, Y. B. Park, Computer simulations of two-dimensional and three-dimensional ideal grain growth, Physical Review E 74 (6) (2006) 061605.

[147] Y. Suwa, Y. Saito, H. Onodera, Parallel computer simulation of three-dimensional grain growth using the multi-phase-field model, Materials transactions (2008) 0802180338–0802180338.

[148] R. D. Kamachali, I. Steinbach, 3-d phase-field simulation of grain growth: Topological analysis versus mean-field approximations, Acta Materialia 60 (6-7) (2012) 2719–2728.

[149] R. D. Kamachali, A. Abbondandolo, K. Siburg, I. Steinbach, Geometrical grounds of mean field solutions for normal grain growth, Acta Materialia 90 (2015) 252–258.

[150] V. Yadav, N. Moelans, Investigation on the existence of a ‘hillert regime’in normal grain growth, Scripta Materialia 142 (2018) 148–152.

[151] V. Yadav, N. Moelans, Analysis of grain topology and volumetric growth rate relation in three-dimensional normal grain growth, Acta Materialia 156 (2018) 275–286.

[152] E. Miyoshi, T. Takaki, M. Ohno, Y. Shibuta, S. Sakane, T. Shimokawabe, T. Aoki, Ultra-large-scale phase-field simulation study of ideal grain growth, NPJ Computational Materials 3 (1) (2017) 1–6.

[153] L.-Q. Chen, D. Fan, Computer simulation model for coupled grain growth and ostwald ripening—application to al2o3-zro2 two-phase systems, Journal of the American Ceramic Society 79 (5) (1996) 1163–1168.

[154] D. Fan, L.-Q. Chen, Diffusion-controlled grain growth in two-phase solids, Acta materialia 45 (8) (1997) 3297–3310.
[155] D. Fan, S. Chen, L.-Q. Chen, P. W. Voorhees, Phase-field simulation of 2-d ostwald ripening in the high volume fraction regime, Acta Materialia 50 (8) (2002) 1895–1907.

[156] S. O. Poulsen, P. W. Voorhees, E. M. Lauridsen, Three-dimensional simulations of microstructural evolution in polycrystalline dual-phase materials with constant volume fractions, Acta materialia 61 (4) (2013) 1220–1228.

[157] V. Yadav, L. Vanherpe, N. Moelans, Effect of volume fractions on microstructure evolution in isotropic volume-conserved two-phase alloys: A phase-field study, Computational Materials Science 125 (2016) 297–308.

[158] H. Ravash, J. Vleugels, N. Moelans, Three-dimensional phase-field simulation of microstructural evolution in three-phase materials with different diffusivities, Journal of materials science 49 (20) (2014) 7066–7072.

[159] H. Ravash, J. Vleugels, N. Moelans, Three-dimensional phase-field simulation of microstructural evolution in three-phase materials with different interfacial energies and different diffusivities, Journal of Materials Science 52 (24) (2017) 13852–13867.

[160] A. Kazaryan, Y. Wang, S. Dregia, B. R. Patton, Generalized phase-field model for computer simulation of grain growth in anisotropic systems, Physical Review B 61 (21) (2000) 14275.

[161] A. Kazaryan, Y. Wang, S. Dregia, B. Patton, Grain growth in anisotropic systems: comparison of effects of energy and mobility, Acta Materialia 50 (10) (2002) 2491–2502.

[162] Y. Suwa, Y. Saito, H. Onodera, Three-dimensional phase field simulation of the effect of anisotropy in grain-boundary mobility on growth kinetics and morphology of grain structure, Computational materials science 40 (1) (2007) 40–50.

[163] N. Moelans, B. Blanpain, P. Wollants, Quantitative phase-field approach for simulating grain growth in anisotropic systems with arbitrary inclination and misorientation dependence, Physical review letters 101 (2) (2008) 025502.
[164] M. A. Zaeem, H. El Kadiri, P. T. Wang, M. F. Horstemeyer, Investigating the effects of grain boundary energy anisotropy and second-phase particles on grain growth using a phase-field model, Computational Materials Science 50 (8) (2011) 2488–2492.

[165] H.-K. Kim, S. G. Kim, W. Dong, I. Steinbach, B.-J. Lee, Phase-field modeling for 3d grain growth based on a grain boundary energy database, Modelling and Simulation in Materials Science and Engineering 22 (3) (2014) 034004.

[166] E. Miyoshi, T. Takaki, Validation of a novel higher-order multi-phase-field model for grain-growth simulations using anisotropic grain-boundary properties, Computational Materials Science 112 (2016) 44–51.

[167] E. Miyoshi, T. Takaki, Extended higher-order multi-phase-field model for three-dimensional anisotropic-grain-growth simulations, Computational Materials Science 120 (2016) 77–83.

[168] H. Salama, J. Kundin, O. Shchyglo, V. Mohles, K. Marquardt, I. Steinbach, Role of inclination dependence of grain boundary energy on the microstructure evolution during grain growth, Acta Materialia 188 (2020) 641 – 651.

[169] D. Fan, L.-Q. Chen, S.-P. P. Chen, Numerical simulation of zener pinning with growing second-phase particles, Journal of the American Ceramic Society 81 (3) (1998) 526–532.

[170] K. Chang, W. Feng, L.-Q. Chen, Effect of second-phase particle morphology on grain growth kinetics, Acta Materialia 57 (17) (2009) 5229–5236.

[171] N. Moelans, B. Blanpain, P. Wollants, A phase field model for the simulation of grain growth in materials containing finely dispersed incoherent second-phase particles, Acta Materialia 53 (6) (2005) 1771–1781.

[172] N. Moelans, B. Blanpain, P. Wollants, Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles, Acta Materialia 54 (4) (2006) 1175–1184.
[173] N. Moelans, B. Blanpain, P. Wollants, Pinning effect of second-phase particles on grain growth in polycrystalline films studied by 3-d phase field simulations, Acta Materialia 55 (6) (2007) 2173–2182.

[174] L. Vanherpe, N. Moelans, B. Blanpain, S. Vandewalle, Pinning effect of spheroid second-phase particles on grain growth studied by three-dimensional phase-field simulations, Computational Materials Science 49 (2) (2010) 340–350.

[175] K. Chang, N. Moelans, Phase-field simulations of the interaction between a grain boundary and an evolving second-phase particle, Philosophical Magazine Letters 95 (4) (2015) 202–210.

[176] Y. Suwa, Y. Saito, H. Onodera, Phase field simulation of grain growth in three dimensional system containing finely dispersed second-phase particles, Scripta Materialia 55 (4) (2006) 407–410.

[177] C. Schwarze, R. D. Kamachali, I. Steinbach, Phase-field study of zener drag and pinning of cylindrical particles in polycrystalline materials, Acta Materialia 106 (2016) 59–65.

