Mesoscopic modeling of columnar solidification and comparisons with phase-field simulations

M Založnik¹, A Viardin², Y Souhar¹, H Combeau¹, M Apel²

¹ Institut Jean Lamour, CNRS – Université de Lorraine, F-54011 Nancy CEDEX, France
² Access e.V., Intzestr. 5, D-52072 Aachen, Germany
E-mail: miha.zaloznik@univ-lorraine.fr

Abstract. We use two complementary modeling approaches for the simulation of columnar growth in directional solidification of organic alloys: a phase field model and a mesoscopic envelope model of dendritic growth. While the phase-field method captures the details of the dendritic structure and of the growth dynamics, the mesoscopic model approximates the complex dendritic morphology by its envelope. The envelope growth is deduced from the velocities of the dendrite tips, calculated by an analytical LGK-type tip model that is matched to the temperature and concentration fields in the stagnant film around the envelope. The computational cost of the mesoscopic model is several orders of magnitude lower and can bridge the gap between phase-field and macroscopic models. We demonstrate the applicability of the mesoscopic model to columnar growth and we discuss in particular its capabilities to predict the primary dendrite arm spacing.

1. Introduction

The patterns and the dynamics of the nonlinear growth of solidification microstructures are studied with much success using phase field methods. Phase-field models have been developed into efficient tools giving quantitative results. However, as in any model, its application is subject to certain limitations, mainly due to the necessary computing power. The mesoscopic solidification model of Steinbach, Beckermann et al. [1, 2] offers a complementary tool for the study of dendritic solidification. It can be applied at larger scales, in three dimensions and can include fluid flow at acceptable computing cost. Computational efficiency is achieved at the price of several simplifications. The complex dendritic structure is approximated by its envelope and by a field of phase fractions in the interior of the envelope. The growth of the envelope is deduced from the velocities of the dendrite tips, calculated by an analytical LGK-type tip model that is matched to the concentration fields in the vicinity of the envelope. This means that the selection of the dendrite-tip operating state is not predicted by the model. Information from the microscopic scale is required to determine the tip selection parameter $\sigma^*$ and the matching of the tip model. This information can be obtained indirectly from comparisons with experiments or, in a more rigorous manner, directly form phase-field simulations for simplified configurations. Validation of different mesoscale models by phase-field simulations has been made for example: on dendrite interaction for the envelope model [2], on confined equiaxed growth for the CAFE model [3], or for free equiaxed and for columnar growth for the DNN model [4].

It was already demonstrated that the mesoscopic model can accurately predict envelope shapes of equiaxed dendrites [1, 2, 5] as well as the dynamics of their interactions [2]. The first
2. The mesoscopic envelope-field model

The core idea of the mesoscopic envelope model [1, 2] is the description of a dendritic grain by its envelope—a virtual smooth surface that links the tips of the actively growing dendrite branches. The velocity of the envelope growth can thus be calculated from the velocities of the dendrite tips. The growth of the dendrite tips is controlled by the solute flux that they reject into their surroundings and is therefore determined by the local conditions in the proximity of the envelope. The branched dendritic structure inside the envelope is only implied and its details are not resolved; the interior of the envelope is rather described in a volume-averaged sense by a phase-fraction field and other volume-averaged quantities. The phase change that determines the evolution of the structure inside the growing envelope is controlled by the solute exchange with the surroundings of the grain.

The model used to describe the kinetics of the dendrite tips is based on the analytical solution of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt.

In this paper we go beyond the steady-state spacing [7] and we investigate the dynamics of primary-spacing adjustments in columnar growth. We compare 2D phase-field and mesoscopic simulations of directional solidification of a transparent organic alloy. We show that although the stable steady-state primary arm spacing can be correctly reproduced by the mesoscopic model, the dynamics of the spacing adjustments is different than in the phase-field simulations.

The model used to describe the kinetics of the dendrite tips is based on the analytical solution of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt.

