Numerical study of the influence of mold filling conditions on the as-cast structure of Al-4 wt.% Cu ingots

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***Abstract*—In the last few decades research efforts were conducted to grasp good understanding about the origin of equiaxed and columnar grains formed during solidification. The morphological evolutions such as globular/cellular to dendritic or columnar-to-equiaxed transition were generally studied. Correspondingly, some empirical models were introduced. Nevertheless, no sufficient attention was paid to incorporation of such models together with macroscopic phenomena. A 5-phase mixed columnar-equiaxed solidification model recently proposed by the current authors was used to predict the macrostructure formation. However previous results showed that the initial melt conditions can influence the predicted structure particularly at low pouring temperature. In the current work, the impact of mold filling conditions on the final solidification structure is numerically verified in two stages: during pouring using 3-phase globular-equiaxed model; and after filling using the 5-phase mixed columnar-equiaxed model. The calculated results are compared to the as-cast structures obtained from experiments. The results demonstrated the significance of the 'big bang' nucleation and the 'premature' solidification occurred during pouring at low melt superheat on the as-cast structure.**

***Keywords*—modeling, as-cast structure, nucleation, CET**

I. INTRODUCTION

The as-cast structure has crucial impact on the mechanical properties of cast products. Researchers and metallurgists studied over decades the factors affecting the as-cast structure [1]-[5]. In recent times, they modeled the micro- and macro-structure formation to predict and improve the properties of the final products. Once the nucleation of equiaxed grains occurs (heterogeneously or under dynamically stimulated conditions), grain grow in either columnar (cellular or dendritic) or in equiaxed (globular or dendritic) form. The final as-cast structure may contain one or more of these morphologies with columnar-to-equiaxed transition (CET). In addition, various interacting multi-phase / multi-scale processes during solidification, e.g. transport of heat, momentum, mass, species, and melt convection increase the complexity of the prediction of the as-cast structure.

Progress was also made in the understanding of CET since the pioneer work of Hunt [6] 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 [7]-[12]. In the meantime, empirical correlations were proposed as indirect criteria to predict the CET for engineering castings [13]-[17].

In the late work of Wu et al. [20]-[22], 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 were compared to Al-Cu alloy ingots poured at various temperatures [23]. The results showed that the model is capable to qualitatively produce similar structures. However, the detailed structural agreement could not be achieved. Further improvement to the model results were obtained after the application of experimentally determined nucleation parameters [24] for the nucleation model instead of the assumed nucleation parameters used in [23]. As a consequence, a good qualitative agreement in addition to satisfactory quantitative agreement between simulation and experiment were obtained for the ingot poured at high temperature [25]. Nevertheless, the results of the ingot poured at lower temperature disagree with the experiment. The authors argued some possible reasons for the disagreement. The initial grain number density, n_o, was the most important parameter that influences the profile of CET-line and the proportion of the formed equiaxed crystals. By recalling the previous experimental investigations on the influence of the mold filling conditions on the as-cast structure [4][5][26], it can concluded that the pouring temperature, mold temperature, and pouring technique play very important role.

In the present work and based on the above discussion, the influence of various mold filling parameters on the initial state of the melt is numerically investigated using a 3-phase flow and solidification model developed at earlier time by current authors. Afterwards, the mold filling simulation outcomes are used as initial conditions for the simulation of the as-cast structure using the 5-phase mixed columnar/equiaxed model.

II. KEY FEATURES OF MODELS

The simulation of the as-cast structure and CET was conducted using a 5-phase mixed columnar/equiaxed model [18][20]-[21]. To get realistic initial conditions instead of the previously assumed ones [23], the mold filling was simulated using a 3-phase globular solidification model. Both models are briefly described below. The volume averaging approach was employed to formulate the conservation equations of mass, momentum, species, and energy for the assigned phases. The former conservation equations, in addition to the grain transport equation, were solved sequentially at each time-step with implicit linearization based on the control volume method. The solidification models were implemented in an Eulerian multiphase CFD code (ANSYS Fluent 6.3.26) [27].

A. The 5-phase model

The 5-phase mixed columnar/equiaxed 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 columnar dendrites start to grow perpendicular to the mold interface, opposite to the direction of heat flow. 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, $\vec{u}_{\mathrm{e}}$, $\vec{u}_{\mathrm{c}}$, and $\vec{u}_{\ell}$. Here $\vec{u}_{\mathrm{c}}$ is predefined (zero in the case of ingot casting), while $\vec{u}_{\mathrm{e}}$ and $\vec{u}_{\ell}$ are solved numerically.