[178] Y. Suwa, Y. Saito, H. Onodera, Phase-field simulation of abnormal grain growth due to inverse pinning, Acta materialia 55 (20) (2007) 6881–6894.

[179] K.-J. Ko, P.-R. Cha, D. Srolovitz, N.-M. Hwang, Abnormal grain growth induced by sub-boundary-enhanced solid-state wetting: Analysis by phase-field model simulations, Acta Materialia 57 (3) (2009) 838–845.

[180] Y. Liu, M. Militzer, M. Perez, Phase field modelling of abnormal grain growth, Materials 12 (24) (2019) 4048.

[181] T. Takaki, A. Yamanaka, Y. Higa, Y. Tomita, Phase-field model during static recrystallization based on crystal-plasticity theory, Journal of Computer-Aided Materials Design 14 (1) (2007) 75–84.

[182] T. Takaki, Y. Hisakuni, T. Hirochi, A. Yamanaka, Y. Tomita, Multiphase-field simulations for dynamic recrystallization, Computational Materials Science 45 (4) (2009) 881–888.
[183] T. Takaki, C. Yoshimoto, A. Yamanaka, Y. Tomita, Multiscale modeling of hot-working with dynamic recrystallization by coupling microstructure evolution and macroscopic mechanical behavior, International Journal of Plasticity 52 (2014) 105–116.

[184] N. Moelans, A. Godfrey, Y. Zhang, D. J. Jensen, Phase-field simulation study of the migration of recrystallization boundaries, Physical Review B 88 (5) (2013) 054103.

[185] G. Abrivard, E. P. Busso, S. Forest, B. Appolaire, Phase field modelling of grain boundary motion driven by curvature and stored energy gradients. part i: theory and numerical implementation, Philosophical magazine 92 (28-30) (2012) 3618–3642.

[186] G. Abrivard, E. P. Busso, S. Forest, B. Appolaire, Phase field modelling of grain boundary motion driven by curvature and stored energy gradients. part ii: application to recrystallisation, Philosophical magazine 92 (28-30) (2012) 3643–3664.

[187] J. Zhang, W. Ludwig, Y. Zhang, H. H. B. Sørensen, D. J. Rowenhorst, A. Yamanaka, P. W. Voorhees, H. F. Poulsen, Grain boundary mobilities in polycrystals, Acta Materialia 191 (2020) 211 – 220.

[188] J. Zhang, S. O. Poulsen, J. W. Gibbs, P. W. Voorhees, H. F. Poulsen, Determining material parameters using phase-field simulations and experiments, Acta Materialia 129 (2017) 229–238.

[189] K. G. Janssens, D. Olmsted, E. A. Holm, S. M. Foiles, S. J. Plimpton, P. M. Derlet, Computing the mobility of grain boundaries, Nature materials 5 (2) (2006) 124–127.

[190] D. L. Olmsted, E. A. Holm, S. M. Foiles, Survey of computed grain boundary properties in face-centered cubic metals—ii: Grain boundary mobility, Acta materialia 57 (13) (2009) 3704–3713.

[191] J. W. Christian, S. Mahajan, Deformation twinning, Progress in materials science 39 (1-2) (1995) 1–157.

[192] R. Lebensohn, C. Tomé, A study of the stress state associated with twin nucleation and propagation in anisotropic materials, Philosophical Magazine A 67 (1) (1993) 187–206.
[193] M. Chen, E. Ma, K. J. Hemker, H. Sheng, Y. Wang, X. Cheng, Deformation twinning in nanocrystalline aluminum, Science 300 (5623) (2003) 1275–1277.

[194] V. Yamakov, D. Wolf, S. Phillpot, A. Mukherjee, H. Gleiter, Deformation-mechanism map for nanocrystalline metals by molecular-dynamics simulation, Nature materials 3 (1) (2004) 43–47.

[195] X. Wu, X. Liao, S. Srinivasan, F. Zhou, E. Lavernia, R. Valiev, Y. Zhu, New deformation twinning mechanism generates zero macroscopic strain in nanocrystalline metals, Physical review letters 100 (9) (2008) 095701.

[196] Y. Zhu, J. Narayan, J. Hirth, S. Mahajan, X. Wu, X. Liao, Formation of single and multiple deformation twins in nanocrystalline fcc metals, Acta materialia 57 (13) (2009) 3763–3770.

[197] J. F. Nie, Y. Zhu, J. Liu, X.-Y. Fang, Periodic segregation of solute atoms in fully coherent twin boundaries, Science 340 (6135) (2013) 957–960.

[198] S. Hu, C. H. Henager Jr, L. Chen, Simulations of stress-induced twinning and de-twinning: a phase field model, Acta Materialia 58 (19) (2010) 6554–6564.

[199] T. W. Heo, Y. Wang, S. Bhattacharya, X. Sun, S. Hu, L.-Q. Chen, A phase-field model for deformation twinning, Philosophical Magazine Letters 91 (2) (2011) 110–121.

[200] Y. Gu, L.-Q. Chen, T. W. Heo, L. Sandoval, J. Belak, Phase field model of deformation twinning in tantalum: Parameterization via molecular dynamics, Scripta Materialia 68 (7) (2013) 451–454.

[201] T. W. Heo, Y. Wang, L.-Q. Chen, Spinodal twinning of a deformed crystal, Philosophical Magazine 94 (9) (2014) 888–897.

[202] J. D. Clayton, J. Knap, A phase field model of deformation twinning: nonlinear theory and numerical simulations, Physica D: Nonlinear Phenomena 240 (9-10) (2011) 841–858.
[203] J. Clayton, J. Knap, Phase field modeling and simulation of coupled fracture and twinning in single crystals and polycrystals, Computer Methods in Applied Mechanics and Engineering 312 (2016) 447–467.

[204] Z. Pi, Q. Fang, B. Liu, H. Feng, Y. Liu, Y. Liu, P. Wen, A phase field study focuses on the transverse propagation of deformation twinning for hexagonal-closed packed crystals, International Journal of Plasticity 76 (2016) 130–146.

[205] H. Liu, F. Lin, P. Zhao, N. Moelans, Y. Wang, J. Nie, Formation and autocatalytic nucleation of co-zone \{101\} deformation twins in polycrystalline mg: A phase field simulation study, Acta Materialia 153 (2018) 86–107.

[206] R. Kondo, Y. Tadano, K. Shizawa, A phase-field model of twinning and detwinning coupled with dislocation-based crystal plasticity for hcp metals, Computational materials science 95 (2014) 672–683.

[207] C. Liu, P. Shanthraj, M. Diehl, F. Roters, S. Dong, J. Dong, W. Ding, D. Raabe, An integrated crystal plasticity–phase field model for spatially resolved twin nucleation, propagation, and growth in hexagonal materials, International Journal of Plasticity 106 (2018) 203–227.