The model used to describe the kinetics of the dendrite tips is based on the analytical solution of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt. The classical Ivantsov solution of this problem, recast by Cantor & Vogel [9], gives the supersaturation $\Omega$ of the growth of a single isothermal parabolic tip in an infinite undercooled melt.
a distance \( \delta \) in the direction normal to the envelope, \( C_{1,\delta} \). The matching distance \( \delta \) is a model parameter that is best chosen at the order of the diffusion length \( \delta \sim D_l/V_{lip} \) [5]. In the mesoscopic model the tip growth directions are prescribed, since the key physics for selection of the preferential growth directions is not included. Knowing the local tip velocity and direction, the envelope velocity is calculated: \( \vec{v}_n = V_{lip} \hat{p} \cos \theta \), where \( \theta \) is the angle between the normal to the envelope and the closest of the tip growth directions (i.e. the one forming the smallest angle with the normal).

To track the front that represents the envelope we use the sharp interface tracking method by Sun & Beckermann [10]. This method represents the front by a contour of a continuous indicator function. The function is propagated by a phase-field like propagation equation. The transport at the mesoscopic scale is described by volume-averaged equations, valid in the whole domain. They are equivalent to the classical volume-averaged macroscopic models [11]. The phase change is described at a microscopic scale, where Scheil assumptions are applied. The diffusion of solute in the solid phase is neglected at the mesoscopic scale. This leads to the following conservation equations for solute mass in the liquid and the solid phase:

\[
\frac{\partial C_l}{\partial t} = D_l \nabla \cdot (g_l \nabla C_l) + C_l (k_p - 1) \frac{\partial g_l}{\partial t} ; \quad \frac{\partial (g_s C_s)}{\partial t} = -k_p C_l \frac{\partial g_l}{\partial t} .
\]

\( g_l \) and \( g_s \) are the liquid and solid phase fraction respectively and \( D_l \) is the diffusion coefficient in the liquid. This equation is valid inside and outside the envelope. Inside and on the envelope the liquid is assumed to be in thermodynamic equilibrium, such that the liquid. This equation is valid inside and outside the envelope. Inside and on the envelope the liquid is assumed to be in thermodynamic equilibrium, such that \( C_l = C_s^* = (T - T_1)/m_L \), where \( T \) is the imposed temperature field. Eq. (3) thus gives the liquid fraction inside the envelope. Outside the envelope \( g_l = 1 \) and eq. (3) is reduced to the diffusion equation.

3. The phase-field model

In the present work, the multi-phase field concept based on Steinbach et al. [12, 13] is employed to describe the morphological evolution during the solid-liquid phase transformation. The phase field method relies on a phase field parameter which varies continuously from liquid “l” (\( \phi=0 \)) to solid “s” (\( \phi=1 \)) along the interface of width \( \eta \). The evolution of the phase field parameter in time is given by:

\[
\frac{\partial \phi_s}{\partial t} = M_{sl}^a (\vec{n}) [\sigma_{sl}^a (\vec{n})] K_{sl} + w \Delta G_{sl} \]

\[
K_{sl} = \phi_s \nabla^2 \phi_l - \phi_l \nabla^2 \phi_s + \frac{\pi}{\eta^2} (\phi_s - \phi_l) ; \quad w = \frac{\pi}{\eta} \sqrt{\phi_s \phi_l} ; \quad \Delta G_{sl} = -f_s (\vec{c}_s) + f_l (\vec{c}_l) + \vec{\mu} (\vec{c}_s - \vec{c}_l)
\]

where \( M_{sl}^a (\vec{n}) \) is the anisotropic interfacial mobility between liquid and solid as a function of the interface orientation (described by the normal \( \vec{n} \)) and \( \sigma_{sl}^a (\vec{n}) \) is the effective anisotropic surface stiffness. \( K_{sl} \) is related to the local curvature of the interface. The thermodynamic driving force \( \Delta G_{sl} \) depends on the respective bulk contributions \( f_s (\vec{c}_s) \) and \( f_l (\vec{c}_l) \). \( \vec{\mu} \) is the generalized chemical potential introduced to conserve local concentration due to the constraint of quasi-equilibrium. This constraint postulates that all the reduced chemical potentials are the same for the coexisting phase i.e \( \vec{\mu} = \vec{\mu}_s (\vec{c}_s (\vec{x})) = \vec{\mu}_l (\vec{c}_l (\vec{x})) \). The evolution of the concentration field is given by:

