Editor's Choice

# Three-dimensional mesoscopic modeling of equiaxed dendritic solidification of a binary alloy

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## ARTICLE INFO

## ABSTRACT

The mesoscopic envelope model is a recent multiscale model that is intended to bridge the gap between purely microscopic and macroscopic approaches for the study of dendritic solidification. It consists of the description of a dendritic grain by an envelope that links the active dendrite branches. The envelope growth is deduced from an analytical microscopic model of the dendrite tip growth kinetics matched to the numerical solution of the mesoscopic solute concentration field in the vicinity of the envelope. The branched dendritic structure inside the envelope is described in a volume-averaged sense by phase fractions and averaged solute concentrations. We present a careful quantitative analysis of the influence of numerical and model parameters on the accuracy of the model predictions. We further perform a validation study through comparisons of 3D simulations to experimental scaling laws giving the shape and the internal solid fraction of freely growing binary alloy dendrites and to analytical solutions for the primary dendrite tip speed. We provide generally valid guidelines for the calibration of the mesoscopic model, enabling reliable control of the accuracy of model predictions over a wide range of undercoolings. The model is applied to simulate strong solutal interactions in large ensembles of equiaxed grains. The potential for mesoscopic simulations to provide refined modeling of microstructures in volume-averaged macroscopic models via scale bridging is demonstrated.

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## 1. Introduction

Dendritic (treelike) crystals or grains are the most common growth form in solidification of metal alloys. Their growth is governed by an intricate interplay between diffusion or convection of heat and chemical species (solutes) and capillary effects. Furthermore, in castings the growth of dendritic crystals is influenced by adjacent grains. The grains can "feel" each other due to the overlap of thermal and solutal fields surrounding each growing grain. Analytical solutions of dendritic growth are limited to the description of a single isolated dendrite tip that grows by diffusion in an infinite, uniformly undercooled melt [1,2].

Complex dendritic structures can be simulated directly by phase-field methods, which directly resolve the dendritic structure in detail but are computationally expensive. These and other microscopic methods thrived and matured in the last decade [3–5]. Phase-fields methods have become the most common approach

to the numerical simulation of dendrite growth. However, because phase-field methods need a very fine mesh, computing and memory requirements are large. Most simulations are limited to the scale of a few dendrites, to two dimensions and purely diffusive conditions. Only recently simulations of large ensembles of grains in 3D have been reported [6,7]. They required complex high-performance parallel computing algorithms and massive supercomputing resources.

Other common approaches are cellular-automaton and volume-averaged models [8–13] that can simulate the growth of multiple dendrites on the scale of an entire casting but at the expense of simplifications. These methods are not able to predict accurate grain shapes and rely on very approximate relations for modeling grain interactions.

A simulation tool for dendritic solidification that is intended to bridge the gap between purely microscopic and macroscopic approaches is given by the so-called mesoscopic solidification model of Steinbach, Beckermann and coworkers [14–16]. This model relies on the description of a dendritic grain by its envelope, which is a smooth surface connecting all of the actively growing dendrite tips. An example of interacting three-dimensional

## Nomenclature

*Greek Letters*

| | |
|---|---|
| $\Gamma$ | Gibbs–Thomson coefficient |
| $\delta$ | stagnant film thickness (distance between the envelope and the confocal envelope) |
| $\delta_{env}$ | distance to the envelope |
| $\delta_l$ | volume-averaged diffusion length at the envelope |
| $\theta$ | angle between the envelope normal and the tip growth direction |
| $\sigma^*$ | tip selection parameter |
| $\tau$ | dimensionless time scaled by $D_l/V_{LGK}^2$ |
| $\tau_d$ | dimensionless time of departure from free growth |
| $\tau_{\psi_{min}}$ | dimensionless time of minimum sphericity |
| $\phi$ | phase indicator field |
| $\Psi$ | average envelope sphericity |
| $\Omega$ | supersaturation |
| $\Omega_0$ | initial supersaturation |
| $\Omega_\delta$ | supersaturation at the confocal envelope |
| $\Omega_\infty$ | supersaturation at infinity |