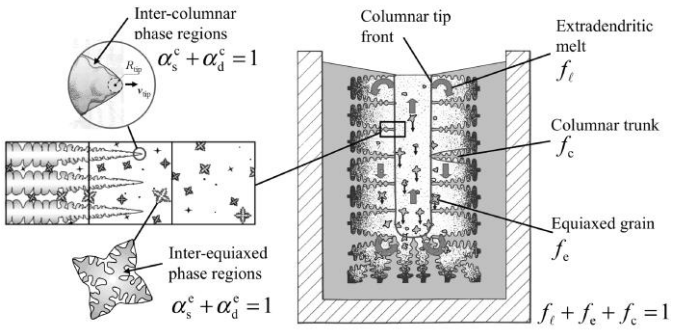


Figure 1. Schematic of the mixed columnar-equiaxed solidification in an ingot casting

A three-parameter heterogeneous nucleation law [28][29] is applied for the origin of equiaxed grains. These nucleation parameters can be obtained experimentally. Since the current model does not include mold filling, its end effect can be resembled by assuming some initial conditions in the as-filled state, e.g. initial grain number density, n_0 , initial phase fractions, etc.

The dendritic growth of crystals is taken into consideration as shown in Figure 1. Two distinct phase regions exist within the crystal envelope: 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. 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. Each region has correspondingly volume fractions: $f_{\mathrm{s}}^{\mathrm{e}}$, $f_{\mathrm{d}}^{\mathrm{e}}$, $f_{\mathrm{s}}^{\mathrm{c}}$, $f_{\mathrm{d}}^{\mathrm{c}}$, f_{ℓ} , and characterized by its corresponding solute concentration: $c_{\mathrm{s}}^{\mathrm{e}}$, $c_{\mathrm{d}}^{\mathrm{e}}$, $c_{\mathrm{s}}^{\mathrm{c}}$, $c_{\mathrm{d}}^{\mathrm{c}}$, c_{ℓ} . Inside an equiaxed grain, volume fractions of interdendritic liquid and solid dendrites are quantified respectively with $\alpha_{\mathrm{d}}^{\mathrm{e}}$, $\alpha_{\mathrm{s}}^{\mathrm{e}}$, hence $f_{\mathrm{d}}^{\mathrm{e}} = \alpha_{\mathrm{d}}^{\mathrm{e}} \cdot f_{\mathrm{e}}$ and $f_{\mathrm{s}}^{\mathrm{e}} = \alpha_{\mathrm{s}}^{\mathrm{e}} \cdot f_{\mathrm{e}}$. Inside a columnar dendrite trunk, $f_{\mathrm{d}}^{\mathrm{c}} = \alpha_{\mathrm{d}}^{\mathrm{c}} \cdot f_{\mathrm{c}}$ and $f_{\mathrm{s}}^{\mathrm{c}} = \alpha_{\mathrm{s}}^{\mathrm{c}} \cdot f_{\mathrm{c}}$.

Both hard blocking [6] and soft blocking [9] mechanisms are implemented and applied to model the CET model. In current simulations, $f_{\mathrm{e,CET}}$ is set to 0.49. For more details regarding growth kinetics, treatment of the dendritic morphology of crystals, algorithm of tracking the columnar tip, etc. refer to previous publications [18]-[21].

B. The 3-phase model

The 3-phase model used during pouring and filling comprises: the air phase that initially fills the mold space, the poured liquid metal, and the solidifying crystals that form as the melt is undercooled. The mass exchange between liquid and solid depends on the growth velocity. The air has no mass or species exchange with the other phases. The presence of air increases the model flexibility as it can substitute metal shrinkage, heat and drag force exchange, which makes the model closer to reality. On the other hand, including the air increases the computational time and requires a finer mesh to account for the distinct and intricate topology of the liquid/air interface. The mass exchange introduces an additional source term for the momentum equation. The latent heat liberated during solidification is taken into account for the source term of the energy equation. A detailed description of the transport equations and the definitions of the corresponding source terms are provided in [30]-[33].

