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Three-dimensional dendritic needle network model for alloy solidification

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ABSTRACT

We present a three-dimensional (3D) formulation of the multiscale Dendritic Needle Network (DNN) model for dendritic microstructure growth. This approach is aimed at simulating quantitatively the solidification dynamics of complex hierarchical networks in spatially extended dendritic arrays, hence bridging the scale gap between phase-field simulations at the scale of a few dendrites and coarse-grained simulations on the larger scale of entire polycrystalline structures. In the DNN model, the dendritic network is represented by a network of branches that interact through the solutal diffusion field. The tip velocity $V(t)$ and tip radius $\rho(t)$ of each needle is determined by combining a standard solvability condition that fixes the product $\rho^2 V$ and a solute flux conservation condition that fixes the product ρV^2 in 2D and ρV in 3D as a function of a solutal flux intensity factor $\mathcal{F}(t)$. The latter measures the intensity of the solute flux in the dendrite tip region and can be calculated by contour (2D) or surface (3D) integration around the tip of each needle. We first present an extended formulation of the 2D DNN model where needles have a finite thickness and parabolic tips. This formulation remains valid for a larger range of tip Péclet number than the original thin needle formulation and is readily extended to 3D needles with paraboloidal tips. The 3D DNN model based on this thick-needle formulation is developed for both isothermal and directional solidification. Model predictions are validated by comparisons with known analytical solutions that describe the early transient and steady-state growth regimes. We exploit the power of the DNN model to characterize the competitive growth of well-developed secondary branches in 3D on the scale of the diffusion length. The results show that the length of active secondary branches increases as a power law of distance behind the tip with an exponent in good quantitative agreement with experimental measurements. Finally, we apply the model to simulate the three-dimensional directional solidification of an Al-7wt% Si alloy, which we directly compare to observed microstructures from microgravity experiments onboard the International Space Station. The predictions of selected microstructural features, such as dendrite arm spacings, show a good agreement with experiments. The computationally-efficient DNN model opens new avenues for investigating the dynamics of large dendritic arrays at length and time scales relevant to solidification experiments and processes.

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1. Introduction

Dendritic microstructures are the most common among cast metals and alloys [1,2]. The geometrical features of these structures arise from a subtle interplay between microscopic interfacial phenomena and macroscopic solute and heat transport, and are crucial to mechanical properties of a cast part, and subsequently to its performance during service [1,3,4]. Within a grain, interactions among individual dendritic branches determine its inner structure, such as the primary spacing crucial for the mechanical strength of a dendritic grain. In polycrystalline microstructures too, long range interactions between the growing dendrites play a key role in shaping the grain structure that critically influences the mechanical properties of a material. Hence, our ability to understand, predict, and control the microstructure selection mechanisms across all critical length and time scales is key to develop innovative materials and processes.

At the scale of an entire solidification process or experiment, computational approaches include continuum models [5–8],

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models based on dynamics of average dendritic grain envelopes [9–13], and approaches coupling cellular automata with finite elements [14–16], finite differences [17], or Lattice Boltzmann methods [18,19]. This type of models can be used at the scale of a dendritic array to investigate mechanisms of intragrain [17] or intergrain [20] microstructure selection up to the scale of entire casting experiments, thus providing average statistical predictions of microstructure selection by complex phenomena such as the columnar-to-equiaxed transition [21]. However, those volume-averaged equilibrium-based models do not resolve quantitatively the transient interactions between individual dendritic branches that are crucial to dendritic microstructure selection.

At a smaller scale, the phase-field (PF) approach is the method of choice to quantitatively simulate complex solid-liquid interface patterns [22]. The theoretical development of the thin-interface limit [23,24] and the anti-trapping current for alloy solidification [25–27], combined with advanced numerical techniques such as adaptive meshing [28,29] and massive parallelization [30,31], now enable quantitative PF predictions at the scale of spatially extended three-dimensional arrays of cells [32,33] and dendrites [34,35]. However, quantitative predictions of dendritic growth dynamics with PF require an accurate morphological description of each dendrite tip, which makes simulations extremely challenging for concentrated alloys that usually solidify as a hierarchical network of thin branches with several orders of magnitude separating the scale of a dendrite tip radius and the larger scale of diffusive transport in the melt.

In order to bridge the scale gap between phase-field and coarse-grained models, we recently developed a multiscale Dendritic Needle Network (DNN) approach that quantitatively predicts the dynamics of individual branches in complex dendritic networks during alloy solidification at a scale much larger than the diffusion length. This model, first developed in 2D [36,37], is rigorously valid as long as the dendrite tip Péclet number remains relatively small, which is the case for many common processing conditions. Hence, the approach is well suited to describe concentrated alloys where dendrites form hierarchical tree-like structures with several generations of needle-like branches.

