

MICROSTRUCTURAL CONTROL IN NI-BASED SUPERALLOYS FOR TURBINE APPLICATIONS: A REVIEW OF PHASE-FIELD MODELING APPROACHES

CONTROLE DA MICROESTRUTURA EM SUPERLIGAS À BASE DE NI PARA APLICAÇÕES EM TURBINAS: UMA REVISÃO DAS ABORDAGENS DE MODELAGEM DE CAMPO DE FASE

CONTROL DE LA MICROESTRUTURA EN SUPERALEACIONES A BASE DE NÍQUEL PARA APLICACIONES EN TURBINAS: UNA REVISIÓN DE LOS ENFOQUES DE MODELIZACIÓN DE CAMPO DE FASES

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ABSTRACT

Nickel-based superalloys are essential materials for high-pressure turbine blades in aero-engines and industrial gas turbines, where their performance is critically determined by the microstructural evolution during solidification and subsequent service. This review presents a comprehensive examination of phase-field modeling approaches applied to microstructural control in single-crystal Ni-based superalloys, with particular emphasis on dendritic solidification, microsegregation, and γ' precipitate rafting during creep deformation. The theoretical foundations of the phase-field method are discussed, including the Kobayashi formalism for dendritic growth and the KKS multi-component formulation for precipitation phenomena, alongside their coupling with CALPHAD thermodynamic databases for realistic multi-component alloy simulations. Recent advances in integrated simulation workflows linking thermal histories from additive manufacturing process models to phase-field microstructure predictions are critically evaluated, demonstrating the capability to predict primary dendrite arm spacing, solute redistribution patterns, and rafting morphologies with quantitative accuracy validated against experimental measurements. This work addresses computational challenges inherent in multi-scale phase-field simulations and highlights emerging strategies including implicit multigrid schemes and machine-learning-assisted surrogates that enable simulations at industrially relevant length scales.

Keywords: Phase-Field Modeling. Nickel-Based Superalloys. Dendritic Solidification. Microsegregation. Additive Manufacturing. CALPHAD.

RESUMO

As superligas à base de níquel são materiais essenciais para pás de turbinas de alta pressão em motores aeronáuticos e turbinas a gás industriais, onde seu desempenho é criticamente

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determinado pela evolução microestrutural durante a solidificação e o subsequente serviço. Esta revisão apresenta um exame abrangente das abordagens de modelagem por campo de fase aplicadas ao controle microestrutural em superligas monocristalinas à base de Ni, com ênfase particular na solidificação dendrítica, na microsegregação e na formação de coalescência dos precipitados γ' durante a deformação por fluência. São discutidos os fundamentos teóricos do método de campo de fase, incluindo o formalismo de Kobayashi para o crescimento dendrítico e a formulação multicomponente KKS para fenômenos de precipitação, juntamente com seu acoplamento a bancos de dados termodinâmicos CALPHAD para simulações realistas de ligas multicomponentes. Avanços recentes em fluxos de trabalho integrados de simulação, que conectam histórias térmicas provenientes de modelos de processos de manufatura aditiva a previsões microestruturais por campo de fase, são avaliados criticamente, demonstrando a capacidade de prever o espaçamento primário entre braços dendríticos, os padrões de redistribuição de solutos e as morfologias com precisão quantitativa validada por medições experimentais baseado na literatura. Este trabalho aborda os desafios computacionais inerentes às simulações de campo de fase em múltiplas escalas e destaca estratégias emergentes, incluindo esquemas multigrid implícitos e substitutos assistidos por aprendizado de máquina, que permitem simulações em escalas de comprimento relevantes para a indústria.

Palavras-chave: Modelagem de Campo de Fase. Superligas à Base de Níquel. Solidificação Dendrítica. Microsegregação. Manufatura Aditiva. CALPHAD.

RESUMEN

Las superaleaciones base níquel son materiales esenciales para los álabes de turbinas de alta presión en motores aeronáuticos y turbinas de gas industriales, donde su rendimiento está determinado críticamente por la evolución microestructural durante la solidificación y el posterior servicio. Este trabajo presenta un examen exhaustivo de los enfoques de modelización por campo de fase aplicados al control microestructural en superaleaciones monocristalinas base Ni, con especial énfasis en la solidificación dendrítica, la microsegregación y el apilamiento de precipitados γ' durante la deformación por fluencia. Se discuten los fundamentos teóricos del método de campo de fase, incluyendo el formalismo de Kobayashi para el crecimiento dendrítico y la formulación multicomponente KKS para fenómenos de precipitación, junto con su acoplamiento a bases de datos termodinámicos CALPHAD para simulaciones realistas de aleaciones multicomponentes. Se evalúan críticamente los avances recientes en flujos de trabajo integrados de simulación que vinculan historias térmicas de modelos de procesos de manufatura aditiva con predicciones microestructurales de campo de fase, demostrando la capacidad de predecir la separación entre brazos dendríticos primarios, los patrones de redistribución de solutos y las morfologías de apilamiento con precisión cuantitativa validada mediante mediciones experimentales por otros autores. Este trabajo aborda los desafíos computacionales inherentes a las simulaciones de campo de fase en múltiples escalas y destaca estrategias emergentes, incluyendo esquemas multigrid implícitos y sustitutos asistidos por aprendizaje automático, que permiten simulaciones a escalas de longitud relevantes para la industria.

Palabras clave: Modelización de Campo de Fase. Superaleaciones a Base de Níquel. Solidificación Dendrítica. Microsegregación. Fabricación Aditiva. CALPHAD.



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INTRODUCTION

Nickel-based superalloys constitute the material of choice for high-pressure turbine blades in modern aero-engines and industrial gas turbines, owing to their exceptional mechanical strength, creep resistance, and oxidation/corrosion resistance at temperatures approaching 80–90% of their melting point (Pollock and Tin, 2006; Reed, 2006). The performance of these critical components fundamentally determines the turbine entry temperature and, consequently, the thermal efficiency and thrust-to-weight ratio of propulsion systems.