III. PROBLEM SETUP

A 2D-axisymmetric grid (Figure 2, left) was constructed and provided with one velocity inlet at the top for pouring the superheated melt. Pouring temperatures were 700, 750, and 800°C. From the casting experiments, pouring speed was estimated to be 1.037 m/s for a corresponding filling time of ~ 5.5 s. The heat is transferred from the mold to the atmosphere through the outer wall by convection with a coefficient of 120 $\mathrm{W \cdot m^{-2} \cdot K^{-1}}$. The heat transfer coefficient at ingot/mold interface is set to 2900 $\mathrm{W \cdot m^{-2} \cdot K^{-1}}$. The mold is initially filled with air (with phase fraction, f_a ~ 1) at ambient temperature. Air is

allowed to scape from mold during filling. Fixed time-stepping scheme was employed with a time step of 10^{-4} s.

For the simulation of columnar/equiaxed solidification using 5-phase model a similar grid was constructed (Figure 2, right) such that the top surface profile is similar to that of the real casting. The heat transfer coefficient at the interface is reduced to 1000 $W \cdot m^{-2} \cdot K^{-1}$. It is further reduced to 125 $W \cdot m^{-2} \cdot K^{-1}$ when the temperature at T1 reaches the liquidus temperature. The initial conditions such as; phase fractions, phase concentrations, grain number density (n), mold and ingot temperatures, etc. were given based on the results of mold filling simulation. The columnar primary dendrites were initialized with tips at the side and bottom mold walls and with $f_c = 10^{-5}$. Adaptive time-stepping scheme was employed with a minimum time step of 10^{-4} s. The grid was provided with some control points and thermocouples, e.g. T1, T2, T3.

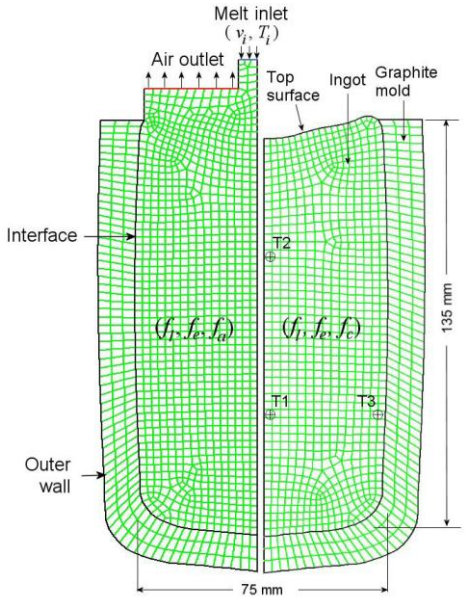


Figure 2. Simulation grid for mold filling (left) and for columnar/equiaxed solidification (right).

IV. Results and Discussion

A. Results of 3-phase model

The calculated temperature after filling time of 5 s for the ingot poured at 700 °C (Figure 3, left) showed that the superheated falling metal jet retains its temperature till it bumps up against the mold base. Thus, it exchanges the heat with the cold mold, cools down and continues to cool while it is streaming upward close to the mold wall. Additional heat losses occur through the melt/air interface at the top. As a result, during the filling the top of the ingot is colder than the bottom. Consequently, the liquid-to-solid mass transfer rate is high at the top compared to the bottom which is almost zero. The grains formed at the top are transported by convection and sedimentation to the bottom. Some of them survive and some are remelted in the hot region of the mold. This complex interaction leads finally to increase of f_e and grain density at the bottom as shown in Figure 3 (right) and Figure 4. The grain nucleation is much sensitive to the temperature fluctuations compared to grain growth. Consequently, the distribution of grains and the maximum grain density are successively changed, which is very obvious by comparing the grain density after 4.5 s and 5.0 s (Figure 4).

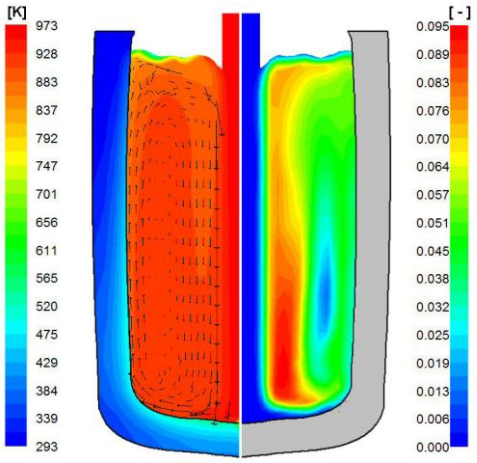


Figure 3. Calculated temperature, left, and equiaxed phase fraction, right, after ~5 s filling time for ingot poured at 700 °C.

