

Home Search Collections Journals About Contact us My IOPscience

Simulation of the as-cast structure of AI-4.0wt.%Cu ingots with a 5-phase mixed columnarequiaxed solidification model

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 2012 IOP Conf. Ser.: Mater. Sci. Eng. 33 012075 (http://iopscience.iop.org/1757-899X/33/1/012075) View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 178.191.204.136 The article was downloaded on 31/05/2013 at 10:23

Please note that terms and conditions apply.

Simulation of the as-cast structure of Al-4.0wt.%Cu ingots with a 5-phase mixed columnar-equiaxed solidification model

M Wu^{1,2}, M Ahmadein², A Kharicha², A Ludwig², J H Li³ and P Schumacher³

¹ Christian-Doppler Lab for Advanced Process Simulation of Solidification & Melting, ² Chair for Simulation and Modelling of Metallurgical Processes,

³ Chair for Casting Research,

Dept. of Metallurgy, Univ. of Leoben, A-8700 Leoben, Austria

E-mail: menghuai.wu@unileoben.ac.at

Abstract. Empirical knowledge about the formation of the as-cast structure, mostly obtained before 1980s, has revealed two critical issues: one is the origin of the equiaxed crystals; one is the competing growth of the columnar and equiaxed structures, and the columnar-to-equiaxed transition (CET). Unfortunately, the application of empirical knowledge to predict and control the as-cast structure was very limited, as the flow and crystal transport were not considered. Therefore, a 5-phase mixed columnar-equiaxed solidification model was recently proposed by the current authors based on modeling the multiphase transport phenomena. The motivation of the recent work is to determine and evaluate the necessary modeling parameters, and to validate the mixed columnar-equiaxed solidification model by comparison with laboratory castings. In this regard an experimental method was recommended for in-situ determination of the nucleation parameters. Additionally, some classical experiments of the Al-Cu ingots were conducted and the as-cast structural information including distinct columnar and equiaxed zones, macrosegregation, and grain size distribution were analysed. The final simulation results exhibited good agreement with experiments in the case of high pouring temperature, whereas disagreement in the case of low pouring temperature. The reasons for the disagreement are discussed.

1. Introduction

The mechanical properties of castings (either in primary or final form) and welded joints are of great importance in the design and manufacture of engineering products. These properties can be modified by controlling the microstructure formed during the solidification. Solidification is a multi-phase / multi-scale process where the transport of heat, momentum, mass, and species interact with each other in a complex manner to provide the final morphology. Therefore, the prediction of the microstructure at the industrial scale represents a big challenge for researchers. Empirical knowledge about the formation of the as-cast structure, mostly obtained before 1980s [1]-[5], rests primarily on two critical issues: one is the origin of equiaxed crystals; one is the columnar-to-equiaxed transition (CET). The most-likely-operating nucleation mechanisms proposed were: (1) heterogeneous nucleation [6]; (2) the 'big band' theory [1]; (3) partial remelting of columnar dendrites [7]; (4) the showering down of dendrite crystals formed from the casting top surface [8]; and (5) the so-called 'separation' theory [3] which has some similarity to the 'big band' theory. Progress was also made in the understanding of CET since the pioneer work of Hunt [9] in 1980s. A CET map, the correlation of the columnar primary dendrite tip growth velocity with the local temperature gradient at the moment of CET, was established to analyze the occurrence of CET. This CET map was later confirmed and further improved by many authors [10][15]. In the meantime, empirical correlations were proposed as indirect criteria to predict the CET for engineering castings [16]-[20].

The current authors [21]-[25] proposed a 5-phase mixed columnar-equiaxed model that treats the solidification as a multiphase transport problem which takes into account the impacts of flow and grain transport based on the above mentioned empirical knowledge. Preliminary simulations showed that the model is capable to qualitatively produce structures similar to those observed in previous experiments [1] [3] [5]. In addition, classical ingot casting experiments on Al-Cu alloy were conducted in a previous work [26] and the results were compared to simulations using the 5-phase model. The macrostructure of Al-Cu ingots could be reproduced by the model, however, the detailed structural quantities and point-to-point validation did not match the experiment. Modeling results have shown that the most sensitive parameters for the macrostructure are the nucleation parameters. Thus, the authors recommend that further evaluations and more detailed analyses of the modeling and experimental results should continue. In the current work a numerical parameter study is carried out to investigate the influence of the nucleation parameters on the as-cast structure. Previous experiments for in-situ determination of the nucleation parameters were also used to validate and improve the modeling results.