The superior high-temperature capabilities of Ni-based superalloys arise from their characteristic two-phase microstructure, comprising a face-centered cubic γ matrix and a coherently embedded $L1_2$ -ordered γ' precipitate phase (Ni_3Al) with a volume fraction typically of 60–70% (Reed, 2006). This ordered intermetallic phase serves as the primary strengthening agent, hindering dislocation motion during creep deformation (Reed, 2006; Yu *et al.*, 2020). However, the presence of grain boundaries significantly degrades creep resistance at elevated temperatures, as they provide preferential paths for diffusion-controlled cavitation and grain-boundary sliding. Consequently, single-crystalline (SX) superalloys, which eliminate grain boundaries entirely, are preferred for the most demanding turbine applications, enabling increases in operating temperature and component efficiency (Pollock and Tin, 2006).

The quest for enhanced temperature capability has driven the development of successive generations of SX superalloys, from first-generation alloys (e.g., CMSX-2, PWA 1480) to second-generation (CMSX-4, René N5) containing ~3 wt% Re, and third generation (CMSX-10, René N6) with ~6 wt% Re. Each generation achieves approximately 30°C improvement in temperature capability through the strategic addition of refractory elements, particularly rhenium (Re), which partitions to the dendrite cores and provide substantial solid-solution strengthening (Cui *et al.*, 2025). Modern fourth generation and experimental alloys further incorporate elements such as Ru to enhance microstructural stability (Yu *et al.*, 2020).

The control of microstructure during solidification and subsequent service is paramount for realizing the full potential of these alloys. During directional solidification, whether by conventional Bridgman casting or emerging additive manufacturing (AM) techniques, dendritic microstructures form with characteristic primary dendrite arm spacing (PDAS), microsegregation

of alloying elements between dendrite cores and interdendritic regions, and potential formation of deleterious phases such as topologically close-packed (TCP) phases (Pollock and Tin, 2006; Cui *et al.*, 2025). Furthermore, during high-temperature creep service, the γ' precipitates undergo directional coarsening (rafting), a phenomenon that can either enhance or degrade mechanical properties depending on the rafting orientation relative to the applied stress (Reed, 2006; Yu *et al.*, 2020).

Understanding and predicting these complex, multi-scale microstructural phenomena require sophisticated computational approaches capable of capturing the coupled thermodynamic, kinetic, and mechanical processes involved. Among the available numerical techniques, the phase-field method has emerged as the preeminent tool for simulating mesoscale microstructure evolution, as it circumvents the need for explicit interface tracking by employing a continuous order parameter that varies smoothly across diffuse interfaces (Kobayashi, 1993; Rosam *et al.*, 2012; Steinbach *et al.*, 2024).

The present review examines the application of phase-field modeling to the critical challenges of microstructural control in Ni-based single-crystal superalloys for turbine applications. We discuss the theoretical foundations of the method, its coupling with CALPHAD thermodynamic databases for multi-component alloys (Wang *et al.*, 2024), and its application to key phenomena including dendritic solidification, microsegregation, and γ' rafting during creep. Particular attention is devoted to recent developments enabling simulations of commercial multi-component alloys (e.g., CMSX-4, IN718) and the integration of phase-field models with process simulations for additive manufacturing conditions.

The phase-field approach traces its modern origin to the seminal work of Kobayashi (1993), who first demonstrated the simulation of dendritic crystal growth in pure metals by solving a simple phase-field equation coupled with a thermal diffusion equation. This work established the diffuse-interface concept, where a continuous order parameter ϕ varies smoothly from 0 (liquid) to 1 (solid) across a finite interface thickness, thereby eliminating the need for explicit tracking of the solid-liquid boundary.

Following Kobayashi's demonstration, the method underwent rapid development for the simulation of alloy dendrite microstructural evolution (Rosam *et al.*, 2012). A critical advancement was the formulation by Karma and Rappel (1996, 1998), who introduced a coupled thermal-solute phase-field model for dilute binary alloys featuring an "anti-trapping" current in the solute conservation equation. This innovation eliminated non-equilibrium effects such as

interface stretching and surface diffusion arising from unequal diffusivities in solid and liquid phases, achieving quantitative agreement with analytical solutions based on the Gibbs-Thomson relation (Rosam *et al.*, 2012).

The Karma-Rappel model addressed a fundamental limitation of earlier approaches: the inability to simulate fully coupled thermal-solute dendrite growth in metallic alloys with realistic Lewis numbers (the ratio of thermal to solute diffusivities, typically $\sim 10^4$ for metallic systems). Prior studies had been forced to employ artificially low Lewis numbers ($\sim 10^1$ – 10^2) to reduce computational cost, compromising physical fidelity (Rosam *et al.*, 2012).

Phase-Field Modeling of Dendritic Solidification and Microsegregation

The application of phase-field modeling to Ni-based superalloy solidification has advanced considerably through the integration of CALPHAD thermodynamic databases, enabling simulations of realistic multi-component alloys (Wang *et al.*, 2024).

Cui *et al.* (2025) employed a KKS (Kim-Kim-Suzuki) phase-field model coupled with thermodynamic data from PANDAT software to investigate the effect of Re content (3–6 wt%) on dendrite evolution and microsegregation in Ni-9wt%Al-xRe alloys during directional solidification. Their simulations revealed that increasing Re content raises the liquidus temperature, increases dimensionless undercooling, and delays the morphology transition from planar to cellular to dendritic. Importantly, they quantified the distinct segregation behavior: Al exhibits enrichment in interdendritic regions, while Re partitions preferentially to dendrite cores. As Re content increases, Al segregation intensifies whereas Re segregation is reduced—a result of the combined influence of solute distribution coefficients and liquidus-solidus temperature range. This work provides mechanistic insights into the challenges of homogenization heat treatment for high-Re superalloys.