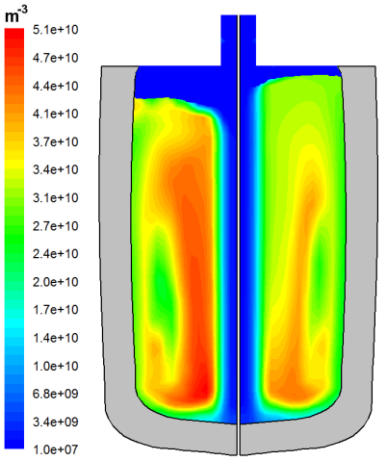


Figure 4. Calculated grain number density of the ingot poured at 700 °C after filling time of 4.5 s, left, and 5.0 s, right.

The development of the average grain number density, n, and equiaxed phase fraction within the mold were tracked during pouring process. The simulation results at various pouring temperatures are plotted as shown in Figure 5 and Figure 6. It is obvious that the reduction of pouring temperature increases the nucleation rate and the final n. At low superheat (pouring temperature of 700°C) nucleation takes place immediately when the falling metal jet touches the cold bottom of the mold and n reaches ~2e+9 m^{-3}. The nucleation rate decreases afterwards as a result of heating up the mold and the continual pouring of hot metal. The grain density is

subjected to fluctuations due to the destruction of some already formed crystals caused by the convection of them into the hot region. For the case of 700 °C and after ~2.8 s, the plenty amount of nucleated crystals grow at high rate leading to the steeper rise of f_e (Figure 6). At this moment the mold is about 50% full and is relatively heated up. On the other hands, pouring continues and much latent heat is released due to grain growth. The mutual effect of the former factors leads to destruction of some solid crystals (n decreases) and reduction of the growth rate (f_e) after 4 s.

In contrast to the ingot poured at 700 °C, the nucleation and growth are delayed for the ingots poured at 750 °C and 800 °C until the melt is sufficiently supercooled. However, in all cases initial solidification (nucleation + growth) with f_e ~ 4e-5 occurs at the same moment (0.2 s) when the hot melt bumps the mold bottom and strongly mixed with the cold air. The obtained solid fraction decreases gradually due to the continual pouring liquid metal with (f_l = 1), which reduces f_e in spite of the progressive solidification. In the case of 800 °C the solid fraction formed after at the end of filling is almost zero although ~7e+8 m^{-3} of stable nuclei are already formed. The grain diameter is kept at the model minimum (1 μm).

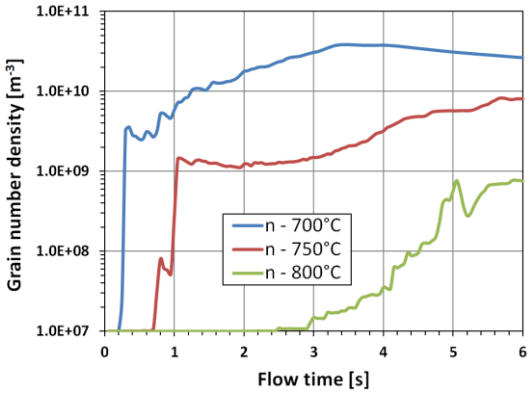


Figure 5. Grain number density at different pouring temperatures versus the filling time.

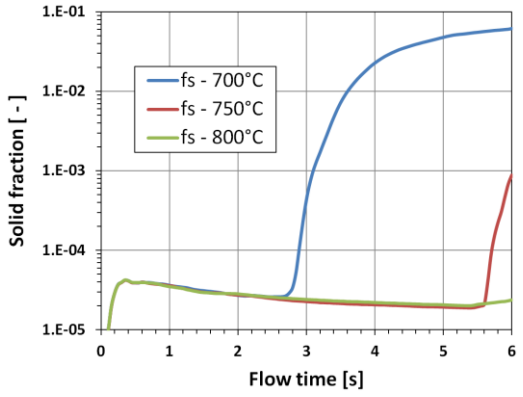


Figure 6. Development in equiaxed phase fraction during mold filling at different pouring temperatures.

