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Numerical study on the prediction of microstructure parameters by multi-scale modeling of directional solidification of binary aluminum–silicon alloys

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Abstract

In order to create a model to predict microstructural quantities like grain size, primary and secondary dendrite arm spacing a multi-phase and multi-scale model based on the work of Wang and Beckermann [C. Wang, C. Beckermann, Metallurgical and Materials Transactions A 27A (1996) 2754–2764] was combined with a front tracking technique [A. Wu, A. Ludwig, in: C.-A. Gandin, M. Bellet (Eds.), Modeling of Casting, Welding, and Advanced Solidification Processes – XI, TMS, 2006, pp. 291–298], micro-models for nucleation [M. Rappaz, P. Thevoz, Acta Metallurgica 35 (7) (1987) 1487–1497], primary [J. Hunt, S.-Z. Lu, Metallurgical and Materials Transactions A 27A (1996) 611–623], secondary [W. Kurz, D. Fisher, Fundamentals of Solidification, Trans Tech Publication, 1986, ISBN 0-87849-522-3] dendrite arm spacing and a control volume based finite element solver for axial-symmetric problems. As most of the micro-models are just valid for pure diffusive conditions, the model just takes into account macroscopic diffusion in the melt and thus neglects the influence of melt flow. The new software was used for a comprehensive comparison to several test cases. The validation includes investigation of the correlation of calculated and measured grain size distributions for inoculated alloys. Experimental and numerical data for the primary and secondary dendrite arm spacing for steady state and transient directional solidification were compared in a second step. A good correlation is found for all test cases.

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Keywords: Directional solidification; Multi-scale modeling; Primary dendrite spacing; Secondary dendrite arm spacing

1. Introduction

The mechanical properties of cast metallic parts are strongly affected by their microstructure which is defined during solidification. Among others grain size, primary and secondary dendrite spacing are one of the most important quantities describing the microstructure. A prediction of these microstructure parameters on the scale of the sample by numerical simulation of a casting process would make the process development and optimization much simpler and more efficient. This would require a physically sound modeling of the processes occurring on different length scales during alloy solidification. On the scale of the sample, macroscopic heat and species transport have to be considered, because it influences the formation of the microstructure in various ways. The formation of the microstructure on the other hand occurs on the scale of fractions of millimeters and bellow. One example is the formation of the spacing of the dendritic array. In order to create a model, which is able to bridge between the scales, a combination of different available macro- and micro-models is used.

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Nomenclature

$a_{ij,i}$	matrix coefficient
$\langle C_k \rangle^k$	intrinsic concentration in phase k [wt.%]
$\overline{C}_{kj}$	area averaged concentration in phase k at the interface of phase j [wt.%]
c_p	heat capacity $[\frac{\mathrm{J}}{\mathrm{kg\ K}}]$
C_0	initial concentration of the alloy [wt.%]
C_E	eutectic concentration [wt.%]
$\overline{C}_\mathrm{e}$	envelope or equilibrium concentration [wt.%]
D_k	diffusion coefficient in phase k $[\frac{\mathrm{m}^2}{\mathrm{s}}]$
ΔH^m	change in enthalpy during a macro-time-step [J]
G	thermal gradient $[\frac{\mathrm{K}}{\mathrm{m}}]$
G'	dimensionless thermal gradient
$\mathrm{Iv}(x)$	Ivantsov function
k	partition coefficient
$\mathscr{L}$	latent heat $[\frac{\mathrm{J}}{\mathrm{kg}}]$
l_{kj}	diffusion length in phase k at the interphase of j [m]
m_l	liquidus line slope $[\frac{\mathrm{K}}{\mathrm{wt.\%}}]$
n	nucleation density $[\frac{1}{\mathrm{m}^3}]$
n_0	maximum nucleation density $[\frac{1}{m^3}]$
N	number of neighbors (phases or nodes)
Pe	Peclet number of the dendritic envelop $Pe = w_\mathrm{ne} R_\mathrm{f}/2D_\mathrm{l}$
Q_ext	external net heat flux over the control volume [J]
R_e	instantaneous grain radius [m]
R_f	final grain radius/ size of the representative cell [m]
S_e	envelope area concentration $[\frac{1}{\mathrm{m}}]$
t	time [s]
t_f	local solidification time [s]
Δt^m	width of a macro-time-step [s]
T	temperature [K]
ΔT	undercooling of the melt [K]
ΔT_0	solidification interval [K]
ΔT_max	maximum undercooling of the melt [K]
ΔT_N	nucleation undercooling [K]
ΔT_σ	half width of Gaussian distribution of the nuclei [K]
ΔT_tip	undercooling of the dendritic growth front [K]
T_j	temperature at node j [K]
T_pure	melting point of pure substance [K]
v_g	velocity of the columnar dendritic front $[\frac{\mathrm{m}}{\mathrm{s}}]$
V_cv	volume of control volume $[\mathrm{m}^3]$
V'	dimensionless growth velocity
w_ne	normal velocity of the dendritic envelope $[\frac{\mathrm{m}}{\mathrm{s}}]$

Greek characters

Γ	Gibbs–Thomson coefficient [m K]
ε_k	volume fraction of phase k
λ	thermal conductivity $[\frac{\mathrm{W}}{\mathrm{m\ K}}]$
λ'	dimensionless primary dendrite arm spacing
λ_1	primary dendrite spacing [m]
λ_1^eff	primary dendrite spacing used in the multi-scale model's micro-loop [m]
λ_2	secondary dendrite arm spacing [m]
ρ_k	density of phase k $[\frac{\mathrm{kg}}{\mathrm{m}^3}]$
$(\rho c_p)_\mathrm{eff}$	effective heat capacity for the energy equation in the micro-loop $[\frac{\mathrm{kg}}{\mathrm{m}^3}]$
Ω	dimensionless solutal undercooling

Sub and superscripts

d	interdendritic melt
e	envelope or equilibrium
f	total fluid (l + d) phase
i	index of node I in the matrix
I	node inside the control volume
j	Index of a neighboring node or phase
l	extradendritic melt
m	macroscopic property constant during a macro-time-step
n	end of the macro-time-step (new value)
o	beginning of the macro-time-step (old value)
s	solid phase
t	value of dendritic tip

In this work it is investigated if such a multi-scale model allows the calculation of the microstructure in terms of the resulting grain size, the primary and secondary arm spacing, within a global model on the scale of the crucible and the furnace. The study was made by using the software package CrysMAS [6], which is specially designed for global modeling of directional solidification in complex axial-symmetric geometries. It offers modeling of conductive and radiative heat transfer including automated control of heating powers and moving of furnace regions for simulation of various processing strategies. For these investigations the software was extended with a multi-phase and multi-scale model, which is briefly described in the following.

The paper is structured as follows: In Section 2, the governing set of transport equations and the model for capturing the dendritic grain growth is briefly summarized. After that the integrated models for calculating microscopic properties, like primary and secondary dendrite arms spacing are presented. Then the numerical procedure is sketched in Section 3. Finally, a numerical parameter study and a comparison with experimental data in Section 4 is presented.

2. Description of the multi-scale model

This section describes the macroscopic model with the transport equations for multi-phase systems together with