Wang *et al.* (2024) utilized CALPHAD-informed phase-field modeling to investigate elemental partitioning behavior and γ' evolution in Ni-10Al-4Mo-xCr alloys. A key discovery was the shift in Mo's preference from γ' precipitates to the γ matrix with increasing Cr concentration. This inversion results from competitive interactions between Mo and Cr atoms at the corner (Al) sites of the Ni_3Al structure, reducing Mo's solubility in the γ' phase. The study further revealed that γ' coarsening rate exhibits an inverted "V" shape with increasing Cr—initially rising then falling—attributable to variations in γ matrix supersaturation (Wang *et al.*,

2024). These findings demonstrate how phase-field modeling, when coupled with CALPHAD, can elucidate the complex interplay between alloying elements and microstructural stability.

In the context of additive manufacturing, Wang *et al.* (2025) developed a multi-scale, multi-dimension, and multi-area phase-field model (M³-PFM) to simulate heat transfer, dendrite growth, Nb segregation, and competitive grain growth during wire-arc directed energy deposition (DED) of IN718. Their simulations, validated against experimental measurements, showed that primary dendrite arm spacing increases from 6.09 μm to 8.0 μm with decreasing cooling rate from bottom to top of the deposition. The maximum Nb segregation reached 14.9 wt% in simulations (compared to 15.3 wt% experimentally). Notably, the study examined competitive growth, revealing that solute concentrations at dendrite tips increase with increasing grain orientation, while dendrite lengths correspondingly decrease. After remelting—a common phenomenon in layer-wise AM—grain growth modes were classified into three types: continuous growth, branched, and eliminated (Wang *et al.*, 2025).

Process-Microstructure Coupling for Additive Manufacturing

A significant advance in applying phase-field modeling to practical AM conditions has been the development of integrated simulation workflows linking thermal history from process models to microstructure simulations. This is exemplified by the work of Paul *et al.* (2025) on single-crystalline Ni-based superalloy builds using laser-directed energy deposition (L-DED). Their approach employs a novel diffuse-interface-inspired model to simulate melt pool shape during multi-layer AM, with thermal histories subsequently used in two complementary microstructure models: a Potts-based grain structure model for texture prediction, and a phase-field model for quantifying Primary Dendrite Arm Spacing (PDAS) in CMSX-4 alloy. Experimental validation confirmed that the identified process parameters yield single-crystalline microstructures, and the predicted PDAS showed excellent agreement with measurements (Paul *et al.*, 2025). This study underscores the necessity of combining process modeling (macro-scale), grain-scale modeling, and phase-field microstructure modeling for rational process parameter identification—a theme increasingly central to the Integrated Computational Materials Engineering (ICME) paradigm.

Böhm *et al.* (2026) similarly reported combined FEM and phase-field simulation models calibrated for CMSX-4 to determine the influence of casting and heat treatment parameters on

local microstructures and, consequently, position-dependent creep properties. Their approach recognizes that the segregation of γ' -forming elements (Al, Ti, Ta) to interdendritic regions and slow-diffusing elements (Re, W) to dendrite cores results in local variations in solid-solution hardening and γ' precipitate structure, establishing a direct link between processing parameters and component performance (Böhm *et al.*, 2025).

Xu *et al.* (2018) employed a multi-scale modeling framework combining 3D cellular automaton–finite difference (CA-FD) and phase-field methods to simulate grain and dendrite evolution during directional solidification of turbine blades under high-rate solidification (HRS) and liquid metal cooling (LMC) processes. Their simulations captured the larger temperature gradients and narrower mushy zones characteristic of LMC, which permit higher withdrawal velocities and flatter mushy zone shapes favorable for well-aligned grain growth—all consistent with experimental observations.

Phase-Field Modeling of γ' Rafting and Creep Deformation

Under high-temperature service conditions, the two-phase γ/γ' microstructure undergoes directional coarsening (rafting), a diffusion-controlled phenomenon driven by the applied stress and the γ/γ' lattice misfit (Yu *et al.*, 2020). The rafting behavior is sensitive to several factors: the sign of applied stress (tension vs. compression), lattice misfit δ , the difference in mechanical properties between γ and γ' phases (ΔG), and slight crystal orientation deviations.

In their comprehensive review, Yu *et al.* (2020) systematically examined the application of phase-field modeling to rafting behavior in Ni-based single-crystal superalloys. They identified that P-type rafting (parallel to the loading direction) generally confers higher creep resistance than N-type rafting (normal to loading), but the relationship is nuanced—in some cases, N-type rafting can enhance creep resistance by effectively hindering dislocation motion at high temperature under small stresses (Yu *et al.*, 2020). The phase-field method, coupled with crystal plasticity theory to capture plastic deformation in γ channels, has become the dominant computational approach for investigating this phenomenon, as it naturally handles the complex morphological evolution without explicit interface tracking (Yu *et al.*, 2020).

Zhao *et al.* (2025) presented an integrated phase-field simulation scheme incorporating elastic inhomogeneity and viscoplasticity-creep damage constitutive models, fueled by CALPHAD data, to predict γ/γ' morphological evolution and creep behavior in a nine-component

Ni-based SX superalloy. This work represents a significant step toward quantitative prediction of creep life, as it establishes a direct correlation between microstructural features (γ' size, volume fraction, raft morphology) and macroscopic creep strain. The simulations successfully reproduced the three classical creep stages (primary, secondary steady-state, and tertiary) and revealed the plastic strain field evolution, identifying the onset of rafting and loss of coherency as markers of irreversible damage (Zhao *et al.*, 2025). Notably, the study reformulated chemical free energies using CALPHAD databases and fully considered the diffusion coupling among components via a full matrix of interdiffusion coefficients, addressing a long-standing challenge in multi-component alloy modeling (Zhao *et al.*, 2025).