2. The numerical model

The model comprises any combination of the hydrodynamically interacting phases: equiaxed crystals, columnar crystals, and liquid melt as explained in Figure 1. It was assumed that immediately following the nucleation of equiaxed crystals in the chill zone, columnar dendrites start to grow from the casting surface. The three phases, denoted as e-, c- and ℓ -phases, are considered and quantified with their volume fractions, f_e , f_c , f_ℓ . They move with corresponding velocities, \vec{u}_e , \vec{u}_c , and \vec{u}_ℓ . Here \vec{u}_c is predefined (zero in the case of ingot casting), while \vec{u}_e and \vec{u}_ℓ are solved numerically. The volume averaging approach was employed to formulate the conservation equations of mass, momentum, species, and energy for the three phases, as described in the Eulerian multiphase model.



Figure 1. Schematic of the mixed columnar-equiaxed solidification in an ingot casting

A three-parameter heterogeneous nucleation law [27] is applied for the origin of equiaxed grains. These nucleation parameters can be obtained experimentally. The e-phase, the equiaxed grains attached to casting surfaces (top or side wall) are allowed to be brought away by the melt convection into the bulk region. Almost all the aforementioned nucleation mechanisms [1][3][6][8] can be taken into account except for the one due to partial remelting of columnar dendrites [7]. As the current model does not include mold filling, hence a simple idea is proposed to consider the equiaxed nuclei which have formed during mold filling, i.e. to pre-set an initial grain number density in the as-filled state, n_0 .

MCWASP XIII	IOP Publishing
IOP Conf. Series: Materials Science and Engineering 33 (2012) 012075	doi:10.1088/1757-899X/33/1/012075

The dendritic growth of crystals is taken into consideration as shown in Figure 1. Two distinct phase regions exist within the envelope of the crystal: the solid dendrites and interdendritic melt. It is assumed that the interdendritic melt is transported with the solid dendrites and is generally more enriched with solute element than the extradendritic melt surrounding the crystals. In this sense, a fictitious crystal boundary envelope is constructed to separate the interdendritic melt from the extradendritic melt. Therefore, five 'thermodynamic' phase regions are defined in the system: the solid dendrites and interdendritic melt in the equiaxed grain, the solid dendrites and interdendritic melt in the columnar dendrite trunk, and the extradendritic melt. They are quantified with their volume fractions, f_s^e , f_d^e , f_s^c , f_d^c , f_ℓ , and characterized by their corresponding solute concentrations, c_s^e , c_d^e , c_s^e , c_d^c , c_ℓ . Inside an equiaxed grain, volume fractions of interdendritic liquid and solid dendrites are quantified respectively with α_d^e , α_s^e , hence $f_d^e = \alpha_d^e \cdot f_e$ and $f_s^e = \alpha_s^e \cdot f_e$. Inside a columnar dendrite trunk, $f_d^c = \alpha_d^c \cdot f_c$ and $f_s^c = \alpha_s^c \cdot f_c$. Both hard blocking [9] and soft blocking [12] mechanisms are implemented and applied to model

Both hard blocking [9] and soft blocking [12] mechanisms are implemented and applied to model the columnar-to-equiaxed transition (CET). The hard blocking mechanism suggests that CET might occur when the equiaxed grains ahead of the columnar dendrite tip exceeds a critical volume fraction ($f_{e,CET} = 0.49$). A recent study [28] has shown that the critical value suggested by Hunt [9] might be too large. Instead, a value of $f_{e,CET} = 0.2$ should be used. In current simulations, $f_{e,CET}$ is set to 0.49 except for the case shown in Figure 8, where $f_{e,CET} = 0.2$. The soft blocking mechanism suggests that the exhausting of the growth driving force (constitutional undercooling) due to the enrichment of solute element (rejected by the growing equiaxed grains) stops the growth of columnar primary dendrite tips. For more details regarding growth kinetics, treatment of the dendritic morphology of crystals, algorithm of tracking the columnar tip, etc. refer to previous publications [21][22]. The above solidification model is implemented in a multiphase CFD code (ANSYS Fluent 6.3.26).