[208] P. Zhao, T. S. E. Low, Y. Wang, S. R. Niezgoda, Finite strain phase-field microelasticity theory for modeling microstructural evolution, Acta Materialia 191 (2020) 253 – 269.

[209] J. S. Langer, Chance and matter, in: Proc. Les Houches Summer School, Session XLVI, North-Holland Amsterdam, 1987.

[210] R. Kobayashi, A numerical approach to three-dimensional dendritic solidification, Experimental mathematics 3 (1) (1994) 59–81.

[211] G. McFadden, A. Wheeler, R. Braun, S. Coriell, R. Sekerka, Phase-field models for anisotropic interfaces, Physical Review E 48 (3) (1993) 2016.

[212] A. Karma, W.-J. Rappel, Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetics, Physical review E 53 (4) (1996) R3017.
[213] B. Böttger, J. Eiken, I. Steinbach, Phase field simulation of equiaxed solidification in technical alloys, Acta materialia 54 (10) (2006) 2697–2704.

[214] T. Haxhimali, A. Karma, F. Gonzales, M. Rappaz, Orientation selection in dendritic evolution, Nature materials 5 (8) (2006) 660–664.

[215] J. Dantzig, P. Di Napoli, J. Friedli, M. Rappaz, Dendritic growth morphologies in al-zn alloys—part ii: phase-field computations, Metallurgical and Materials Transactions A 44 (12) (2013) 5532–5543.

[216] A. Karma, W.-J. Rappel, Quantitative phase-field modeling of dendritic growth in two and three dimensions, Physical review E 57 (4) (1998) 4323.

[217] B. Echebarria, R. Folch, A. Karma, M. Plapp, Quantitative phase-field model of alloy solidification, Physical Review E 70 (6) (2004) 061604.

[218] A. Karma, Phase-field formulation for quantitative modeling of alloy solidification, Physical Review Letters 87 (11) (2001) 115701.

[219] G. Caginalp, P. Fife, Phase-field methods for interfacial boundaries, Physical Review B 33 (11) (1986) 7792.

[220] G. Caginalp, P. Fife, Higher-order phase field models and detailed anisotropy, Physical review B 34 (7) (1986) 4940.

[221] Z. Bi, R. F. Sekerka, Phase-field model of solidification of a binary alloy, Physica A: Statistical Mechanics and its Applications 261 (1-2) (1998) 95–106.

[222] M. Plapp, Unified derivation of phase-field models for alloy solidification from a grand-potential functional, Physical Review E 84 (3) (2011) 031601.

[223] A. Choudhury, B. Nestler, Grand-potential formulation for multicomponent phase transformations combined with thin-interface asymptotics of the double-obstacle potential, Physical Review E 85 (2) (2012) 021602.
[224] W. L. George, J. A. Warren, A parallel 3d dendritic growth simulator using the phase-field method, Journal of Computational Physics 177 (2) (2002) 264–283.

[225] B. Nestler, A 3d parallel simulator for crystal growth and solidification in complex alloy systems, Journal of Crystal Growth 275 (1-2) (2005) e273–e278.

[226] A. Vondrous, M. Selzer, J. Hötzer, B. Nestler, Parallel computing for phase-field models, The International journal of high performance computing applications 28 (1) (2014) 61–72.

[227] A. Yamanaka, T. Aoki, S. Ogawa, T. Takaki, Gpu-accelerated phase-field simulation of dendritic solidification in a binary alloy, Journal of Crystal Growth 318 (1) (2011) 40–45.

[228] T. Shimokawabe, T. Aoki, T. Takaki, T. Endo, A. Yamanaka, N. Maruyama, A. Nukada, S. Matsuoka, Peta-scale phase-field simulation for dendritic solidification on the tsubame 2.0 supercomputer, in: Proceedings of 2011 International Conference for High Performance Computing, Networking, Storage and Analysis, 2011, pp. 1–11.

[229] N. Provatas, N. Goldenfeld, J. Dantzig, Efficient computation of dendritic microstructures using adaptive mesh refinement, Physical Review Letters 80 (15) (1998) 3308.

[230] N. Provatas, N. Goldenfeld, J. Dantzig, Adaptive mesh refinement computation of solidification microstructures using dynamic data structures, Journal of computational physics 148 (1) (1999) 265–290.

[231] M. Greenwood, K. Shampur, N. Ofori-Opoku, T. Pinomaa, L. Wang, S. Gurevich, N. Provatas, Quantitative 3d phase field modelling of solidification using next-generation adaptive mesh refinement, Computational Materials Science 142 (2018) 153–171.

[232] C. Lan, Y. Chang, C.-J. Shih, Adaptive phase field simulation of non-isothermal free dendritic growth of a binary alloy, Acta Materialia 51 (7) (2003) 1857–1869.
[233] J. Rosam, P. Jimack, A. Mullis, An adaptive, fully implicit multigrid phase-field model for the quantitative simulation of non-isothermal binary alloy solidification, Acta Materialia 56 (17) (2008) 4559–4569.

[234] P. Bollada, C. E. Goodyer, P. K. Jimack, A. M. Mullis, F. Yang, Three dimensional thermal-solute phase field simulation of binary alloy solidification, Journal of Computational Physics 287 (2015) 130–150.

[235] Z. Guo, J. Mi, P. Grant, Phase field simulation of multi-dendrite growth in a coupled thermal-solute-convective environment, in: IOP Conference Series: Materials Science and Engineering, Vol. 33, IOP Publishing, 2012, p. 012101.

[236] J. S. Langer, Instabilities and pattern formation in crystal growth, Reviews of modern physics 52 (1) (1980) 1.

[237] E. Ben-Jacob, N. Goldenfeld, B. Kotliar, J. Langer, Pattern selection in dendritic solidification, Physical review letters 53 (22) (1984) 2110.

[238] M. Ben Amar, E. Brener, Theory of pattern selection in three-dimensional nonaxisymmetric dendritic growth, Physical review letters 71 (4) (1993) 589.

[239] E. Brener, Needle-crystal solution in three-dimensional dendritic growth, Physical review letters 71 (22) (1993) 3653.

[240] W. Kurz, D. J. Fisher, R. Trivedi, Progress in modelling solidification microstructures in metals and alloys: dendrites and cells from 1700 to 2000, International Materials Reviews 64 (6) (2019) 311–354.

[241] A. Karma, Y. H. Lee, M. Plapp, Three-dimensional dendrite-tip morphology at low undercooling, Physical Review E 61 (4) (2000) 3996.

[242] M. Plapp, A. Karma, Multiscale random-walk algorithm for simulating interfacial pattern formation, Physical review letters 84 (8) (2000) 1740.

[243] M. Ode, S. G. Kim, W. T. Kim, T. Suzuki, Numerical prediction of the secondary dendrite arm spacing using a phase-field model, ISIJ international 41 (4) (2001) 345–349.
[244] T. F. Bower, H. Brody, M. C. Flemings, et al., Measurements of solute redistribution in dendritic solidification, AIME MET SOC TRANS 236 (5) (1966) 624–634.