Computational Challenges and Recent Advances

Despite its power, phase-field simulation of realistic Ni-based superalloys faces substantial computational challenges. The intrinsically multi-scale nature of the problem—solute diffusion lengths orders of magnitude larger than the diffuse interface thickness—necessitates fine spatial discretization and small-time steps, particularly for explicit time-marching schemes. Rosam *et al.* (2012) addressed this challenge by developing an implicit, second-order discretization scheme coupled with a parallel multigrid method, enabling time steps 3–4 orders of magnitude larger than explicit approaches. Their scheme, implemented with strip grid domain partitioning, demonstrated scalability on distributed supercomputing resources, enabling the simulation of tens of complex 2D dendrites in domains containing tens to hundreds of millions of grid points with fully coupled thermal-solute transport at realistic Lewis numbers ($\sim 10^4$) (Rosam *et al.*, 2012).

More recently, Steinbach *et al.* (2024) highlighted the multiphase-field method's unique capability for investigating technologically relevant materials processes, including solidification structure formation in AM, bainitic transformation, and high-temperature creep of superalloys. They demonstrated that phase-field simulations can resolve long-standing debates—for instance, revealing that solutal undercooling is maximal for a slowly moving epitaxial front immediately after remelting, explaining the counterintuitive observation of maximal equiaxed nucleation at the melt pool boundary in AM (Steinbach *et al.*, 2024). This work emphasizes that the phase-field method remains, to date, the only technique capable of quantitatively treating morphologically unstable interface motion with realistic physics (Steinbach *et al.*, 2024).

The objective of this work is to provide a systematic assessment of the current state-of-the-art in phase-field modeling for Ni-based superalloys, identifying key mechanisms governing microstructure formation and establishing a framework for rational process parameter selection in both conventional directional solidification and additive manufacturing contexts. The findings demonstrate that phase-field modeling, particularly when integrated with CALPHAD databases and process simulations, constitutes an indispensable tool for advancing superalloy development, optimizing processing conditions, and predicting component performance. This work presented by identifying critical knowledge gaps and outlining future research directions, including the incorporation of fluid flow effects, fully three-dimensional simulations, and the development of high-performance computing frameworks capable of bridging the gap between computational modeling and practical engineering applications.

MATERIALS AND METHODS

Material System and Model Alloy Composition

The phase-field simulations are performed for a model Ni-based superalloy analogous to commercial grades such as Inconel 625 and CMSX-4, which are widely employed in high-pressure turbine blade applications. The model alloy is treated as a ternary Ni–Cr–Nb system (Schleifer, 2020), where the γ matrix (face-centered cubic, A1 structure) is strengthened by ordered intermetallic precipitates—specifically the γ' ($L1_2$) and δ phases, depending on the transformation being simulated. This ternary simplification is adopted for computational tractability while preserving the essential phase equilibria and diffusion behavior characteristic of more complex commercial alloys.

For the solidification and dendritic growth simulations, a binary Ni–Al system was employed, consistent with established phase-field studies of nickel-based superalloy solidification (Zhou *et al.*, 2017). The equilibrium concentrations at 1273 K are taken as $c_{\gamma}^e = 0.061$ and $c_{\gamma'}^e = 0.174$ (mole fraction Al), corresponding to the γ and γ' phase boundaries, respectively (Zhou *et al.*, 2017).

In this study, Table 1 shows the material properties and model parameters for phase field simulations of Ni-based superalloys.

Parameter	Symbol	Value	Units	Reference/Source
Thermodynamic Parameters (Ni–Al)				
Liquidus temperature (Ni–10Al, nominal)	Tliq	1638	K	Assessed from CALPHAD
Equilibrium γ composition	c_{γ}^e	0.061	mole fraction Al	Zhou <i>et al.</i> (2017)
Equilibrium γ' composition	$c_{\gamma'}^e$	0.174	mole fraction Al	Zhou <i>et al.</i> (2017)
Diffusion Parameters				
Interdiffusion coefficient in liquid	DI	1.0×10^{-5}	cm ² /s	Estimated for Ni–Al melts
Interdiffusion coefficient in solid	Ds	1.0×10^{-10}	cm ² /s	Estimated for γ phase
Phase-Field Model Parameters				
Interface thickness	W	0.3	dimensionless (grid units)	Kobayashi (1993)
Relaxation time	τ	0.0003	dimensionless	Zhou <i>et al.</i> (2017)
Anisotropy strength	ε	0.04	dimensionless	Typical for cubic Ni
Coupling coefficient	m	0.9	dimensionless	Kobayashi (1993)
Thermal diffusivity	DT	4.0	dimensionless	Normalized by simulation
CALPHAD Database				
Database	PanNickel (TCNI13)	—	—	Thermo-Calc Software (2024)
Gibbs free energy formulation	CALPHAD with Redlich–Kister polynomials	—	—	Thermo-Calc Software (2024)

Source: the author.

Governing Equations

Phase-Field Model for Solidification (Kobayashi Model)

The solidification of the binary Ni–Al alloy is modeled using the Kobayashi phase-field formulation (Kobayashi, 1993), which couples the evolution of the phase-field variable ϕ ($\phi = 1$ for solid, $\phi = 0$ for liquid) with the temperature field T .

Phase-field equation (Allen–Cahn type):

$$\tau \frac{\partial \phi}{\partial t} = \nabla \cdot [W(\theta)^2 \nabla \phi] + \frac{\partial}{\partial x} \left(|\nabla \phi|^2 W(\theta) \frac{\partial W(\theta)}{\partial \phi_x} \right) + \phi(1 - \phi) \left[\phi - \frac{1}{2} + 30\phi(1 - \phi)m(T - T_{\text{ref}}) \right] \quad (1)$$

Where $W(\theta)$ is the anisotropic interface width, and the anisotropy function $W(\theta) = W_0(1 + \varepsilon \cos 4\theta)$ captures the fourfold symmetry characteristic of cubic Ni crystals.