To study the influence of mold temperature on the possible 'premature' solidification during mold filing, simulation boundary conditions of the 700 °C poured ingot are kept the same and only the initial mold temperature is increased to 300 °C. The calculated grain number density and the development in f_e are plotted as per Figure 7. It is clear that increasing the mold temperature from 20 °C to 300 °C decreases the nucleation and the growth rate as well. The grain number density is ~3.5 times decreased with n = 6.2e+9 representing a solid fraction of ~0.00003. The relative jump in f_e at 0.2 s decreases gradually afterwards similar to the above cases.

The above results reveal that the severity of what is called "big bang" nucleation is much reduced as the pouring temperature increased and/or the mold temperature is increased, which agree with the experimental evidences [4][5][26].

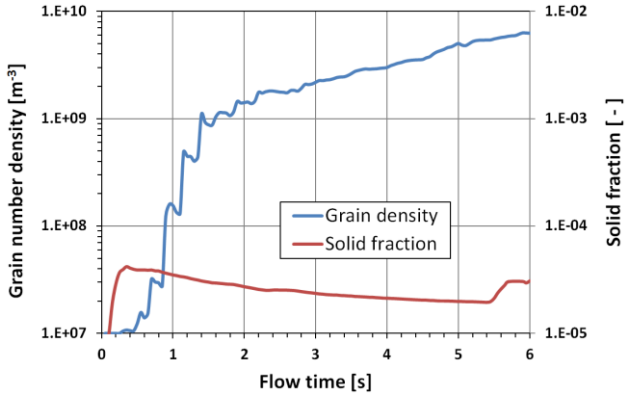


Figure 7. The calculated n and fe for the ingot poured at 700 °C in a mold preheated to 300 °C.

B. Results of 5-phase model

The predicted results of mold filling obtained above are used to initialize the solution of the solidification using the 5-phase mixed columnar/equiaxed one. The initialization quantities are summarized in Table.1.

TABLE 1. CONDITIONS FOR SOLUTION INITIALIZATION OF 5-PHASE MODEL.

$T_{pouring}$ [°C]	$T_{casting}$ [°C]	T_{mold} [°C]	n_o [m^{-3}]	f_e [-]	d_e [mm]	c_{solid} [wt.%]	c_l [wt.%]
700	675	102	2e+10	0.055	0.017	1.7	4.15
800	775	150	5e+9	0.00002	0.001	2.3	4

The calculated cooling curves at the thermocouple T1 (Figure 2) are plotted along with those of recorded from experiments as explained in Figure 8. Both results have approximately similar cooling rates and exhibited solidification plateau at the equilibrium liquidus temperature. Slight undercooling can be revealed, in particular for the ingot poured at 700 °C.

The predicted macrostructures after solidification of the 700 °C and 800°C poured ingots using $f_{e,CET}$ = 0.49 are shown in Figure 9. The calculated as-cast structure of the ingot poured at 700 °C (Figure 9a) consists mainly of equiaxed grains. Very few columnar dendrites with maximum f_c < 0.5 are formed at the ingot peripheral and extended just few millimeters into the ingot. These dendrites are blocked by the equiaxed crystals growing competitively ahead of the columnar tips, leading to the formation of the CET-line.

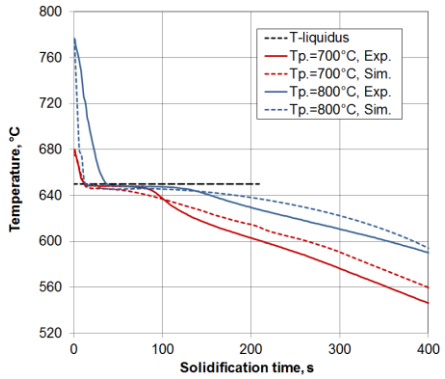
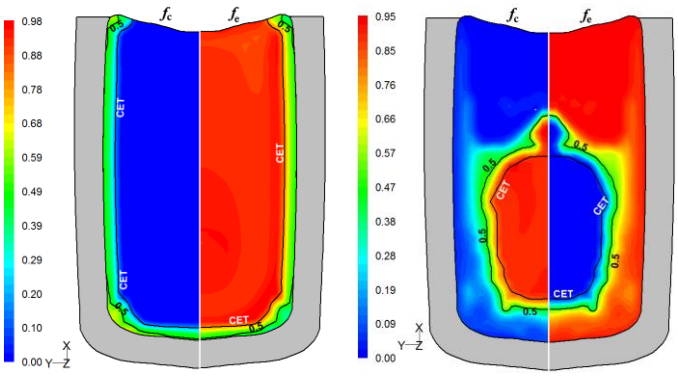


Figure 8. The calculated and measured cooling curves at point T1 for ingots poured at 700 °C and 800 °C.