[245] M. Greenwood, M. Haataja, N. Provatas, Crossover scaling of wavelength selection in directional solidification of binary alloys, Physical review letters 93 (24) (2004) 246101.

[246] L. Liu, J. Kirkaldy, Thin film forced velocity cells and cellular dendrites—i. experiments, Acta metallurgica et materialia 43 (8) (1995) 2891–2904.

[247] J. Kirkaldy, L. Liu, A. Kroupa, Thin film forced velocity cells and cellular dendrites—ii. analysis of data, Acta metallurgica et materialia 43 (8) (1995) 2905–2915.

[248] A. Clarke, D. Tourret, Y. Song, S. Imhoff, P. Gibbs, J. Gibbs, K. Fezzaa, A. Karma, Microstructure selection in thin-sample directional solidification of an Al-Cu alloy: In situ x-ray imaging and phase-field simulations, Acta Materialia 129 (2017) 203–216.

[249] A. K. Boukellal, J.-M. Debierre, G. Reinhart, H. Nguyen-Thi, Scaling laws governing the growth and interaction of equiaxed Al-Cu dendrites: A study combining experiments with phase-field simulations, Materialia 1 (2018) 62–69.

[250] J. Bragard, A. Karma, Y. H. Lee, M. Plapp, Linking phase-field and atomistic simulations to model dendritic solidification in highly undercooled melts, Interface Science 10 (2-3) (2002) 121–136.

[251] J. Hoyt, M. Asta, A. Karma, Method for computing the anisotropy of the solid-liquid interfacial free energy, Physical review letters 86 (24) (2001) 5530.

[252] J. Hoyt, M. Asta, A. Karma, Atomistic and continuum modeling of dendritic solidification, Materials Science and Engineering: R: Reports 41 (6) (2003) 121–163.

[253] J. Hoyt, B. Sadigh, M. Asta, S. Foiles, Kinetic phase field parameters for the Cu-Ni system derived from atomistic computations, Acta materialia 47 (11) (1999) 3181–3187.
[254] J. W. Lum, D. M. Matson, M. C. Flemings, High-speed imaging and analysis of the solidification of undercooled nickel melts, Metallurgical and Materials Transactions B 27 (5) (1996) 865–870.

[255] R. Willnecker, D. Herlach, B. Feuerbacher, Evidence of nonequilibrium processes in rapid solidification of undercooled metals, Physical review letters 62 (23) (1989) 2707.

[256] J. Herenguel, Les procédés de coulée semi-continue et continue des métaux non ferreux et leurs conséquences métallurgiques, Revue de Métallurgie 45 (5-6) (1948) 139–146.

[257] S. Henry, T. Minghetti, M. Rappaz, Dendrite growth morphologies in aluminium alloys, Acta Materialia 46 (18) (1998) 6431–6443.

[258] A. Sémoroz, Y. Durandet, M. Rappaz, Ebsd characterization of dendrite growth directions, texture and misorientations in hot-dipped al–zn–si coatings, Acta materialia 49 (3) (2001) 529–541.

[259] F. Gonzales, M. Rappaz, Dendrite growth directions in aluminum-zinc alloys, Metallurgical and Materials Transactions A 37 (9) (2006) 2797–2806.

[260] C. Becker, D. Olmsted, M. Asta, J. Hoyt, S. Foiles, Atomistic underpinnings for orientation selection in alloy dendritic growth, Physical review letters 98 (12) (2007) 125701.

[261] D. Sun, M. Mendelev, C. Becker, K. Kudin, T. Haxhimali, M. Asta, J. Hoyt, A. Karma, D. Srolovitz, Crystal-melt interfacial free energies in hcp metals: A molecular dynamics study of mg, Physical Review B 73 (2) (2006) 024116.

[262] J. R. Morris, Complete mapping of the anisotropic free energy of the crystal-melt interface in al, Physical Review B 66 (14) (2002) 144104.

[263] R. Napolitano, S. Liu, R. Trivedi, Experimental measurement of anisotropy in crystal-melt interfacial energy, Interface Science 10 (2-3) (2002) 217–232.

[264] M. Becker, J. Dantzig, M. Kolbe, S. Wiese, F. Kargl, Dendrite orientation transition in alge alloys, Acta Materialia 165 (2019) 666–677.
[265] L. Wang, J. J. Hoyt, N. Wang, N. Provatas, C. W. Sinclair, Controlling solid-liquid interfacial energy anisotropy through the isotropic liquid, Nature communications 11 (1) (2020) 1–7.

[266] D. Casari, W. Mirihanage, K. V. Falch, I. G. Ringdalen, J. Friis, R. Schmid-Fetzer, D. Zhao, Y. Li, W. H. Sillekens, R. Mathiesen, α-mg primary phase formation and dendritic morphology transition in solidification of a mg-nd-gd-zn-zr casting alloy, Acta Materialia 116 (2016) 177–187.

[267] M. Yang, S.-M. Xiong, Z. Guo, Effect of different solute additions on dendrite morphology and orientation selection in cast binary magnesium alloys, Acta Materialia 112 (2016) 261–272.

[268] J. Du, Z. Guo, A. Zhang, M. Yang, M. Li, S. Xiong, Correlation between crystallographic anisotropy and dendritic orientation selection of binary magnesium alloys, Scientific reports 7 (1) (2017) 1–13.

[269] S. Shuai, E. Guo, J. Wang, A. Phillion, T. Jing, Z. Ren, P. D. Lee, Synchrotron tomographic quantification of the influence of zn concentration on dendritic growth in mg-zn alloys, Acta Materialia 156 (2018) 287–296.

[270] M. Bedel, G. Reinhart, A.-A. Bogno, C.-A. Gandin, S. Jacomet, E. Boller, H. Nguyen-Thi, H. Henein, Characterization of dendrite morphologies in rapidly solidified al–4.5 wt.% cu droplets, Acta Materialia 89 (2015) 234–246.

[271] G. IVANTSOV, Temperature field around a spherical cylindrical and a cubic crystal growing in a supercooled melt, in: Dokl. Akad. Nauk SSSR, Vol. 58, 1947, pp. 567–569.

[272] R. Mehrabian, M. Keane, M. Flemings, Interdendritic fluid flow and macrosegregation; influence of gravity, Metallurgical and Materials Transactions B 1 (5) (1970) 1209–1220.

[273] H. N. Thi, B. Billia, H. Jamgotchian, Influence of thermosolutal convection on the solidification front during upwards solidification, Journal of Fluid Mechanics 204 (1989) 581–597.
[274] M. Dupouy, D. Camel, J. Favier, Natural convection in directional dendritic solidification of metallic alloys—i. macroscopic effects, Acta Metallurgica 37 (4) (1989) 1143–1157.