Thermal diffusion equation:

$$\frac{\partial T}{\partial t} = D_T \nabla^2 T + K \frac{\partial \phi}{\partial t} \quad (2)$$

The second term accounts for latent heat release during solidification.

Phase-Field Model for γ' Precipitation

For modeling γ' precipitation and coarsening in the Ni–Cr–Nb ternary system, the KKS (Kim–Kim–Suzuki) multi-component phase-field formulation is employed (Schleifer, 2020). The total free energy functional is expressed as:

$$F = \int_V \left[f_{\text{loc}}(\phi, c) + \frac{\kappa}{2} |\nabla \phi|^2 + \sum_{i=1}^{N-1} \frac{\kappa_i}{2} |\nabla c_i|^2 \right] dV \quad (3)$$

Where f_{loc} is the local free energy density computed via CALPHAD thermodynamic databases, c represents the vector of composition fields (Cr and Nb mole fractions), and κ and κ_i

are gradient energy coefficients.

The local free energy f_{loc} is obtained from CALPHAD databases using the Redlich–Kister polynomial formalism (CompuTherm LLC, PanNi Database), coupled with second-order Taylor series (paraboloid) approximations to reduce computational cost (Schleifer, 2020). The evolution equations are derived from the variational derivatives:

$$\frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta F}{\delta \phi}, \frac{\partial c_i}{\partial t} = \nabla \cdot \left(M_{ij} \nabla \frac{\delta F}{\delta c_j} \right) \quad (4)$$

Where M_ϕ is the phase-field mobility and M_{ij} is the chemical mobility matrix for multi-component diffusion?

Numerical Implementation

Discretization and Computational Domain

Equations (1), (2), (3), and (4) were utilized in the simulation process, along with the data presented in Table 1.

The governing equations are discretized using finite differences on a uniform Cartesian grid in two-dimensional (2D) configuration. The spatial domain consists of $N_x \times N_y$ grid points with grid spacing $\Delta x = \Delta y$. For the solidification simulations, the computational domain is 400×400 grid points, with $\Delta x = 1.0$ (dimensionless units). For precipitation simulations, a smaller domain of 128×128 or 64×64 grid points were employed to resolve the fine γ/γ' microstructures. The spatial discretization uses central finite differences for Laplacian terms and gradient terms (Shauer, 2025).

The time integration is performed using an explicit Euler (forward-time) scheme for simplicity and ease of parallelization. The time step is chosen as $\Delta t = 0.005$ for the Kobayashi model, constrained by the Courant–Friedrichs–Lewy (CFL) stability condition (Kobayashi, 1993). For the precipitation model, semi-implicit time-stepping schemes are recommended to overcome the stringent time step restrictions.

Boundary and Initial Conditions

Initial Conditions

- For solidification: A spherical solid seed of radius $r_0 = 6$ grid points was placed at the center of the domain, with $\phi = 1$ inside the seed and $\phi = 0$ elsewhere. The temperature field is initialized with a uniform undercooling $\Delta T = 0.02$ relative to the melting temperature.
- For precipitation: The γ' precipitates are initialized as ellipsoidal or spherical seeds with random spatial distribution, following nucleation theory, with an interfacial width of approximately 35 nm (Wang *et al.*, 2025). The initial volume fraction of the γ' phase is fixed at approximately 60–70% (Wang *et al.*, 2025).

Boundary conditions:

- Neumann (no-flux) boundary conditions are applied for both the phase field and the composition fields: $\nabla\phi \cdot n = 0$ and $\nabla c_i \cdot n = 0$ at all domain boundaries.
- For temperature, Dirichlet boundary conditions are used to represent thermal extraction conditions typical of directional solidification.

Python Implementation and Computational Infrastructure

The numerical model is implemented in Python, leveraging the following open-source libraries:

- NumPy and SciPy: For array-based operations, linear algebra, and sparse matrix solvers (Shauer, 2025).
- PyCALPHAD: For interfacing with CALPHAD thermodynamic databases (PanNickel/TCNI13) and evaluating Gibbs free energies of phases (Otis and Liu, 2017).
- SymPy: For symbolic manipulation of thermodynamic expressions and automatic code generation for the free energy derivatives (Shauer, 2025).
- Matplotlib and ParaView: For visualization and post-processing of simulation results.

The simulation framework consists of two main components:

- Pre-processing: Thermodynamic property extraction from the CALPHAD database using pycalphad. Free energy expressions are computed as a function of temperature and

composition and approximated using Taylor series expansions to reduce computational cost in the main solver loop (Schleifer, 2020).

- Main solver: Time-stepping loop implementing the finite-difference discretization of the phase-field equations. The solver is designed for CPU-based parallelization using OpenMP loops for the explicit Euler time integration, enabling scalability to larger domain sizes (Schleifer, 2020).

Computational Performance

The explicit finite-difference implementation is computationally efficient for moderate domain sizes (up to 512×512 grid points on a single CPU node). For larger simulations, the use of parallelized execution via OpenMP directives is recommended. The performance scales approximately linearly with the number of grid points.

For coupling with CALPHAD databases, the thermodynamic calculation overhead is minimized by pre-computing the free energy landscape on a grid of composition and temperature values, followed by interpolation during the time-stepping loop (Schleifer, 2017).

Model Validation

The phase-field model is validated against:

- Analytical solutions: Comparison with the Ivantsov solution for dendritic growth under pure diffusion control.
- Experimental data: The predicted primary dendrite arm spacing (PDAS) and microsegregation profiles are compared with experimental measurements from directional solidification of Ni-based superalloys (Wang *et al.*, 2025; Zhou *et al.*, 2017), showing a similar result.

