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# Macrostructure Modeling of Al-20 % Sn Alloy

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## Abstract

In metallic alloys, the formation of macrostructure involves different length and time scales. The macrostructure strongly influences the mechanical properties of the materials. Modeling of macrostructure provides valuable insights for tailoring of the structure. In the present study simulation of macrostructure in Al-20Sn has been carried out. Expression for nucleation rate and growth rate were tuned to get a match with the experimentally observed macrostructure. The study incorporates the motion of grains due to Brownian motion. Incorporation of Brownian motion resulted in more uniform distribution locally, which has been experimentally observed. Both simulation and macrograph showed few columnar grains and absence of sharp columnar to equiaxed transition.

**Key words**: Brownian motion, Al-Sn system, Macrostructure, Cellular Automaton (CA)

## Introduction

In metallic alloys systems, the study of macrostructure evolution involves different length and time scales. The final macrostructure strongly influences the mechanical properties of the materials. Modeling of macrostructure provides valuable insights for tailoring of the macrostructure.

Microstructural evolution during solidification processing primarily depends upon the thermal and solutal fields. Fluid flow due to forced or natural convection also influences the microstructural evolution. It does so in two ways. Firstly, it influences the thermal-solutal fields which in turn influence the microstructural evolution. Secondly, due to the fluid flow isolated grains get redistributed.

Modeling of microstructural evolution during solidification[(1)] mostly involves computation of thermal-solutal fields using continuum equations and prediction of microstructure based on thermal-solutal fields, using cellular automaton (CA) based models. CA based modeling was initially developed by Rappaz, et al.[(2)] The model was modified by Zhu, et al.[(3)] and some researchers[(4-7)] for the prediction of dendritic structures. It is interesting to note that modeling of microstructural evolution has been attempted at different lengths scales ie from atomistic to macro scale.

The present work involves solution of continuum equations for computation of temperature fields (using FLUENT or control-volume heat transfer models), and coupling it with a CA based model that computes the evolution of grain structure with solidification time. The measured flux values (obtained by the Data Acquisition System) can be fed into FLUENT to derive the evolution of thermal fields with solidification time. Using measured temperature values at specific points along the mold-metal interface, realistic flux values at the mold-metal interface can be derived which can then be fed to FLUENT to obtain accurate thermal fields across the casting domain. These fields are used in the Cellular Automaton model to predict macrostructure evolution as solidification proceeds.

It was felt that unlike solid state transformation the nuclei formed will get transported due to Brownian motion and fluid flow-which has a significant role in the case of immiscible alloy systems, due to the large solidification range. So the present model incorporates the Brownian motion of nuclei when their size is below a critical value ie the size of the nuclei is below submicron. The effect of Brownian motion ceases to be significant once the liquid fraction decreases below a critical limit-henceforth due to excessive grain crowding and grain growth, grain redistribution becomes less probable.

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Solidification modeling of Al-Sn alloy systems has not been widely investigated. Solidification occurs over a large range of temperature-giving sufficient time for grain redistribution to occur. It influences the microstructure in a significant manner. The simulated macrostructures incorporating Brownian motion closely match the observed macrographs in three key aspects-absence of a distinct columnar zone at the mold-metal interface, absence of the columnar-to-equiaxed transition zone and presence of larger grains midway between the central mold axis and the mold-metal interface.

Incorporation of Brownian motion results in better uniformity and overall homogeneity in the final macrostructures. The model was validated for Al-20%Sn alloy. The grain size distribution was mapped both for observed and simulated macrographs. The one incorporating Brownian motion better resembled the experimentally observed macrographs. Hence, incorporation of Brownian motion results in better prediction of solidification macrostructures of immiscible alloy systems.