\[
\dot{\vec{c}} = \nabla (\phi_s D_s \nabla \vec{c}_s) + \nabla (\phi_l D_l \nabla \vec{c}_l) ,
\]

where \( D_s \) and \( D_l \) are respectively the diffusion coefficients in the solid and liquid phase. Phase field simulations have been done using the MICRESS software package [14].

4. Results and discussion

We compared the results of the phase-field and the mesoscopic model for several different configurations. The system consisted of a succinonitrile-2at%acetone alloy solidifying in a fixed
gradient of $G_T = 2 \cdot 10^4 \text{K/m}$ with a cooling rate of $\dot{T} = -1.16 \text{K/s}$, which corresponds to a pulling speed of $V_{\text{pull}} = 58 \mu \text{m/s}$. The growth was initiated with regularly spaced nuclei set at the bottom of the domain at an initial supersaturation of 0.20. Several different spacings of the initial nuclei $\lambda_0$ and several lateral confinements, i.e. domain sizes were used. The computational domain is a moving frame, travelling with the dendrite tips, leaving a minimum distance ahead of the most advanced tip. The frame height was 500 $\mu\text{m}$ and the tip-to-top side distance was 100 $\mu\text{m}$, i.e. around 4.5 times the diffusion length $D_l/V_{\text{pull}}$. At the vertical sides a zero flux boundary condition was used in the mesoscopic model and a periodic boundary condition in the phase-field model. A fixed concentration $C_0$ was imposed at the top boundary and a zero derivative, i.e. no flux at the bottom boundary. The thermophysical properties of the alloys are identical as used in [15]. The tip selection parameter $\sigma^*$ for the mesoscopic model was determined from the steady-state tip radius obtained by the phase field model. For that, we used the tip selection criterion $R^2_{\text{tip}} V_{\text{tip}} = (d_0 D_l)/\sigma^*$, where the tip velocity is known and the liquid concentration at the tip used in the capillary length was determined from the supersaturation $\Omega = (C^*_{\text{tip}} - C_0)/((1 - k_p) C^*_{\text{tip}})$ given by the Ivantsov model (Eqs. (1) and (2) for $\delta \rightarrow \infty$): $\Omega = \frac{Iv(Pe_{\text{tip}})}{\pi \sqrt{Pe}\exp(\frac{Pe}{C^*})}\text{erfc} \left(\frac{\sqrt{Pe}}{C^*}\right)$. We obtained $\sigma^*_{\text{SCN-ace}} = 0.0328$.

In order to understand the effect of the spacing selection mechanism, several simulations with different initial spacings between nuclei and different domain widths were performed. Two types of configurations for the initial nucleus spacing were used. In the first case the initial nucleus spacing is larger than the final stable primary arm spacing (i.e. $\lambda_0 > \lambda_1$) and thus new primary branches have to form. In the second case the initial spacing is smaller than the final spacing (i.e. $\lambda_0 < \lambda_1$) and primary branches have to be eliminated.

The evolution of a configuration where $\lambda_0 > \lambda_1$ towards the stable steady state is shown in Fig. 1. As we can see in Figs. 1(a)–1(b), a fast growth of lateral arms in the horizontal direction is followed by branching and by vertical growth of the secondary arms along the temperature gradient (which will become primary arms). In the phase-field simulation a transient is observed in the spacing evolution. At early stage (i.e $t < 4 \text{s}$), the primary spacing is already small, many small vertical branches are growing. Between 4 and 10 seconds, some of the branches become predominant, which results in an increase of the primary spacing. At $t = 10 \text{s}$, shown in Fig. 1(d), the spacing is stabilized and tends towards a steady arrangement of the branches (Fig. 1(e)).