3. Experiments

The nucleation parameters for the Al-4.0 wt.%Cu alloy were obtained from a previous work [29] by conducting a series of experiments based on the works of Rappaz and Gandin [30] and Rappaz [27]. The casting samples were cooled at different rates. The resulting maximum undercooling and the corresponding grain number density were experimentally determined and plotted to provide a Gaussian curve, from which the nucleation characteristic parameters were deduced (Table 1).

Classical ingot casting experiments on Al-4.0 wt.%Cu were additionally conducted. The alloy was prepared by mixing the suitable proportions of Cu and Al with commercial purity. The alloy was melted and poured into a clay-bonded graphite crucible at different pouring temperatures, namely 800, 750, and 700 °C. The initial mold temperature was about 20 °C for all samples. Ingots were cooled down in normal atmosphere. After solidification specimens were cut, ground, polished and etched for macroscopic examination. The resulting macrographs are shown in Figure 3. In addition, macrosegregation was studied for one sample (poured at 800 °C) using spectrometer analysis.



Figure 2. Ingot geometry and configuration of simulation.

 IOP Conf. Series: Materials Science and Engineering 33 (2012) 012075
 doi:10.1088/1757-899X/33/1/012075

Thermodynamic data: $T_{\text{liquidus}} = 922.5 \text{ K}$ $T_{\text{solidus}} = 847.15 \text{ K}$ $T_{\text{eutectic}} = 821.35 \text{ K}$ $c_0 = 4.0 \text{ wt.\%}$ $c_0 = 4.0 \text{ wt.\%}$ $c_{\text{eutectic}} = 0.332 \text{ wt.\%}$ Liquidus slope, $m = -260 \text{ K/wt.\%}$	Boundary conditions: $T_0 = 800, 700^{\circ}\text{C}$ $H_t = 10 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$ $T_t = 290 \text{ K}$ $H_w = 120 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$ $T_w = 290 \text{ K}$ $H_b = 120 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$ $T_b = 290 \text{ K}$				
Partition coefficient, $k = 0.145$ Latent heat = 389.32 kJ/kg	Morphological parameters & hard blocking criterion:				
Nucleation parameters: $n_{max} = 1.48 \times 10^{11} \text{ m}^{-3}$ $n_{min} = 10^7, 10^8 \text{ and } 10^9 \text{ m}^{-3}$ $\Delta T_{\sigma} = 10.17 \text{ K}$ $\Delta T_N = 28.84 \text{ K}$ $n_0 = 10^7, 10^8 \text{ and } 10^9 \text{ m}^{-3}$	$\Phi_{env}^{e} = 0.48 \qquad \Phi_{sph}^{e} = 0.4 \qquad \lambda_{1} = 500 \ \mu m$ $\Phi_{env}^{c} = 0.80 \qquad \Phi_{circ}^{c} = 0.5 \qquad \lambda_{2} = 100 \ \mu m$ $f_{e,CET} = 0.49, \ 0.2$				

Table 1. Parameters used for the simulation of the Al-4.0 wt.%Cu ingot

From a first glance at Figure 3 it seems that a lower pouring temperature favors the formation of equiaxed structure, and the equiaxed grain size is reduced with the decreasing pouring temperature. In Figure 3(a) for the ingot poured at 800 °C the region marked (A+B) contains mainly equiaxed grains. Finer equiaxed grains are located in the bottom half, 'region-A', while coarser grains are in the top, 'region-B'. It can also be observed that the equiaxed zone extended upwards to near the mold wall to form the 'region-C', where it interferes with the outer columnar structure zone. In the outer region the columnar trunks growing perpendicular to mold walls are evident, especially in the upper part of the ingot. The structure of the ingot poured at 750 °C (Figure 3 (b)) is mainly very fine equiaxed in the core 'region-A', and relatively coarse equiaxed in the exterior and upper (region-B), where it interferes with columnar structure. Further reduction of pouring temperature (Figure 3(c), poured at 700 °C) introduces even finer equiaxed grains in the core 'region-A', a band of relatively coarse equiaxed grains in the core 'region-C', where it interferes with some fine columnar structure. The variation in equiaxed/columnar zones and the grain size are mainly due to the different temperature gradient, the cooling rate and grain movement during solidification.