In this approach, a dendritic grain, such as the crystal in Fig. 1a [38], is modeled as a network of thin needles, as in Fig. 1b. The dynamics of each needle tip is prescribed by two conditions that jointly determine the evolution of its velocity $V(t)$ and radius $\rho(t)$.

The first condition is a solute conservation equation formulated at an intermediate scale much larger than the dendrite tip radius ρ and much smaller than the diffusion length D/V, with D the solute diffusion coefficient in the liquid (Fig. 1c). In 2D, this condition links the product ρV^2 to a flux intensity factor $\mathcal{F}(t)$ that measures the strength of the incoming solute flux at the tip [36]. The value of $\mathcal{F}(t)$ can be calculated using a contour integral around the tip, e.g. in Ref. [36] using the J-integral classically used in fracture mechanics to compute stress intensity factors at the tip of a crack [40].

The second condition, formulated at the scale of the dendrite tip (Fig. 1d), is a standard microscopic solvability condition for the existence of a solution to the shape-preserving growth of a parabola/paraboloid. It relates the product $\rho^2 V$ to the strength of surface tension anisotropy [41–43]. While $\rho^2 V$ remains constant in the DNN model, the flux intensity factor $\mathcal{F}(t)$ at each needle tip evolves with the surrounding solutal field, hence enabling the approach to capture long-range diffusive interactions between branches in both transient and steady-state growth regimes.

The DNN model derives its efficiency from the fact that the solid-liquid interface is not explicitly tracked and that the diffusion field can be discretized on a scale comparable to or larger than ρ. In comparison, phase-field typically requires a computational grid size one order of magnitude smaller than the tip radius for a reliable

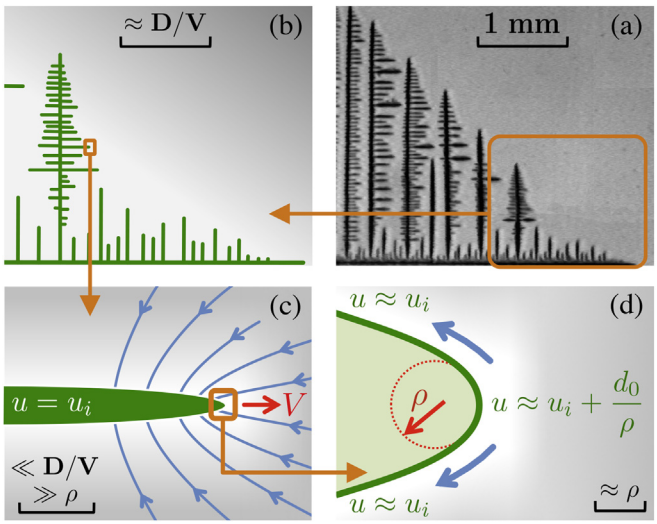

Fig. 1. The Dendritic Needle Network model represents a dendritic grain, like the ammonium-bromide crystal from Ref. [38] in (a), as a hierarchical network of needle-like branches interacting through the long range diffusion field, as illustrated in (b). The instantaneous tip radius $\rho(t)$ and velocity $V(t)$ of each branch is established by combining two conditions at distinct length scales: (c) a solute conservation condition at an intermediate scale larger than the tip radius ρ, but smaller than the diffusion length D/V (indicated with the $\gg\rho$ and $\ll D/V$ scale bar labels, respectively), and (d) a solvability condition at the scale of the tip radius ρ.

morphological description of the dendrite tip and hence of its growth dynamics [24,44]. This leads to DNN simulations faster than PF simulations by four to five orders of magnitude in 2D and 3D, respectively, if both models are discretized on a finite-difference grid using an explicit time stepping.

In this article, we present a three-dimensional formulation of the DNN model. In Section 2, we summarize the sharp interface solidification problem and the two-dimensional model as presented in Ref. [36]. Then, we propose a new 2D formulation for thick branches with parabolic tips. This thick-needle formulation has the dual benefit that it increases the range of tip Péclet number where the DNN approach is quantitatively valid and that it can be readily extended to 3D where branches have paraboloidal tips. We provide details of our first numerical implementation in Section 3. In Section 4, we validate the DNN predictions through comparisons with analytical solutions in a steady-state growth regime and with an analytical scaling law for the early stage transient growth of an equiaxed 3D grain with six branches growing along principal crystal axes. In Section 5, we compare the predicted dynamics of secondary sidebranches against experimental measurements of dendritic envelope shapes. Then, in Section 6, we apply the DNN model to a fully three-dimensional directional solidification experiment of an Al-7wt% Si alloy, and directly compare the results to microgravity experiments performed in the framework of the CETSOL project [45–47] (Columnar-to-Equiaxed Transition in SOLidification Processing). Finally, in Section 7, we summarize our results and discuss further investigations made possible by this new modeling approach.

2. Modeling

2.1. Sharp-interface solidification model

We consider the solidification of a binary alloy in a purely diffusive regime with negligible diffusion in the solid phase, such that the solute concentration c in the liquid follows the diffusion equation