[275] H. Jamgotchian, N. Bergeon, D. Benielli, P. Voge, B. Billia, R. Guerin, Localized microstructures induced by fluid flow in directional solidification, Physical review letters 87 (16) (2001) 166105.

[276] A. Bogno, H. Nguyen-Thi, A. Buffet, G. Reinhart, B. Billia, N. Mangelinck-Noël, N. Bergeon, J. Baruchel, T. Schenk, Analysis by synchrotron x-ray radiography of convection effects on the dynamic evolution of the solid–liquid interface and on solute distribution during the initial transient of solidification, Acta Materialia 59 (11) (2011) 4356–4365.

[277] M. Glicksman, M. Koss, E. Winsa, Dendritic growth velocities in microgravity, Physical review letters 73 (4) (1994) 573.

[278] H. N. Thi, Y. Dabo, B. Drevet, M. Dupouy, D. Camel, B. Billia, J. Hunt, A. Chilton, Directional solidification of al–1.5 wt% ni alloys under diffusion transport in space and fluid-flow localisation on earth, Journal of crystal growth 281 (2-4) (2005) 654–668.

[279] H. Nguyen-Thi, G. Reinhart, B. Billia, On the interest of microgravity experimentation for studying convective effects during the directional solidification of metal alloys, Comptes Rendus Mécanique 345 (1) (2017) 66–77.

[280] R. Marcout, A. S. Transportation, Declic: a facility to investigate fluids and transparent materials in microgravity conditions on iss, Proceedings of the 57th IAC IAC-06-A2 (5.02).

[281] N. Bergeon, A. Ramirez, L. Chen, B. Billia, J. Gu, R. Trivedi, Dynamics of interface pattern formation in 3d alloy solidification: first results from experiments in the declic directional solidification insert on the international space station, Journal of materials science 46 (19) (2011) 6191–6202.

[282] K. Jackson, J. Hunt, Transparent compounds that freeze like metals, Acta Metallurgica 13 (11) (1965) 1212–1215.
[283] N. Bergeon, D. Tourret, L. Chen, J.-M. Debierre, R. Guérin, A. Ramirez, B. Billia, A. Karma, R. Trivedi, Spatiotemporal dynamics of oscillatory cellular patterns in three-dimensional directional solidification, Physical review letters 110 (22) (2013) 226102.

[284] D. Tourret, J.-M. Debierre, Y. Song, F. L. Mota, N. Bergeon, R. Guerin, R. Trivedi, B. Billia, A. Karma, Oscillatory cellular patterns in three-dimensional directional solidification, Physical Review E 92 (4) (2015) 042401.

[285] J. Pereda, F. Mota, L. Chen, B. Billia, D. Tourret, Y. Song, J.-M. Debierre, R. Guérin, A. Karma, R. Trivedi, et al., Experimental observation of oscillatory cellular patterns in three-dimensional directional solidification, Physical Review E 95 (1) (2017) 012803.

[286] M. Georgelin, A. Pocheau, Oscillatory instability, limit cycle, and transition to doublets in directional solidification, Physical review letters 79 (14) (1997) 2698.

[287] J. Pereda, F. L. Mota, J.-M. Debierre, B. Billia, R. Trivedi, A. Karma, N. Bergeon, Experimental characterization and theoretical analysis of cell tip oscillations in directional solidification, Physical Review E 102 (3) (2020) 032804.

[288] F. L. Mota, N. Bergeon, A. Karma, R. Trivedi, J.-M. Debierre, Oscillatory-nonoscillatory transitions for inclined cellular patterns in three-dimensional directional solidification, Physical Review E 102 (3) (2020) 032803.

[289] F. Mota, N. Bergeon, D. Tourret, A. Karma, R. Trivedi, B. Billia, Initial transient behavior in directional solidification of a bulk transparent model alloy in a cylinder, Acta Materialia 85 (2015) 362–377.

[290] Y. Song, D. Tourret, F. Mota, J. Pereda, B. Billia, N. Bergeon, R. Trivedi, A. Karma, Thermal-field effects on interface dynamics and microstructure selection during alloy directional solidification, Acta Materialia 150 (2018) 139–152.

[291] F. Mota, J. Pereda, K. Ji, Y. Song, R. Trivedi, A. Karma, N. Bergeon, Effect of sub-boundaries on primary spacing dynamics during 3d direc-
tional solidification conducted on declc-dsi, Acta Materialia 204 (2021) 116500.

[292] J. Strickland, B. Nenchev, S. Perry, K. Tassenberg, S. Gill, C. Panwisawas, H. Dong, N. D'Souza, S. Irwin, On the nature of hexagonality within the solidification structure of single crystal alloys: Mechanisms and applications, Acta Materialia 200 (2020) 417–431.

[293] B. Bellón, A. Boukellal, T. Isensee, O. Wellborn, K. Trumble, M. Krane, M. Titus, D. Tourret, J. LLorca, Multiscale prediction of microstructure length scales in metallic alloy casting, Acta Materialia 207 (2021) 116686.

[294] G. B. Olson, Computational design of hierarchically structured materials, Science 277 (5330) (1997) 1237–1242.

[295] T. Pollock et al., Integrated Computational Materials Engineering, The National Academy Press, Washington DC, USA., 2008.

[296] J. Allison, Integrated computational materials engineering: A perspective on progress and future steps, Jom 63 (4) (2011) 15.

[297] I. J. Beyerlein, S. Xu, J. Llorca, J. A. El-Awady, J. R. Mianroodi, B. Svendsen, Alloy design for mechanical properties: Conquering the length scales, MRS Bulletin 44 (2019) 257 – 265.

[298] J. Zhu, Z. Liu, V. Vaithyanathan, L. Chen, Linking phase-field model to calphad: application to precipitate shape evolution in ni-base alloys, Scripta Materialia 46 (5) (2002) 401–406.

[299] I. Steinbach, B. Böttger, J. Eiken, N. Warnken, S. Fries, Calphad and phase-field modeling: a successful liaison, Journal of phase equilibria and diffusion 28 (1) (2007) 101–106.

[300] S. G. Fries, B. Boettger, J. Eiken, I. Steinbach, Upgrading calphad to microstructure simulation: the phase-field method, International journal of materials research 100 (2) (2009) 128–134.

[301] Z.-K. Liu, L.-Q. Chen, Integration of first-principles calculations, calphad modeling, and phase-field simulations, in: Applied Computational Materials Modeling, Springer, 2007, pp. 171–213.
[302] D. D. J. N. A. Zarkevich, On the early stages of precipitation in dilute Mg-Nd alloys, Physical Review B 67 (2003) 064104.

[303] A. Natarajan, E. Solomon, B. Puchala, A. Van der Ven, On the early stages of precipitation in dilute Mg-Nd alloys, Acta Materialia 108 (2016) 367 – 379.

