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Short note

Simulating dendritic solidification using an anisotropy-free meshless front-tracking method

K. Reuther *, M. Rettenmayr

Otto Schott Institute of Materials Research, Löbdergraben 32, 07743 Jena, Germany

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Dendritic morphologies are by far the most frequently observed structures during solidification of metals and alloys. The simulation of dendritic solidification, however, places strong requirements on the applied models, as the formation of the complex morphology is the result of the weakly anisotropic interfacial energy of the solid–liquid interface. The difference in equilibrium solute concentration along the interface is usually much smaller than the difference between the concentration at the interface and the liquid bulk. This results in small differences in the solute fluxes to or from the interface, which need to be accounted for with a sufficiently high accuracy to reproduce dendritic structures by a spatially resolved simulation method.

Common simulation models for dendritic solidification (e.g. Cellular Automaton or Phase Field models) usually operate on Cartesian grids which may affect the simulation results by introducing an anisotropic error. In Phase Field models it is attempted to reduce this error by choosing fine grids, whereas in Cellular Automata special modifications for the reduction of the anisotropy error are usually incorporated into the model (e.g. [1–4]). Another approach (as demonstrated by Schönfisch for Cellular Automata [5]) is the adoption of stochastic, quasi-isotropic grids that can be expected to introduce no direction-dependent error at all. This approach has been taken up in a recent publication [6] by the present authors in the form of a Meshless Front Tracking (MFT) method.

In the MFT method the spatial domain is discretized by nodes on random positions throughout the domain, with the constraint of a minimum pairwise distance between all nodes. These nodes do not have any connectivity as would be required for e.g. FEM methods. The diffusion equation is instead discretized by the meshless Diffuse Approximation Method (DAM) [7,8], with additional stability handling [9] for the reduction of numerical noise that is introduced by the use of an irregular grid. The DAM represents the solute concentration field by a weighted Least Squares fit of the nodes' concentration

* Corresponding author.
E-mail address: klemens.reuther@uni-jena.de (K. Reuther).

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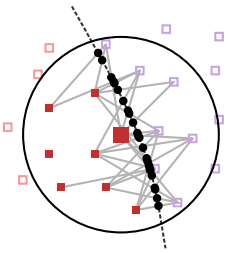

Fig. 1. Neighborhood of a grid node (large square) near the interface, consisting of nodes on the same side of the interface (filled squares) and all tracking particles (dots) between all nodes inside the neighborhood. Only filled objects participate in the interpolation calculations at this node.

using a complete monomial base of second order. The derivatives required for the solution of the diffusion equation are taken directly from the fit. The diffusion equation is integrated by an explicit time-forward scheme.

The interface is represented by a Front Tracking (FT) method using moving particles. These particles, contrary to common FT methods, are neither ordered nor connected. Each of them is instead linked to two grid nodes. This approach allows for a straightforward test for the location of the interface with respect to a given grid node and also simplifies the bookkeeping of particles which are close to each other. The interface geometry is determined by a two-step algorithm: in the first step, the interface normal is calculated by a weighted Total Least Squares fit [6,10]. The interface curvature is calculated in the second step by a weighted Least Squares fit for a parabola. This fit is conducted in the coordinate system of the interface normal. The local velocity of the interface is calculated by the mass balance at the position of the particles, which are then moved accordingly. The implemented particle tracking method does not yet include explicit algorithms for topology changes.

To attain the accuracy required for the simulation of dendritic solidification, two minor modifications were introduced to the model of Ref. [6]: (1) The neighborhood of a grid node, which contains all elements that contribute to the DAM, is set to include a larger selection of the particles. Although in Ref. [6] only particles belonging to the node itself contributed to the DAM, in the present implementation particles between all pairs of nodes which belong to the nodes' neighborhood are included (Fig. 1). (2) The weighting for all Least Squares fits both of the DAM and of the interface geometry calculation is modified to depend inversely on the actual object density. This density is calculated as a sum of contributions from all objects (particles and/or nodes) participating in the respective calculation. All contributions are Gaussian functions of their distance to the node or particle where the density is calculated.

Equiaxed solidification in an undercooled binary alloy melt is simulated here as a proof of concept for the ability of the present model to simulate anisotropic, unstable interface problems. Solute diffusion in the solid and liquid bulk is described by Fick's second law. The interface velocity, v, is described by the mass balance that depends on the solute fluxes, $j_{s,l}$, on either side of the interface [11]:

$$v = \frac{1}{C_l^\Gamma - C_s^\Gamma}(j_s + j_l) \tag{1}$$

The fluxes are calculated by Fick's first law. The interface concentrations, $C_{s,l}^\Gamma$, are equal to the equilibrium concentration according to the phase diagram, including capillarity and anisotropy effects. The Al–Cu system with linearized solidus and liquidus lines is chosen as an example for the simulation. Its parameters are as follows [11]: melting temperature of pure aluminum $T_m = 933.47$ K; liquidus slope $m = -2.6$ K/wt%; partition coefficient $k = 0.14$. The diffusion coefficients in solid and liquid are $D_s = 3.0 \cdot 10^{-13}$ m^2/s and $D_l = 3.0 \cdot 10^{-9}$ m^2/s, respectively. The capillarity undercooling, ΔT_c, of the solid–liquid interface is described in dependence of its normal, $\vec{n}$, and curvature, κ, by

$$\Delta T_c = \gamma(\vec{n})\kappa \tag{2}$$

with γ representing the sum of the interfacial energy and its stiffness (i.e., its second derivative with respect to the normal angle). In two dimensions it is described by the interface energy-density modulus, γ^0, and an anisotropy parameter, ϵ. Choosing fourfold symmetry, γ is given by

$$\gamma = \gamma^0\big[1 - 15\epsilon\cos\big(4[\Theta_0 - \arccos n_x]\big)\big], \tag{3}$$

with Θ_0 describing the direction of the maximum of the anisotropic interfacial energy with respect to the coordinate system in which $\vec{n}$ is noted. The anisotropy parameter ϵ is chosen to be 0.01.

The simulation domain is a square with a side length of 100 μm and periodic boundaries. It consists of 2.7 million nodes with a minimum pairwise distance of 0.05 μm and the corresponding radius of the circular neighborhood used for the Least Squares calculations of 0.25 μm. The time step of the simulation is 0.2 μs.

A circular seed with a diameter of 1.0 μm is placed in the melt with a Cu concentration of 2.1 wt%, the equilibrium concentration of a plane front at 928.0 K. At the start of the simulation, the domain temperature is set to 920.0 K. A smooth initial concentration gradient is introduced between the seed and the bulk liquid to ensure the quality of the meshless interpolation of the concentration field. The length scale of this transition is chosen as 1.25 μm, which is on the order of