## Materials and Experimental Procedures

### *Modeling of Microstructural Evolution*

FLUENT software version 6.2.16 has been used to compute the thermal and flow field at different locations within the casting. The boundary condition(s) used for the solidification process is shown in Figure 1. The heat flux at the mold-casting interface was calculated on the basis of temperature recorded by data acquisition system. Based on the thermal field calculated by FLUENT a Cellular Automata based model was used for predicting the microstructure, similar to that developed by Rapaaz and other co-workers. (2-6) However here Brownian motion of small nuclei was taken into consideration.

### *Undercooling, Nucleation and Growth*

In the current model the, the undercooling ($\Delta T$) in a cell is determined as $\Delta T = T_{eq} - T_{cell}$. The equilibrium liquidus temperature ($T_{eq}$) is calculated from the phase diagram and $T_{cell}$ is obtained from the Fluent 6.2.16 at each time step. During the simulation the local undercooling is updated in each cell at every time step to determine the nucleation rate. The nucleation rate has been assumed to be linear and depends upon the undercooling. The nucleation is defined as below.

$$N = k(\Delta T)^n$$

where $k$ = constant that has been determined experimentally
$\Delta T$ = undercooling required for nucleation to start
$n$ = exponent that determines the order of nucleation rate
For $n$ = 1, the nucleation rate is linear

The growth velocity at certain undercooling is determined using the KGT model.[2] Once the cell is nucleated it will grow in preferential direction corresponding to its crystallographic orientation depending on heat flow. The detail of growth algorithm is given in the literature.[2]

### *In Corporation of Brownian Motion*

Brownian motion, in terms of physics, is the random motion of particulate matter suspended in a fluid. Einstein predicted that the random motions of molecules in a liquid impacting on larger suspended particles would result in irregular,

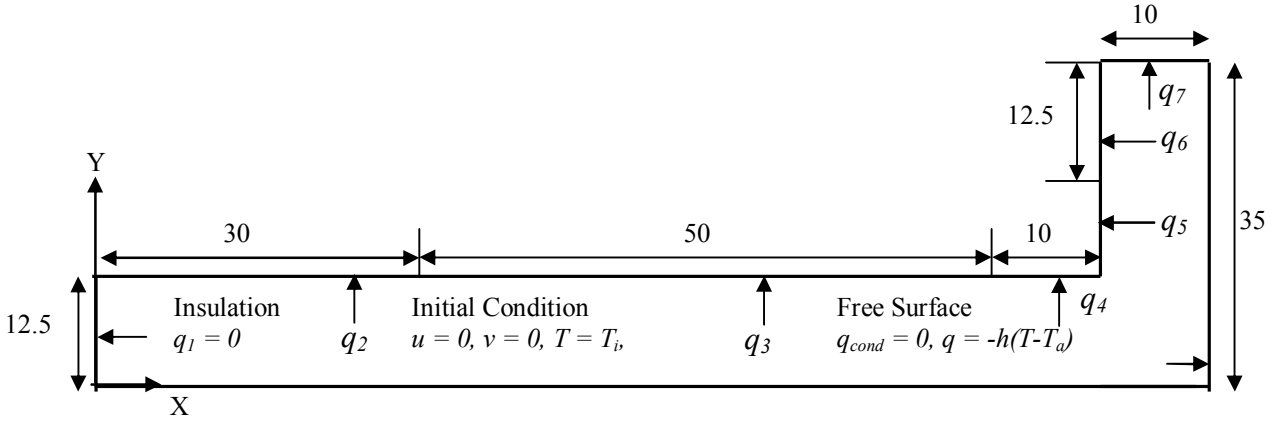



**Figure 1.** Initial and boundary condition (All dimensions are in mm)

random motions of the particles, which could be directly observed under a microscope. The algorithm of Brownian movement of the nucleus was given as below.