Figure 3. Macrostructure of the Al-4.0%Cu ingots poured at (a) 800, (b) 750, and (c) 700° C.

4. Simulation and discussion

A 2D-axisymmetric grid (Figure 2) with 1197 volume elements was constructed such that the top surface profile is similar to that of the real casting. Some parameters used for the simulation are listed in Table 1. For more details about other simulation parameters refer to [21][22]. Calculations started with a mini phase volume fraction ($f_e = f_c = 10^{-5}$), an initial grain number density of n_0 and grain diameter of 1 µm. The columnar primary dendrite tips were initialized at the side and bottom mold walls. Mold filling is not considered in the simulation. Instead, the mold was assumed to be initially filled with the molten alloy of an initial temperature, T_0 , equal to the pouring temperature. Simulations were conducted for the castings with different pouring temperatures (800 and 700 °C). Adaptive time-stepping scheme was employed with a minimum time step of 10^{-4} s.

The numerically predicted macrostructure for the ingot poured at 800 °C is shown in Figure 4(a). Two zones could be easily distinguished: the equiaxed phase in the core region and the columnar phase in the exterior region. Both regions are separated by a mixed columnar-equiaxed zone. The final position of the columnar primary dendrite tips is indicated by the CET-line. The equiaxed zone is extended vertically near the sidewall with a lower volume fraction. It is additionally found that the current results based on the experimentally in-situ determined grain nucleation parameters matches better with the experiment than the previous result that was based on estimated nucleation parameters Figure 4(b) [26]. Thus the macrostructure with distinguished columnar and equiaxed zones is reproducible by the numerical model.



Figure 4. Predicted macrostructure of the Al-4.0wt.%Cu ingot poured at 800 °C: distribution of f_c (left-half) and f_e (right-half) phases. The CET line indicates the final position of the columnar primary dendrite tips. Simulations were performed (a) using experimentally in-situ determined nucleation parameters (Table 1); and (b) using estimated nucleation parameters $n_{max} = 10^{11} \text{ m}^{-3}$, $\Delta T_N = 3.5 \text{ K}$, $\Delta T_{\sigma} = 0.5 \text{ K}$ [26].

IOP Publishing

Further structural quantities of this ingot are shown in Figure 5. The calculated grain size, d_e , shows good qualitative agreement to experiments. The grain size in the bottom half is finer than that in the top half. Coarse columnar structure (Figure 5(b)) was predicted in the upper and peripheral regions of the ingot, similar to the as-cast result in Figure 3(a). Close to the CET-line the diameter of the columnar trunk, d_c , gets smaller, and the amount of equiaxed phase becomes dominant. The calculated grain number density, n_e , as shown in Figure 5(c) agrees with the real macrograph (Figure 3(a)). The grain number density in upper region (10^7 m^{-3}) is equivalent to the minimum of each volume element allowed by the model, which virtually means that no equiaxed grains. The maximum grain number density is obtained in the lower bottom. Lowest grain number density with coarsest grain size appears at CET peak 'region-B' in Figure 3(a). A quantitative comparison of n_e , d_e , and d_c at some selected positions (a-d) as marked in Figure 3(a) is given in Table 2. The results confirmed the above discussions. The predicted volume fraction of the formed eutectic is also shown in Figure 5(d).

doi:10.1088/1757-899X/33/1/012075



Figure 5. Additional structural quantities for the ingot poured at 800 °C: (a) d_{e} , (b) d_{c} , (c) n_{e} , (d) $f_{eutectic}$.

 Table 2. Measured microstructural quantities vs. calculated.