[304] S. Liu, E. Martínez, J. LLorca, Prediction of the al-rich part of the al-cu phase diagram using cluster expansion and statistical mechanics, Acta Materialia 195 (2020) 317–326.

[305] D. Sun, M. Asta, J. Hoyt, Crystal-melt interfacial free energies and mobilities in fcc and bcc fe, Physical Review B 69 (17) (2004) 174103.

[306] H. Zhou, X. Lin, M. Wang, W. Huang, Calculation of solid–liquid interfacial free energy of cu by two different methods, Journal of crystal growth 377 (2013) 107–111.

[307] E. Asadi, M. A. Zaeem, S. Nouranian, M. I. Baskes, Two-phase solid–liquid coexistence of ni, cu, and al by molecular dynamics simulations using the modified embedded-atom method, Acta Materialia 86 (2015) 169–181.

[308] E. Asadi, M. A. Zaeem, S. Nouranian, M. I. Baskes, Quantitative modeling of the equilibration of two-phase solid-liquid fe by atomistic simulations on diffusive time scales, Physical Review B 91 (2) (2015) 024105.

[309] E. Asadi, M. A. Zaeem, The anisotropy of hexagonal close-packed and liquid interface free energy using molecular dynamics simulations based on modified embedded-atom method, Acta Materialia 107 (2016) 337–344.

[310] S. Kavousi, B. R. Novak, M. I. Baskes, M. A. Zaeem, D. Moldovan, Modified embedded-atom method potential for high-temperature crystal-melt properties of ti–ni alloys and its application to phase field simulation of solidification, Modelling and Simulation in Materials Science and Engineering 28 (1) (2019) 015006.

[311] J. Hoyt, M. Asta, Atomistic computation of liquid diffusivity, solid-liquid interfacial free energy, and kinetic coefficient in au and ag, Physical Review B 65 (21) (2002) 214106.
[312] J. Monk, Y. Yang, M. Mendelev, M. Asta, J. Hoyt, D. Sun, A. Stukowski, Y. Lei, H. Liu, W. Xiao, et al., Determination of the crystal-melt interface kinetic coefficient from molecular dynamics simulations, Modelling Simul. Mater. Sci. Eng 18 (2010) 015004.

[313] M. Mendelev, M. Rahman, J. Hoyt, M. Asta, Molecular-dynamics study of solid–liquid interface migration in fcc metals, Modelling and Simulation in Materials Science and Engineering 18 (7) (2010) 074002.

[314] Y. Gao, Y. Yang, D. Sun, M. Asta, J. Hoyt, Molecular dynamics simulations of the crystal–melt interface mobility in hcp mg and bcc fe, Journal of crystal growth 312 (21) (2010) 3238–3242.

[315] S. Kavousi, B. R. Novak, M. A. Zaeem, D. Moldovan, Combined molecular dynamics and phase field simulation investigations of crystal-melt interfacial properties and dendritic solidification of highly undercooled titanium, Computational Materials Science 163 (2019) 218–229.

[316] S. Kavousi, B. R. Novak, J. Hoyt, D. Moldovan, Interface kinetics of rapid solidification of binary alloys by atomistic simulations: Application to ti-ni alloys, Computational Materials Science 184 (2020) 109854.

[317] L. Q. Chen, J. Shen, et al., Applications of semi-implicit fourier-spectral method to phase field equations, Computer Physics Communications 108 (2) (1998) 147–158.

[318] J. Zhu, L.-Q. Chen, J. Shen, V. Tikare, Coarsening kinetics from a variable-mobility cahn-hilliard equation: Application of a semi-implicit fourier spectral method, Physical Review E 60 (4) (1999) 3564.

[319] W. Feng, P. Yu, S. Hu, Z.-K. Liu, Q. Du, L.-Q. Chen, Spectral implementation of an adaptive moving mesh method for phase-field equations, Journal of Computational Physics 220 (1) (2006) 498–510.

[320] A. Finel, Y. Le Bouar, B. Dabas, B. Appolaire, Y. Yamada, T. Mohri, Sharp phase field method, Physical review letters 121 (2) (2018) 025501.

[321] A. Dimokrati, Y. Le Bouar, M. Benyoucef, A. Finel, S-pfm model for ideal grain growth, Acta Materialia 201 (2020) 147–157.
[322] R. Folch, M. Plapp, Quantitative phase-field modeling of two-phase growth, Physical Review E 72 (1) (2005) 011602.

[323] S. G. Kim, A phase-field model with antitrapping current for multi-component alloys with arbitrary thermodynamic properties, Acta Materialia 55 (13) (2007) 4391–4399.

[324] R. Almgren, Siam (soc. ind. appl. math.) j, Appl. Math 59 (1999) 2086.

[325] M. Ohno, K. Matsuura, Quantitative phase-field modeling for dilute alloy solidification involving diffusion in the solid, Phys. Rev. E 79 (2009) 031603.

[326] M. Ohno, T. Takaki, Y. Shibuta, Variational formulation and numerical accuracy of a quantitative phase-field model for binary alloy solidification with two-sided diffusion, Phys. Rev. E 93 (2016) 012802.

[327] A. Fang, Y. Mi, Recovering thermodynamic consistency of the antitrapping model: A variational phase-field formulation for alloy solidification, Physical Review E 87 (1) (2013) 012402.

[328] E. A. Brener, G. Boussinot, Kinetic cross coupling between nonconserved and conserved fields in phase field models, Phys. Rev. E 86 (2012) 060601.

[329] G. Boussinot, E. A. Brener, Achieving realistic interface kinetics in phase-field models with a diffusional contrast, Physical Review E 89 (6) (2014) 060402.

[330] K. Wang, G. Boussinot, C. Hüter, E. A. Brener, R. Spatschek, Modeling of dendritic growth using a quantitative nondiagonal phase field model, Phys. Rev. Materials 4 (2020) 033802.

[331] D. Morgan, R. Jacobs, Opportunities and challenges for machine learning in materials science, Annual Review of Materials Research 50 (2020) 71–103.

[332] T. Mueller, A. G. Kusne, R. Ramprasad, Machine learning in materials science: Recent progress and emerging applications, Reviews in Computational Chemistry 29 (2016) 186–273.
[333] K. T. Butler, D. W. Davies, H. Cartwright, O. Isayev, A. Walsh, Machine learning for molecular and materials science, Nature 559 (7715) (2018) 547–555.

[334] D. M. de Oca Zapiain, J. A. Stewart, R. Dingreville, Accelerating phase-field-based microstructure evolution predictions via surrogate models trained by machine learning methods, npj Computational Materials 7 (1) (2021) 1–11.

[335] Z.-H. Shen, J.-J. Wang, J.-Y. Jiang, S. X. Huang, Y.-H. Lin, C.-W. Nan, L.-Q. Chen, Y. Shen, Phase-field modeling and machine learning of electric-thermal-mechanical breakdown of polymer-based dielectrics, Nature communications 10 (1) (2019) 1–10.