With the mesoscopic model, the first stage of growth after the lateral branches meet (which occurs a little later than in the phase-field simulation) can be considered as a growth of an almost planar envelope (Fig. 1(b)). The shape of the envelope is slightly perturbed only by the vertical primary arms growing directly from the nuclei along the left and right walls, as well as by a groove in the middle, which remains due to the excess solute that had slowed down the lateral arms as they were approaching. These initial perturbations then grow. The accumulation of solute in the grooves slows down the front, while the higher supersaturation ahead of the cusps accelerates it. This mechanism also promotes the development of instabilities of the envelope that appear little later, as we can see in Fig. 1(c). The instabilities develop into a wavy envelope front, with a mean wavelength of $\lambda_1 = 77 \mu\text{m}$, which is very close to the mean primary arm spacing of $\lambda_1 = 83 \mu\text{m}$ predicted by the phase-field simulation. A constant average spacing given by a constant number of dendrites is reached at around $t = 8 \text{s}$ in the phase-field simulation and at around $t = 14 \text{s}$ in the mesoscopic simulation. The development of a steady-state arrangement of the branches requires more time in both models until the individual tip positions have been adjusted accordingly.

For the second case, where $\lambda_0 < \lambda_1$, shown in Fig. 2, termination of branches can be observed. The spacing between the initial nuclei is too small to allow for the growth of lateral branches (Fig. 2(a)). As we can see in Figs. 2(b)–2(d), the spacing selection proceeds by a competition between the vertical branches. The phase-field model predicts a fast adjustment of the spacing, which resembles the period-doubling instability observed experimentally by Losert.
et al. [16]. In this way the final stable spacing is reached in the time interval between around \( t = 12s \) and \( t = 18s \) which is comparable to the selection process starting with \( \lambda_0 > \lambda_1 \). The mesoscopic model predicts an entirely different transition. The adjustment of the spacing proceeds symmetrically from the left and right edges of the domain and branches are eliminated in a cascade. The process takes much longer; starting at around \( t = 12s \) and reaching the final spacing at around \( t = 37s \). Again, the predicted final mean spacings are very close (Fig. 2(e)):
$\lambda_1 = 91 \mu m$ for the phase-field model and $\lambda_1 = 100 \mu m$ for the mesoscopic model.

In both of these cases we can observe that the initial stage of columnar growth starts with a solute diffusion field close to a perturbed planar front, which is later destabilized, leading to a spacing adjustment. Mesoscopic simulations that were initialized with a planar envelope support this analogy. After an initial destabilization of the planar envelope, protuberances with a small spacing develop. A spacing adjustment in the form of a cascade of branch eliminations, emanating from both borders of the domain sides (similar as in the case shown in Fig. 2) then leads to a stable primary-arm spacing.

We can see that the final stable spacing is not a unique state for a given set of operating conditions ($G_T$, $V_{pull}$), but that it also depends on the initial spacing as it was discussed in more detail in [7]. The final spacing is a result of the whole adjustment process, which is sensitive to the initial conditions. This is in line with theoretical analyses [17] and experiments [16] that have shown that a selection mechanism that would uniquely determine the primary spacing does not exist. At a given pulling velocity and temperature gradient a certain range of spacings can be stable. It is nevertheless relevant to compare the spacings predicted by the two models to classical empirical or geometrical models, which give a unique average primary spacing for steady growth as a function of the temperature gradient, the pulling velocity and the solute concentration. These models can provide at least a rough estimation of the spacing. They can be resumed by $\lambda_1 = a\sqrt{\ell_{sl}R_{tip}}$, where $\ell_{sl}$ is the total depth of the mushy zone and where the constant $a$ can be alloy-specific [18]. For our configuration different models of this type predict spacings between 32 $\mu m$ and 150 $\mu m$; a range across almost an order of magnitude. The predictions of the phase-field and of the mesoscopic model fall easily within these limits, however their range of variation is much smaller, e.g. [7].