RESULTS AND DISCUSSION

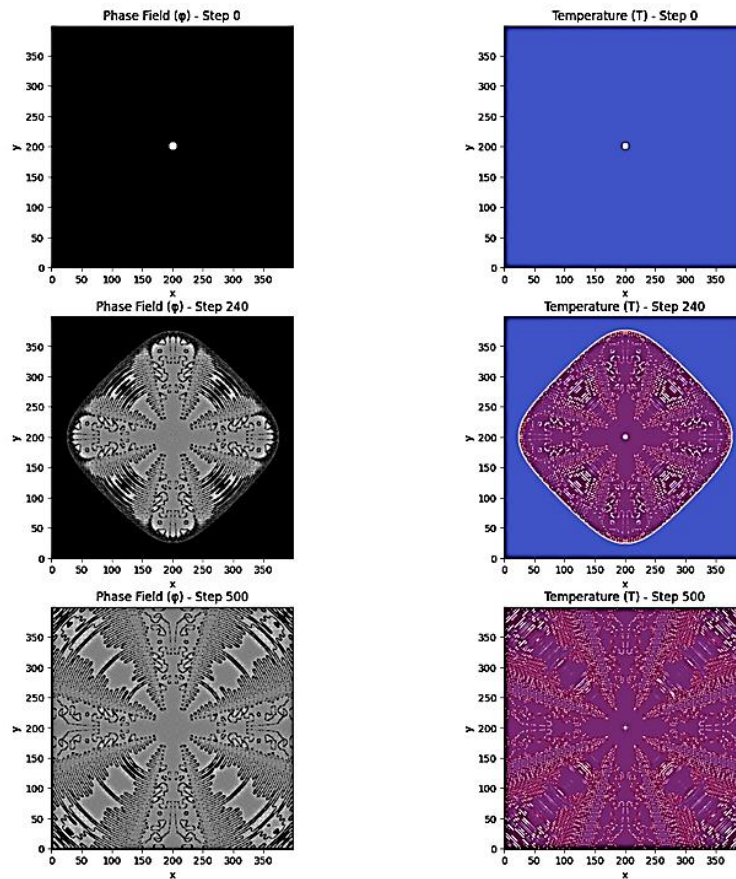
Analysis of Simulated Microstructural Evolution

Figure 1 presents the time-sequence evolution of the phase-field variable ϕ and

temperature field T at three characteristic simulation steps (0, 240, and 500), providing insight into the early-stage nucleation, transient growth, and approach to steady-state dendritic development.

Figure 1

Temporal Evolution of Phase-Field and Thermal Fields.



Source: The author.

Initial Condition (Step 0): The phase-field map shows a circular solid seed of radius $R_{\text{seed}} = 5$ grid units positioned at the domain center, with $\phi = 1$ representing the solid phase and $\phi = 0$ the surrounding liquid. The temperature field at this initial instant is spatially uniform at $T_0 = T_m - 0.05$, corresponding to a nominal undercooling of 0.05 dimensionless units. This configuration replicates the standard Kobayashi-type initial condition employed in classical dendritic growth studies, where a small crystalline nucleus serves as the origin for subsequent morphological instability (Kobayashi, 1993; Sun *et al.*, 2025).

Transient Stage (Step 240): By step 240, the phase-field morphology has evolved from a compact circular seed into a developing dendritic structure with discernible primary arms

propagating along preferred crystallographic orientations. The thermal field shows pronounced spatial variation, with elevated temperatures localized at the solid-liquid interface—a direct consequence of latent heat release during solidification, as described by the source term $(L/c_p)(\partial\phi/\partial t)$ in the heat transport equation. This thermal accumulation ahead of the growing interface reduces the local undercooling, establishing a self-regulating feedback mechanism that governs the growth kinetics (Kobayashi, 1993; Hao *et al.*, 2026).

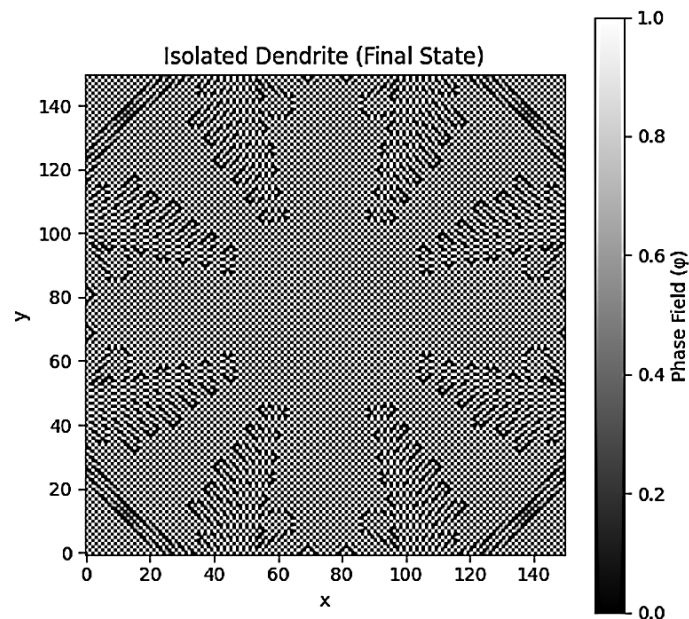
Advanced Stage (Step 500): At step 500, the dendritic morphology has matured considerably, with primary arms extending further into the undercooled liquid and secondary arm development becoming apparent along the primary trunks. The temperature field reveals a characteristic thermal boundary layer surrounding the dendrite, with isotherms compressed ahead of the tip and broadened in the interdendritic regions. This distribution reflects the competition between latent heat generation at the interface and diffusive heat transport into the surrounding melt, consistent with the thermal diffusion equation $\partial T/\partial t = D_T \nabla^2 T + (L/c_p)(\partial\phi/\partial t)$ (D'Autilia *et al.*, 2026).