Position	a [*]		b*		c*		d*	
	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.
$n_{\rm e},{\rm m}^{-3}$	8.5x10 ⁸	4.6×10^{8}	9x10 ⁸	5.7x10 ⁸				
$d_{\rm e},{ m mm}$	1.2	1.7	1.05	1.56				
$d_{\rm c}$, mm					0.73	0.58	0.65	0.52

Refer to Figure 3(a) for the positions.

The calculated solute concentration of the solid mixture, c_{mix} , shown in Figure 6, exhibited good agreement compared to the readings of the spark analysis of the cast sample shown in Figure 6 (right). The calculated highest positive segregation is located at the top of CET and the lowest negative segregation is close to the center of CET. The top and bottom of the ingot have relatively low c_{mix} . The extremes of macrosegregation do not agree but are close to each other. The c_{mix} values at some odd locations do not agree as well. The analysis of macrosegregation formation mechanisms is out of the scope of the current paper.



Figure 6. c_{mix} of the ingot poured at 800 °C: measurement (left) *vs.* calculation (right).

The same modeling parameters for the case poured at 800 °C are applied to the case poured at 700 °C. Nevertheless, similar CET profile and similar macrostructure distribution to those shown in Figure 4(a) were obtained in contrast to the expectations. It is well established that lowering the pouring temperature increases the proportion of the equiaxed zone, i.e. promotes an earlier CET. This contradiction may be owed to the ignorance of the pouring effect. During real mold filling, nucleation of equiaxed grains starts when the molten metal hits and contacts the cold walls of the mold. In the current simulation the mold filling was ignored for the purpose of simplification and reduction of the calculation time. To compensate this ignored effect in the current simulation, the initial state of grain number density, n_0 , was customized. Reasonably, n_0 is dependent on the pouring temperature and

IOP Conf. Series: Materials Science and Engineering 33 (2012) 012075 doi:10.1088/1757-899X/33/1/012075

pouring method [3, 26]. Numerical parameter study was performed to investigate the influence of n_0 on the macrostructure, as shown in Figure 7. The assumption of small n_0 (10⁷ m⁻³) matches well with the case of high pouring temperature (800 °C), while a quite large n_0 (10⁹ m⁻³) should be chosen for the case poured at 700 °C, as shown in Figure 7(a) and (d). The macrostructure as predicted in Figure 7(d) agrees satisfactorily with the experimental result of Figure 3(c). One point needs mentioning here is that a minimum grain number density, $n_{\min} = 10^7$ m⁻³ (default) is numerically preset for the incoming melt in the current nucleation model. Initialization of n_e with ' $n_0 = n_{\min}$ ' is necessary for solving the grain transport equation. This numerical parameter, n_{\min} , seems to show some influence on the modeling results as shown in Figure 7(c) and (d). This influence is not yet fully understood, and it demands further investigation.



The hard blocking of the columnar dendrite tip growth is also an important issue that impacts the prediction of the CET [26, 28]. Reduction of the blocking criterion, $f_{e,CET}$, from the originally suggested 0.49 [9] to the newly proposed 0.2 [28] seems to predict a larger equiaxed zone as shown in Figure 8 for the ingot poured at 700°C. Hence, lower $f_{e,CET}$ better matches with the experiment in the current ingot.

The above results and discussion highlight that simulation results of the high pouring temperature ingot exhibited better agreement with experiments in comparison with those of the lower pouring temperature ingot. The high superheat (~185°C) in the former case heats up the mold walls and reduces the opportunity of melt undercooling and nucleation during the filling of mold. Moreover, it can even re-melt the previously formed nuclei. As a result, this case matches well the model assumptions, where no filling is taken into account. On the other hands, calculated results at the lower pouring temperature (superheat ~85°C) deviate from reality, since nucleation is more likely to occur during mold filling, which is already ignored in the simulation.

Figure 7. Calculated macrostructural quantities for the ingot poured at 700 °C. (a) f_e and (b) n_e calculated using $n_{\min} = 10^7$ and n_0 $= 10^9$, (c) f_e using $n_{\min} = n_0 = 10^8$, (d) f_e using $n_{\min} = n_0 = 10^9$.