[336] A. Kunwar, Y. A. Coutinho, J. Hektor, H. Ma, N. Moelans, Integration of machine learning with phase field method to model the electromigration induced Cu6Sn5 IMC growth at anode side Cu/Sn interface, Journal of Materials Science & Technology 59 (2020) 203–219.

[337] G. H. Teichert, K. Garikipati, Machine learning materials physics: Surrogate optimization and multi-fidelity algorithms predict precipitate morphology in an alternative to phase field dynamics, Computer Methods in Applied Mechanics and Engineering 344 (2019) 666–693.

[338] S. Goswami, C. Anitescu, S. Chakraborty, T. Rabczuk, Transfer learning enhanced physics informed neural network for phase-field modeling of fracture, Theoretical and Applied Fracture Mechanics 106 (2020) 102447.

[339] M. Raissi, G. E. Karniadakis, Hidden physics models: Machine learning of nonlinear partial differential equations, Journal of Computational Physics 357 (2018) 125–141.

[340] E. Samaniego, C. Anitescu, S. Goswami, V. M. Nguyen-Thanh, H. Guo, K. Hamdia, X. Zhuang, T. Rabczuk, An energy approach to the solution of partial differential equations in computational mechanics via machine learning: Concepts, implementation and applications, Computer Methods in Applied Mechanics and Engineering 362 (2020) 112790.
[341] V. Attari, P. Honarmandi, T. Duong, D. J. Sauceda, D. Allaire, R. Arroyave, Uncertainty propagation in a multiscale calphad-reinforced elastochemical phase-field model, Acta Materialia 183 (2020) 452–470.

[342] C. Shen, J. Li, Y. Wang, Finding critical nucleus in solid-state transformations, Metallurgical and materials transactions A 39 (5) (2008) 976–983.

[343] L. Gránásy, T. Börzsönyi, T. Pusztai, Nucleation and bulk crystallization in binary phase field theory, Physical review letters 88 (20) (2002) 206105.

[344] L. Gránásy, T. Börzsönyi, T. Pusztai, Crystal nucleation and growth in binary phase-field theory, Journal of crystal growth 237 (2002) 1813–1817.

[345] L. Gránásy, T. Pusztai, D. Saylor, J. A. Warren, Phase field theory of heterogeneous crystal nucleation, Physical review letters 98 (3) (2007) 035703.

[346] J. A. Warren, T. Pusztai, L. Környei, L. Gránásy, Phase field approach to heterogeneous crystal nucleation in alloys, Physical Review B 79 (1) (2009) 014204.

[347] J. Simmons, C. Shen, Y. Wang, Phase field modeling of simultaneous nucleation and growth by explicitly incorporating nucleation events, Scripta materialia 43 (10) (2000) 935–942.

[348] Y. Wen, J. Simmons, C. Shen, C. Woodward, Y. Wang, Phase-field modeling of bimodal particle size distributions during continuous cooling, Acta materialia 51 (4) (2003) 1123–1132.

[349] J. Simmons, Y. Wen, C. Shen, Y. Wang, Microstructural development involving nucleation and growth phenomena simulated with the phase field method, Materials Science and Engineering: A 365 (1-2) (2004) 136–143.

[350] A. Jokisaari, C. Permann, K. Thornton, A nucleation algorithm for the coupled conserved–nonconserved phase field model, Computational Materials Science 112 (2016) 128–138.
[351] L. Gránásy, G. I. Tóth, J. A. Warren, F. Podmaniczky, G. Tegze, L. Rátkai, T. Pusztai, Phase-field modeling of crystal nucleation in undercooled liquids–a review, Progress in Materials Science.

[352] M. Plapp, Remarks on some open problems in phase-field modelling of solidification, Philosophical Magazine 91 (1) (2011) 25–44.

[353] W. J. Boettinger, Microstructural variations in rapidly solidified alloys, Materials Science and Engineering 98 (1988) 123–130.

[354] L. A. Jacobson, J. McKittrick, Rapid solidification processing, Materials Science and Engineering: R: Reports 11 (8) (1994) 355–408.

[355] W. Kurz, R. Trivedi, Rapid solidification processing and microstructure formation, Materials Science and Engineering: A 179 (1994) 46–51.

[356] M. Aziz, W. Boettinger, On the transition from short-range diffusion-limited to collision-limited growth in alloy solidification, Acta metallurgica et materialia 42 (2) (1994) 527–537.

[357] M. J. Aziz, T. Kaplan, Continuous growth model for interface motion during alloy solidification, Acta metallurgica 36 (8) (1988) 2335–2347.

[358] W. Boettinger, M. Aziz, Theory for the trapping of disorder and solute in intermetallic phases by rapid solidification, Acta Metallurgica 37 (12) (1989) 3379–3391.

[359] P. Galenko, S. Sobolev, Local nonequilibrium effect on undercooling in rapid solidification of alloys, Physical Review E 55 (1) (1997) 343.

[360] P. Galenko, D. Danilov, Model for free dendritic alloy growth under interfacial and bulk phase nonequilibrium conditions, Journal of crystal growth 197 (4) (1999) 992–1002.

[361] N. Ahmad, A. Wheeler, W. J. Boettinger, G. B. McFadden, Solute trapping and solute drag in a phase-field model of rapid solidification, Physical Review E 58 (3) (1998) 3436.

[362] S. G. Kim, W. T. Kim, T. Suzuki, Phase-field model for binary alloys, Physical review e 60 (6) (1999) 7186.
[363] I. Steinbach, L. Zhang, M. Plapp, Phase-field model with finite interface dissipation, Acta Materialia 60 (6-7) (2012) 2689–2701.

[364] L. Zhang, I. Steinbach, Phase-field model with finite interface dissipation: Extension to multi-component multi-phase alloys, Acta Materialia 60 (6-7) (2012) 2702–2710.

[365] L. Zhang, M. Stratmann, Y. Du, B. Sundman, I. Steinbach, Incorporating the calphad sublattice approach of ordering into the phase-field model with finite interface dissipation, Acta Materialia 88 (2015) 156–169.

[366] K. Reuther, S. Hubig, I. Steinbach, M. Rettenmayr, Solute trapping in non-equilibrium solidification: A comparative model study, Materialia 6 (2019) 100256.

[367] L. Zhang, E. V. Danilova, I. Steinbach, D. Medvedev, P. K. Galenko, Diffuse-interface modeling of solute trapping in rapid solidification: Predictions of the hyperbolic phase-field model and parabolic model with finite interface dissipation, Acta materialia 61 (11) (2013) 4155–4168.

[368] S. G. Kim, W. T. Kim, P.-R. Cha, B.-J. Lee, J. S. Lee, J. Park, C.-S. Oh, Phase-field model with relaxation of the partition coefficient, Computational Materials Science 188 (2021) 110184.