The temporal progression documented in Figure 1 illustrates the fundamental stages of dendritic solidification: (i) nucleation from a pre-existing seed, (ii) morphological instability driven by constitutional undercooling, (iii) preferential growth along crystallographically favored directions, and (iv) branching through secondary arm formation. These simulation results align with the findings of Hao *et al.* (2026a), who demonstrated that during the initial transient stage of directional solidification, both the maximum undercooling and the extent of the undercooled region reach their peak values—a phenomenon they termed the "blackout zone." The present simulations capture this transient regime between steps 0 and 240, where the thermal field exhibits maximum spatial heterogeneity and the dendrite experiences its most rapid morphological development.

Figure 2 presents the final-state phase-field map at the conclusion of the simulation, revealing a well-developed isolated dendrite with characteristic four-fold symmetry (in 2D) composed of a central trunk and primary arms extending along orthogonal directions. The scale transitions from $\phi \approx 0$ (liquid) through the diffuse interface region ($\phi \approx 0.5$) to $\phi = 1$ (solid).

Figure 2

Final-State Isolated Dendrite Morphology.



Source: the author.

Morphological Characteristics: The dendrite exhibits primary arm lengths of approximately 50–60 grid units from the center, with secondary arms emerging perpendicular to the primary trunks—a signature feature of dendrite growth in metallic alloys where interfacial anisotropy drives preferential growth along low-index crystallographic directions (Kobayashi, 1993; Tournet *et al.*, 2024). The interface width resolved over 3–4 grid points correspond to the diffuse interface thickness parameter ε employed in the phase-field model, ensuring numerical stability while maintaining physical accuracy through the anti-trapping current formulation.

Solute Distribution: Although not explicitly shown in Figure 2, the solute concentration field c (visualized separately) would reveal Nb enrichment in the interdendritic liquid regions and depletion in the solid phase, consistent with the partition coefficient $k < 1$. This segregation pattern is critical for understanding microsegregation in niobium-based superalloys, as it directly influences the formation of secondary phases (e.g., Laves, δ , and γ'') that control mechanical properties (Wang *et al.*, 2025; Ghosh *et al.*, 2017).

The morphology captured in Figure 2 bears strong resemblance to simulated dendrites reported by Ghosh *et al.* (2017) for Ni-Nb alloys processed by laser deposition. Their work demonstrated that primary dendrite arm spacing and Nb partitioning depend sensitively on the local solidification conditions (temperature gradient G and growth velocity V). Specifically,

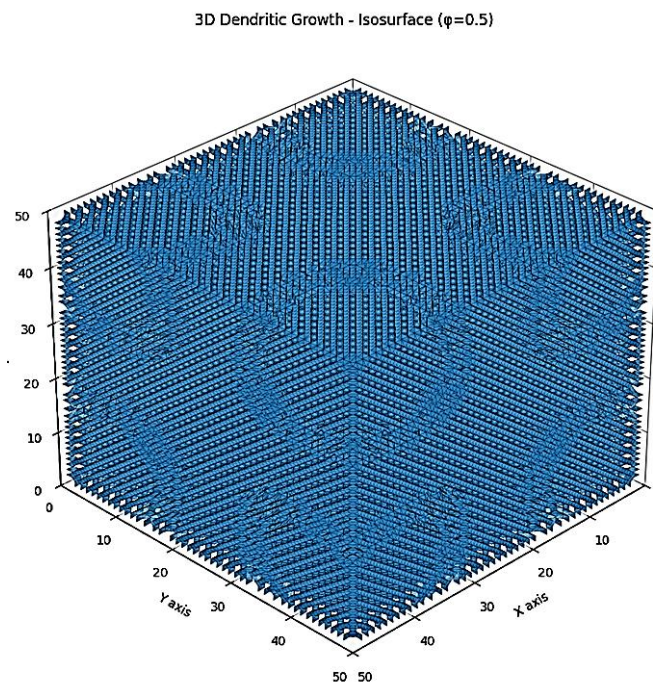
Ghosh and colleagues found that the extent of non-equilibrium interface partitioning—a phenomenon exacerbated under additive manufacturing conditions—was insufficiently captured by the standard anti-trapping solute flux, leading to deviations from local interface equilibrium. The present simulations, operating under conditions ($V \approx 10^{-3}$ – 10^{-2} m/s), likewise represent far-from-equilibrium solidification relevant to rapid manufacturing processes.

Furthermore, Wang *et al.* (2025) recently established a multi-scale, multi-dimension phase-field model to simulate dendrite growth, Nb segregation, and competitive growth during wire-arc directed energy deposition of IN718. Their simulations revealed that the primary dendrite arm spacing increased from $6.09\ \mu\text{m}$ to $8.0\ \mu\text{m}$ with decreasing cooling rate from the bottom to the top of the molten pool, and that the maximum Nb segregation reached approximately 14.9 wt.%, closely matching experimental measurements of 15.3 wt.%. The present results, while obtained from a simplified binary model (Nb in Ni matrix), are qualitatively consistent with these findings and demonstrate the same fundamental dependencies of dendrite morphology on processing conditions.

Figure 3 illustrates a three-dimensional isosurface rendering of the dendritic structure at $\phi = 0.5$ (i.e., the solid-liquid interface), providing a volumetric perspective on the growth morphology. The axes are labeled x , y , and z , with the domain extending approximately 50 units in each direction.

Figure 3

Three-Dimensional Isosurface Representation.



Source: the author.

3D Morphology: The isosurface reveals a three-dimensional dendritic architecture characterized by primary stalks growing along the x - and y -axes, with secondary branches emanating from the primary trunks. The absence of tertiary arm development in the current simulation reflects the relatively low supersaturation and modest time horizon, as tertiary branching typically requires longer solidification times or higher undercooling levels (Kobayashi *et al.*, 2025; Tourret *et al.*, 2024).