Figure 8. Influence of hard blocking criterion on CET. Predicted f_e using $f_{e,CET} = 0.2$ (left) and $f_{e,CET} = 0.49$ (right).

IOP Publishing

5. Conclusion

The as-cast structure, CET and macrosegregation in an Al-4.0 wt.% Cu ingot were successfully predicted using the 5-phase mixed columnar-equiaxed solidification model. As a further step to the previous work [26], it is found that the nucleation parameters for the equiaxed phase play a critical role, and therefore, an experimental method [29] is recommended to determine the nucleation parameters. Calculations with the in-situ determined nucleation parameters improved the modelling results to a large extent. The simulation results exhibited very good agreement with experiments at high pouring temperature. However, modeling results for the ingot poured at low pouring temperature demonstrated the importance of the effect of mold filling in the formation of the as-cast structure. Further verifications for the hard blocking criterion are also desired.

Acknowledgement

This work was financially supported by the FWF Austrian Science Fund (P23155-N24). Casting experiments were performed by Georg Nunner and Gerhard Hochleithner.

References

- [1] Chalmers B 1963 J. Austral. Inst. Met. 8 255
- [2] Flemings M 1974 Solidification Processing (New York: McGraw-Hill)
- [3] Ohno A 1987 Solidification: The Separation Theory and its Practical Applications (Berlin: Springer-Verlag)
- [4] Spittle J, Dellamore G and Smith R 1967 Proc. *The Solidification of Metals* (The Iron and Steel Institute London) 318
- [5] Morando R, Biloni H, Cole G and Bolling G 1970 *Metall. Trans.* **1** 1407
- [6] Winegard W and Chalmers B 1954 Trans. ASM-AIME 46 1214
- [7] Jackson K, Hunt J, Uhlmann D, Seward III T 1966 Trans. TMS-AIME 236 149
- [8] Southin R 1967 Trans. TMS-AIME **239** 220
- [9] Hunt J 1984 Mater. Sci. Eng. 65 75
- [10] Gäumann M, Trivedi R and Kurz W 1997 Mater. Sci. Eng. A 226-228 763
- [11] Wang C and Beckermann C 1994 Metall. Mater. Trans. A 25A 1081
- [12] Martorano M, Beckermann C and Gandin Ch-A 2003 Metall. Mater. Trans. A 34A 1657
- [13] Martorano M and Biscuola V 2009 Acta Mater. 57 607
- [14] Wu M and Ludwig A 2006 Metall. Mater. Trans. A 37A 1613
- [15] Wu M and Ludwig A 2007 Metall. Mater. Trans. A 38A 1465
- [16] Gandin Ch-A. 2000 Acta Mater. 48 2483
- [17] Gandin Ch-A 2000 ISIJ Int. 40 971
- [18] McFadden A, Browne D and Gandin Ch-A 2009 *Metall. Mater. Trans.* A **40A** 662
- [19] McFadden A and Browne D 2009 Applied Math. Modell. 33 1397
- [20] Siqueira C, Cheung N and Garcia A 2002 Metall. Mater. Trans. A 33A 2107
- [21] Wu M, Fjeld A and Ludwig A 2010 Comp. Mater. Sci. 50 32
- [22] Wu M, Ludwig A and Fjeld A 2010 Comp. Mater. Sci. 50 43
- [23] Wu M and Ludwig A 2009 Acta Mater. 57 5621
- [24] Wu M and Ludwig A 2009 Acta Mater. 57 5632
- [25] Wu M and Ludwig A 2009 Int. J. Cast Metals Research 22 323
- [26] Wu M Nunner G Ludwig A Li JH Schumacher P 2011 IOP Conf. Series: Mater. Sci. Eng. 27 012018
- [27] Rappaz M 1989 Int. Mater. Rev. 34 93
- [28] Martorano M and Biscuola V 2008 Metall. Mater. Trans .A 39A 2885
- [29] Ahmadein M Pustal B Berger R Subasic E Bührig-Polaczek A 2009 Metall. Mater. Trans. A 40A 646
- [30] Rappaz M and Gandin C-A 1993 Acta Metall. Mater., 41 345