*Latin letters*

| | |
|---|---|
| $A_1$, $A_2$ | amplification factors in the dendrite scaling laws |
| $b$, $b_{lim}$ | stabilization parameter and its stability limit |
| $C$ | solute concentration |
| $\langle C_l \rangle^e$ | average solute concentration in the extradendritic liquid |
| $Co_\phi$ | courant number of the phase indicator field |
| $D$ | solute diffusion coefficient |
| $d_0$ | capillary length |
| $\bar{d}_{cc}$ | mean distance between grain centers |
| $F$ | projection area of the solid phase |
| $Fo_{\Delta x}$ | grid Fourier number |
| $g$ | volume fraction |
| $k_p$ | equilibrium solute partition coefficient |

| | |
|---|---|
| $l_{diff}$ | theoretical (LGK) solutal diffusion length at the primary tip at the initial supersaturation |
| $m_L$ | slope of the liquidus line |
| $n_1$, $n_2$ | exponents in the dendrite scaling laws |
| $\vec{n}$ | outward drawn normal of the envelope surface |
| $N_V^{ldiff}$ | dimensionless grain density |
| Pe | Péclet number |
| $R$ | radius |
| $S_{V,env}$ | volume averaged specific envelope surface area |
| $T$ | temperature |
| $T_f$ | melting temperature of the pure solvent |
| $t$ | time |
| $V$, $\vec{V}$ | speed, velocity |
| $W$ | characteristic width of the hyperbolic-tangent profile |
| $X_{act}$ | width of the envelope formed by active sidebranches |
| $\vec{x}_\delta$ | position of the confocal envelope point |
| $x$, $y$, $z$ | cartesian coordinates |
| $\Delta x$, $\Delta t$ | grid spacing, timestep |

*Subscripts*

| | |
|---|---|
| $e$ | envelope |
| env | envelope surface |
| LGK | theoretical LGK primary dendrite tip |
| $l$ | liquid phase |
| $s$ | solid phase |
| tip | dendrite tip |

*Superscripts*

| | |
|---|---|
| * | solid–liquid interface |
| ~ | dimensionless quantity |

*Special functions*

| | |
|---|---|
| Iv | Ivantsov function: $Iv(Pe) = Pe \exp(Pe) E_1(Pe)$ |

equiaxed dendritic grain envelopes predicted by the mesoscopic model is shown in Fig. 1. The driving force for the envelope growth is obtained as a function of the temperature or solute concentration in the liquid at a certain distance ahead of the envelope. As shown in Fig. 2, this distance is denoted as the stagnant film thickness $\delta$ and is the principal model parameter. This model has been shown to provide physically realistic results for both equiaxed [14,15] and columnar [16,17] dendritic growth.

Steinbach et al. [14] applied the mesoscopic model to the thermally driven growth of dendritic grains into a supercooled melt of a pure substance. They validated the predictions of the model for the case of a single grain growing into an essentially infinite melt through comparisons with previously obtained scaling laws for the grain envelope shape and the internal solid fraction, derived from microgravity experimental data [19–22]. Later they investigated the transient interactions between equiaxed grains of a pure substance and validated some of their results with phase-field calculations [15]. More recently, Delaleau et al. [16] extended the mesoscopic model to the solidification of a binary alloy with a prescribed temperature field. They applied the model to simulate the columnar dendritic microstructures observed in *in situ* synchrotron X-ray imaging experiments [23,24]. Relatively good agreement was found between the predicted and measured dendrite envelope shapes, solid fractions and solute concentration fields.

These studies have shown the potential of the mesoscopic model for accurate prediction of dendrite envelope shapes and

grain interactions at a computational cost that is up to several orders of magnitude smaller than that of phase-field methods [17]. An interesting future application of this model is the upscaling from mesoscopic simulations to volume-averaged macroscopic models, in order to provide laws of microstructure growth dynamics that account for interactions in large ensembles of grains. This can be done, for example, by simulations of large ensembles of grains across wide parameter ranges and by subsequent averaging of these simulations. However, on the way to such a wide application of this model, a comprehensive investigation of the accuracy of the model predictions, particularly of the dependence of the simulations on the model and numerical parameters, is still necessary. This has not been systematically addressed in previous studies. In the present paper we perform a careful quantitative analysis of the influence of numerical and model parameters on the accuracy of the model predictions. We also validate the model for free dendritic growth in a binary alloy over a wide range of undercoolings. This is accomplished through comparisons of 3D simulations to recently published experimental scaling laws giving the shape and the internal solid fraction of freely growing binary alloy dendrites [18] and to classical analytical solutions for the primary dendrite tip speed. We provide generally valid guidelines for the calibration of the numerical and model parameters of the mesoscopic model, enabling reliable control of the accuracy of model predictions over a wide range of undercoolings. Finally, we apply the model to large ensembles of equiaxed grains growing in the