In the case of ingot poured at 800 °C (Figure 9b), greater columnar zone is formed in account of the equiaxed zone which is limited to the ingot core. Several factors favor the formation of this structure: the low initial f_e; the low initial n obtained from the 3-phase filling simulation; the relatively low cooling rate. Under these conditions, the growing columnar crystals win the competition and advance for a longer distance into till they are blocked either by the accumulative equiaxed crystals (hard blocking) or by the high solute pile up at the advancing front (soft blocking). Thus, the CET-line is formed and the equiaxed crystals are confined within the ingot core.

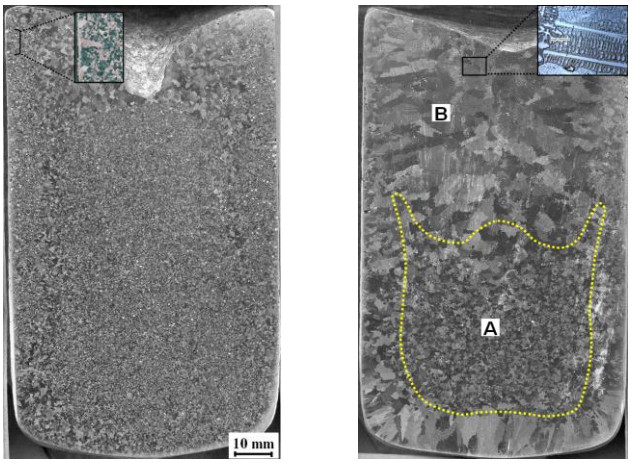


(a) (b)

Figure 9. The calculated fractions of columnar and equiaxed phases within the ingots poured at (a) 700 °C and (b) 800 °C

The actual as-cast structures of both ingots obtained from experiments are shown in Figure 10. It is evident that the macrostructure of ingot poured with smaller superheat is fully equiaxed except for very little columnar dendrites that form in particular close to mold corners and peripherals (look at the zoomed region in Figure 10a). However, pouring at higher temperature (800°C) as shown in Figure 10b introduces a mixed structure with fully equiaxed grains at the ingot core (region A) surrounded by columnar grains growing from the mold walls (region B). Both regions are separated with a mixed structure zone and of course the CET can be easily distinguished.

The present results exhibited a good qualitative agreement with experiments. In a previous study [25] using the 5-phase model alone and assumed initial conditions, the authors could successfully reproduce the as-cast structure of the ingot poured at 800 °C numerically. Nevertheless, they failed obtain the as-cast structure of the ingot poured at 700 °C, even when the assumed initial grain number density was drastically increased.



(a) (b)

Figure 10. The actual as-cast structure of the Al - 4wt.% Cu ingots poured at (a) 700 °C and (b) 800 °C

From the above results it is obvious that the ‘premature’ solidification occurred during mold filling is an unignorable. During mold filling several factors interact simultaneously in a very complex manner and influence the calculated n, f_e, solute concentration, and grain diameter, e.g. heat added by hot melt, heat extracted by the mold, heat transferred to the air at the top, release of the latent heat, nucleation and destruction of grains, growth and remelting of grains, etc. The 3-phase model accounts for all of them and provide an improved estimation for the initial conditions required to simulate the ingot solidification using the 5-phase model.

V. Conclusion

Mold filling conditions, e.g. pouring temperature, mold temperature, influence the as-filled state of ingot. Pouring with low superheat or in cold molds may lead to ‘premature’

solidification. Results reveal the significance of the 'premature' solidification on the as-cast structure. The 3-phase flow and solidification model can successfully account for the various mold filling conditions and can provide improved initial conditions for the prediction of the as-cast structure using 5-phase mixed columnar/equiaxed model. By considering the results of mold filling, better qualitative agreement between simulation and experiment could be achieved.

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