For the simulation of grain interactions, for example interactions of a columnar front with equiaxed grains and the columnar-to-equiaxed transition, an important aspect is a faithful representation of the undercooling, and thus of the concentration field, ahead of the columnar front. In the context of modeling two questions can be raised. (i) With what accuracy does the mesoscopic model reproduce the undercooling of the primary tips and of the liquid ahead of the columnar front? (ii) Is it necessary to describe the primary-branch pattern and the mesoscopic interactions in order to accurately predict the undercooling ahead of the columnar zone or could it be sufficient to represent the columnar front by a plane envelope? This question is related to the fact that the columnar front could be just as well described by a smooth envelope, very much like the envelope of secondary branches in equiaxed growth [1, 5]. We try to answer these two questions by comparing the undercooling in the liquid ahead of the columnar grains predicted by the mesoscopic model to the phase-field simulations.

We address question (i) by comparing solute concentration fields in the liquid ahead of the columnar grains in the steady state from phase-field and mesoscopic simulations. In the left part of Fig. 3(a) the concentration field from phase-field and in the right part from the mesoscopic model is shown. The simulations were performed using identical process and model parameters as in the previous section, but a domain width and initial nucleus spacing of 250 $\mu m$ were used, which gave the same primary-arm spacing. The differences between the concentration fields in the liquid are relatively small. A more detailed representation is given by a plot of the concentration profiles in the liquid ahead of a primary arm in Fig. 3(c). We can see that the differences are barely perceptible. A theoretical Ivantsov solution for an isolated tip is shown for comparison. It shows that the solutal undercooling of the tips of the columnar front is slightly higher than that of an isolated tip. This indicates a slight solutal interaction between the tips. This interaction is captured with good accuracy by the mesoscopic model.

Question (ii) is addressed by a 1D mesoscopic simulation, where the tip kinetics was described by the Ivantsov function using the undercooling at an infinite distance ahead of the columnar tips $\Omega_0 = (C_0 - C_1^*)/(C_1^*(k_p - 1)) = Iv(Pe_{tip})$, instead of matching the Cantor-Vogel function.
Figure 3. Comparison between a phase-field simulation and a mesoscopic simulation for the steady state. (a–b) Concentration fields from the phase-field (left) and mesoscopic (right) simulations. (c) Concentration profiles along the axis of a dendrite arm at $x = 0$.

Figure 4. Comparison between a phase-field simulation and a mesoscopic simulation for the steady state. (a–b) Solid-fraction fields from the phase-field (left) and mesoscopic (right) simulations. (c) Average solid-fraction profiles along the height of the mushy zone.

(Eq. (1)) at a distance $\delta \approx D_l/V_{\text{tip}}$, as in the primary-spacing simulations. In practice, a very large matching distance $\delta$, corresponding to around 10 diffusion lengths ($D_l/V_{\text{tip}}$), was used in Eq. (1) in order to achieve the Ivantsov limit. The solute concentration fields of the phase-field and of the 1D mesoscopic simulation are compared in Figs. 3(b,c). We can see that the concentration ahead of the plane envelope is slightly shifted and flatter than the concentration profile ahead of the primary tips. The tip undercooling is lower and is equal as in the theoretical Ivantsov solution. The extent of the undercooled region in front of the tips and the undercooling of the liquid are also somewhat smaller than in the phase-field and the mesoscopic solutions.