[369] H. Wang, F. Liu, G. Ehlen, D. Herlach, Application of the maximal entropy production principle to rapid solidification: a multi-phase-field model, Acta materialia 61 (7) (2013) 2617–2627.

[370] T. Pinomaa, N. Provatas, Quantitative phase field modeling of solute trapping and continuous growth kinetics in quasi-rapid solidification, Acta Materialia 168 (2019) 167–177.

[371] S. Kavousi, M. A. Zaeem, Quantitative phase-field modeling of solute trapping in rapid solidification, Acta Materialia 205 (2021) 116562.

[372] O. Güvenc, M. Bambach, G. Hirt, Coupling of crystal plasticity finite element and phase field methods for the prediction of srX kinetics after hot working, Steel Research International 85 (2014) 999–1009.
A. Vondrous, P. Bienger, S. Schreijäg, M. Selzer, D. Schneider, B. Nestler, D. Helm, R. Mönig, Combined crystal plasticity and phase-field method for recrystallization in a process chain of sheet metal production, Computational Mechanics 55 (2015) 439–452.

H. Lim, F. Abdeljawad, S. J. Owen, B. W. Hanks, J. W. Foulk, C. C. Battaile, Incorporating physically-based microstructures in materials modeling: Bridging phase field and crystal plasticity frameworks, Modelling and Simulation in Materials Science and Engineering 24 (2016) 045016.

N. C. Admal, G. Po, J. Marian, A unified framework for polycrystalline plasticity with grain boundary evolution, International Journal of Plasticity 106 (2018) 1–30.

H. Neumann-Heyme, K. Eckert, C. Beckermann, General evolution equation for the specific interface area of dendrites during alloy solidification, Acta Materialia 140 (2017) 87–96.

T. Takaki, S. Sakane, M. Ohno, Y. Shibuta, T. Aoki, Permeability prediction for flow normal to columnar solidification structures by large-scale simulations of phase-field and lattice boltzmann methods, Acta Materialia 164 (2019) 237–249.

Y. Mitsuyama, T. Takaki, S. Sakane, Y. Shibuta, M. Ohno, Permeability tensor for columnar dendritic structures: Phase-field and lattice boltzmann study, Acta Materialia 188 (2020) 282–287.

A. Pineau, G. Guillemot, D. Tourret, A. Karma, C.-A. Gandin, Growth competition between columnar dendritic grains–cellular automaton versus phase field modeling, Acta Materialia 155 (2018) 286–301.

C. Schwarze, R. D. Kamachali, M. Kühbach, C. Mießen, M. Tegeler, L. Barrales-Mora, I. Steinbach, G. Gottstein, Computationally efficient phase-field simulation studies using rve sampling and statistical analysis, Computational Materials Science 147 (2018) 204–216.

A. M. Jokisaari, P. W. Voorhees, J. E. Guyer, J. Warren, O. Heinonen, Benchmark problems for numerical implementations of phase field models, Computational Materials Science 126 (2017) 139–151.
[382] A. M. Jokisaari, P. W. Voorhees, J. E. Guyer, J. A. Warren, O. G. Heinonen, Phase field benchmark problems for dendritic growth and linear elasticity, Computational Materials Science 149 (2018) 336–347.

[383] A. Jokisaari, W. Wu, P. Voorhees, J. E. Guyer, J. A. Warren, O. G. Heinonen, Phase field benchmark problems targeting fluid flow and electrochemistry, Computational Materials Science 176 (2020) 109548.

[384] R. D. Kamachali, C. Schwarze, M. Lin, M. Diehl, P. Shanthraj, U. Prahl, I. Steinbach, D. Raabe, Numerical benchmark of phase-field simulations with elastic strains: precipitation in the presence of chemomechanical coupling, Computational Materials Science 155 (2018) 541–553.

[385] J. Eiken, Standardization of fundamental benchmark tests for validation of phase-field models in materials science and engineering, 55th Annual Technical Meeting of the Society of Engineering Science (SES), Madrid, Spain (2018).

[386] L.-X. Lu, N. Sridhar, Y.-W. Zhang, Phase field simulation of powder bed-based additive manufacturing, Acta Materialia 144 (2018) 801–809.

[387] Y. Ji, L. Chen, L.-Q. Chen, Understanding microstructure evolution during additive manufacturing of metallic alloys using phase-field modeling, in: Thermo-mechanical modeling of additive manufacturing, Elsevier, 2018, pp. 93–116.

[388] K. Karayagiz, L. Johnson, R. Seede, V. Attari, B. Zhang, X. Huang, S. Ghosh, T. Duong, I. Karaman, A. Elwany, et al., Finite interface dissipation phase field modeling of ni–nb under additive manufacturing conditions, Acta Materialia 185 (2020) 320–339.

[389] S. Vakili, I. Steinbach, F. Varnik, Controlling bubble coalescence in metallic foams: a simple phase field-based approach, Computational Materials Science 173 (2020) 109437.

[390] S. Vakili, I. Steinbach, F. Varnik, Multi-phase-field simulation of microstructure evolution in metallic foams, Scientific reports 10 (1) (2020) 1–12.
[391] A. A. Kulkarni, E. Hanson, R. Zhang, K. Thornton, P. V. Braun, Archimedean lattices emerge in template-directed eutectic solidification, Nature 577 (7790) (2020) 355–358.

[392] A. Karma, 3d phase-field simulations of pattern formation during freeze casting, tMS Annual Meeting (2021).

[393] K. Yin, P. Divakar, U. G. Wegst, Freeze-casting porous chitosan ureteral stents for improved drainage, Acta biomaterialia 84 (2019) 231–241.

[394] K. Yin, B. A. Reese, C. R. Sullivan, U. G. Wegst, Superior mechanical and magnetic performance of highly anisotropic sendust-flake composites freeze cast in a uniform magnetic field, Advanced Functional Materials 31 (8) (2021) 2007743.

[395] U. G. Wegst, H. Bai, E. Saiz, A. P. Tomsia, R. O. Ritchie, Bioinspired structural materials, Nature materials 14 (1) (2015) 23–36.

[396] V. Schoeppler, R. Lemanis, E. Reich, T. Pusztai, L. Gránásy, I. Zlotnikov, Crystal growth kinetics as an architectural constraint on the evolution of molluscan shells, Proceedings of the National Academy of Sciences 116 (41) (2019) 20388–20397.

[397] C.-Y. Sun, L. Gránásy, C. A. Stifler, T. Zaquin, R. V. Chopdekar, N. Tamura, J. C. Weaver, J. A. Zhang, S. Goffredo, G. Falini, et al., Crystal nucleation and growth of spherulites demonstrated by coral skeletons and phase-field simulations, Acta biomaterialia 120 (2021) 277–292.