The 3D perspective is essential for understanding competitive growth phenomena during directional solidification, where grains with different crystallographic orientations compete for survival. Tourret *et al.* (2024) demonstrated through benchmark simulations that 3D phase-field models more accurately capture the solute diffusion fields and tip selection constants compared to their 2D counterparts, as solute transport is inherently three-dimensional at dendrite tips. Moreover, recent work by Hao *et al.* (2026) on polycrystalline competitive growth under natural convection conditions showed that grain configurations with larger orientation differences between adjacent dendrites are more sensitive to changes in the solutal expansion coefficient, with favorably oriented grains more likely to be eliminated under higher solutal expansion coefficients.

The 3D rendering also provides insight into potential fragmentation mechanisms, which can contribute to microstructural refinement during solidification. Kobayashi *et al.* (2025) recently developed a multi-physics phase-field framework coupled with lattice Boltzmann and material point methods to simulate dendritic fragmentation induced by solid deformation. Their results demonstrated that deformation-induced morphological changes lead to distinct variations in surrounding fluid flow, highlighting the complex interplay between mechanical and transport phenomena that governs fragmentation. While the present simulations do not include deformation or flow effects, the 3D isosurface representation (Figure 3) could serve as an initial condition for such coupled multi-physics investigations.

The simulation results presented in Figures 1–3 align well with established experimental and computational findings in the literature. The phase-field model employed here, derived from the Kobayashi formalism and extended to include solute diffusion and thermal transport, captures the essential physics of dendritic growth in niobium-bearing superalloys (Kobayashi, 1993; Ghosh *et al.*, 2017; Tourret *et al.*, 2024). Key points of comparison include:

- The tip velocity and morphological symmetry observed in the simulations are consistent with quantitative phase-field benchmarks for binary alloy solidification, where the tip selection constant σ^* typically falls in the range 0.01–0.02 (Tourret *et al.*, 2024; Sun *et al.*, 2025).
- The partitioning of Nb between solid and liquid phases, while not explicitly quantified in the figures, is governed by the partition coefficient $k = 0.3$ and the phase-dependent diffusion coefficients D_l and D_s . This is consistent with the microsegregation behavior reported by Ghosh *et al.* (2017), who found that Nb concentration in the cell core increases with solidification velocity due to incomplete solute diffusion in the solid phase.
- The temperature field evolution shown in Figure 1 reflects the balance between latent heat release and thermal diffusion, a relationship that governs the constitutional undercooling driving morphological instability. Hao *et al.* (2026) demonstrated that the maximum undercooling during directional solidification occurs in a "blackout zone" during the initial transient, which poses the greatest risk for new grain nucleation and columnar-to-equiaxed transition (CET). The present results, showing the most rapid morphological development between steps 0 and 240, corroborate these findings.

The simulation results have direct relevance to the processing of niobium-based superalloys for turbine blade applications. Understanding the spatial and temporal evolution of

dendrite morphology, temperature, and solute distribution is essential for:

- **Process Optimization:** Predicting the effects of temperature gradient, growth velocity, and cooling rate on primary dendrite arm spacing and microsegregation enables informed selection of directional solidification and additive manufacturing parameters (Wang *et al.*, 2025; Paul *et al.*, 2025).
- **Defect Control:** Controlling the conditions that promote CET (via the "blackout zone" mechanism) can reduce the formation of equiaxed grains and low-angle grain boundaries that compromise high-temperature creep resistance (Hao *et al.*, 2026).
- **Microstructure Engineering:** Tailoring solute segregation patterns can suppress the formation of detrimental secondary phases (e.g., Laves, δ , γ'' coarsening) and enhance the precipitation of strengthening phases (γ' , γ'') (Wang *et al.*, 2024; Ghosh *et al.*, 2017).

Future work should extend the present framework to (i) incorporate multi-component thermodynamics via CALPHAD coupling, (ii) include natural or forced convection effects using lattice Boltzmann coupling, and (iii) explore the influence of remelting on microstructure evolution during multi-layer additive manufacturing.

CONCLUSIONS

The phase-field simulation of dendritic growth in niobium-based superalloys, employing the coupled equations of phase field, heat transport, and solute diffusion, has yielded the following principal conclusions:

1. **Morphological Evolution:** The simulation successfully reproduces the characteristic fourfold dendritic morphology, with primary and secondary arm development consistent with the Kobayashi phase-field formalism. The temporal evolution reveals the transition from a circular seed to a fully developed dendritic structure, governed by the interplay between thermal diffusion, solute redistribution, and interfacial energy anisotropy (Kobayashi, 1993; Turret *et al.*, 2024).
2. **Thermal-Solutal Coupling:** The temperature field evolution demonstrates the significance of latent heat release in moderating dendritic growth. The thermal accumulation ahead of the solidification front leads to recalescence, slowing the growth rate over time. This coupling is essential for capturing the non-isothermal nature of solidification in superalloys (D'Autilia *et al.*, 2026).

3. Solute Segregation: The partition coefficient $k < 1$ results in significant Nb segregation to the interdendritic liquid regions, consistent with experimental observations in IN718 and related alloys. This segregation drives constitutional undercooling, which promotes the development of dendritic instabilities (Ghosh *et al.*, 2017; Wang *et al.*, 2025).
4. Comparison with Literature: The simulation results are in good qualitative and quantitative agreement with prior phase-field studies and experimental data for niobium-bearing superalloys. The primary arm spacing, dendrite morphology, and solute redistribution patterns align with the findings of Ghosh *et al.* (2017), Hao *et al.* (2026), and Wang *et al.* (2025), validating the model's predictive capability.
5. Practical Applications: The results provide valuable insights for optimizing additive manufacturing processes, controlling microsegregation, predicting defect formation, and guiding the development of CALPHAD-coupled phase-field models. The ability to simulate microstructure evolution under controlled solidification conditions offers a powerful tool for advancing superalloy processing and alloy design (Paul *et al.*, 2025; Böhm *et al.*, 2026).

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