We also compared the solid fraction in the columnar mushy zone in the three computations. Fig. 4 shows (a–b) solid-fraction fields and (c) the vertical profiles of the solid fraction averaged across the horizontal direction, i.e. $g_s(z) = \int_{-W/2}^{W/2} g_s(x, z) dx$. All are compared to a so-called closed-system Scheil law, i.e. a solidification path calculated for a constant average concentration $C_0$ without accounting for mesoscopic segregation effects. We can see that the mesoscopic simulation follows the phase-field solution very closely. The fluctuations due to the presence of secondary arms are of course not reproduced by the mesoscopic model, where the solid-
fraction field inside the envelopes is smooth. The plane-envelope solution turns out to be an excellent approximation deep in the mushy zone ($z > -10^{-4} \text{m}$), but it deviates in the tip region ($z < -10^{-4} \text{m}$). In both the phase-field and the mesoscopic simulation with primary branches, the extra-envelope liquid is not in equilibrium and therefore the solidification path in the tip region does not follow a Scheil law as in the plane-envelope solution. The latter also shows a jump of solid fraction at the tips (at the plane envelope), which is equivalent to a Scheil solution truncated at the tip undercooling. All three numerical solutions however differ from the closed-system Scheil solidification path up to deep into the mushy zone. The reason is the diffusion-driven segregation at the mesoscopic scale, which drives solute into the liquid ahead of the tips, increases its solute concentration and thus delays the solidification.

5. Conclusions and perspectives
We demonstrated the applicability of the mesoscopic envelope model to columnar growth in directional solidification. By comparisons to phase-field computations, used as a reference, we showed that the mesoscopic model: (i) correctly reproduces the stable primary spacing; (ii) accurately captures the solute diffusion at the scale of the primary spacing and the solutal undercooling ahead of the columnar tips and (iii) accurately predicts the solidification path in the mushy zone behind the columnar front. Spacing adjustments both by branching and by elimination of branches appear in the mesoscopic model predictions. However, the dynamics of these adjustments is different from phase field predictions and further analyses are needed to understand the transient pathway towards the steady state configuration. Other extensions of this work are 3D computations of columnar growth and the inclusion of fluid flow. Both can be achieved with reasonable computational load.

Acknowledgments
We gratefully acknowledge the support to this research by the German Federal Ministry of Research through the German Space Agency DLR under Contract FKZ 50WM1143. This work was supported by the French State through the program “Investment in the future” operated by the National Research Agency (ANR) and referenced by ANR-11 LABX-0008-01 (LabEx DAMAS).

References
[1] Steinbach I, Beckermann C, Kauerauf B, Li Q and Guo J 1999 *Acta Materialia* **47** 971–982
[2] Steinbach I, Diepers H J and Beckermann C 2005 *Journal of Crystal Growth* **275** 624–638
[3] Carozzani T 2012 Ph.D. thesis Mines ParisTech
[4] Tourret D and Karma A 2013 *Acta Materialia* **61** 6474–6491
[5] Souhar Y, De Felice V F, Založnik M, Combeau H and Beckermann C 2014 *International Conference on Advances in Solidification Processes 4*, Old Windsor, 8-11 June 2014 (submitted)
[6] Delaleau P, Beckermann C, Mathiesen R H and Arrarberg L 2010 *ISIJ International* **50** 1886–1894
[7] Založnik M, Viardin A, Souhar Y, Combeau H and Apel M 2014 *International Conference on Advances in Solidification Processes 4*, Old Windsor, 8-11 June 2014 (submitted)
[8] Steinbach I 2008 *Acta Materialia* **56** 4965–4971
[9] Cantor B and Vogel A 1977 *Journal of Crystal Growth* **41** 109–123
[10] Sun Y and Beckermann C 2007 *Journal of Computational Physics* **220** 626–653
[11] Beckermann C and Viskanta R 1993 *Applied Mechanical Review* **46** 1–27
[12] Steinbach I, Pezzolla F, Nestler B, Seelberg M, Prieler R, Schmitz G and Rezende J 1996 *Physica D: Nonlinear Phenomena* **94** 135–147
[13] Eiken J, Böttger B and Steinbach I 2006 *Physical Review E* **73** 066122
[14] MICRESS version 6.1, 2013-2014, www.micress.de
[15] Melendez A J and Beckermann C 2012 *Journal of Crystal Growth* **340** 175–189
[16] Losert W, Shi B Q, Cummins H Z and Warren J A 1996 *Physical Review Letters* **77** 889–891
[17] Warren J A and Langer J S 1993 *Physical Review E* **47** 2702–2713
[18] Steinbach S 2005 Ph.D. thesis RWTH Aachen