Step I : Calculation of temperature field
Step II : Calculation of the probability field for each particle/cell

$$P(x_i, \Delta t) = \frac{1}{\sqrt{4\pi D_i \Delta t}} \exp(-x_i^2 / 4D_i \Delta t)$$

$$P(y_i, \Delta t) = \frac{1}{\sqrt{4\pi D_i \Delta t}} \exp(-y_i^2 / 4D_i \Delta t)$$

where, $D_i = k_B T / 6\pi\eta R$

$\Delta t$ = time increment
$T$ = temperature in the cell
$\eta$ = viscosity of the melt
$R$ = radius of the grain

Step III : Movement of nuclei to new position (random walk)
Step IV : Update the parameters for all nuclei

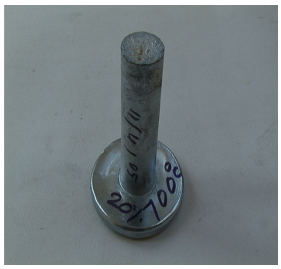
**Experimental Procedure**

A T-section (Inner) and I section (out side) mold was used in the experimental set-up as shown in Figure2(b). An insulator was placed at the bottom of the mold, and the free surface of the melt was exposed to atmospheric cooling. The pouring temperature of the melt was above the liquidus temperature of the alloy system. During the progress of solidification, thermocouples were placed at different positions to measure the unidirectional heat flux values. The heat flux at the mold-casting interface was calculated on the basis of temperature recorded by data acquisition system. After the completion of solidification, the cast was cut both in transverse as well as in longitudinal planes for microstructural observations.

The Al alloy with 20-wt% Sn was melted in a clay graphite crucible up to the temperature about 700°C in an electric furnace and poured in mold. The experimental set up is shown in Figure 2(a). The pouring temperature was recorded as 671°C. The cast was cut both in transverse as well as in longitudinal section for microstructural studies. Temperature at the mold-metal interface is measured at three distinct positions, at an interval of a second, with the help of a Data Acquisition System (DAS). A schematic representation of the points at which flux values have been measured is shown in Figure 2(a). The as cast T section after solidification is shown in Figure 2(c).

The measured flux values can then be fed into FLUENT as a function of solidification time to predict the evolution of thermal fields within the casting domain. Using an inverse model, we can use the temperature values at the mold-metal interface to determine flux values at the interface which can be fed into FLUENT to obtain realistic temperature fields. These can then be used in the Cellular Automaton model to predict macrostructure evolution during solidification.

(a)



(b) (c)

**Figure 2.** (a) Experimental set-up of casting with temperature recording using data acquisition system (b) Mild steel mold (I shape) (c) Al-20Sn casting (T shape)

## Results and Discussion

The simulated temperature profile at t = 328.69s is shown in Figure 3. The macrostructure of the casting is shown in Figure 4 and the corresponding simulated macrostructure after incorporating Brownian motion and without incorporating it, are shown in Figure 5(a) and (b) respectively. The nucleation

and the growth rates have been tuned according to the experimentally observed microstructure.

Both the predicted structure and macrograph show uniformity in macrostructure across the entire casting. They also show very few columnar grains and absence of sharp columnar to equiaxed transition. In the macrostructure, simulated without incorporating the Brownian motion, distributions were more non-uniform locally. Incorporating of Brownian motion resulted in more uniformity in the macrostructure locally. The CA based model predicts the presence of larger grain in between the edge and the centre. The experimental macrograph shows the same. In this sense the CA model incorporating the Brownian motion was closer to the experimental results. On the whole incorporation of Brownian motion appears to be giving a better prediction. The macrostructure of Al-20%Sn alloy is shown in Figure 4.It is observed that the Al grains are distributed in the Sn matrix as in the case of composites. As solidification proceeds, aluminium segregates as nuclei in the tin matrix, which move following Brownian dynamics, depending on local undercooling. The absence of a distinct columnar zone predicts the movement of the nuclei, which were formed near the mold wall, towards the interior of the melt. Both the predicted structure and macrograph show uniformity in macrostructure across the entire casting, and the absence of a sharp columnar to equiaxed transition thus confirming Brownian motion.

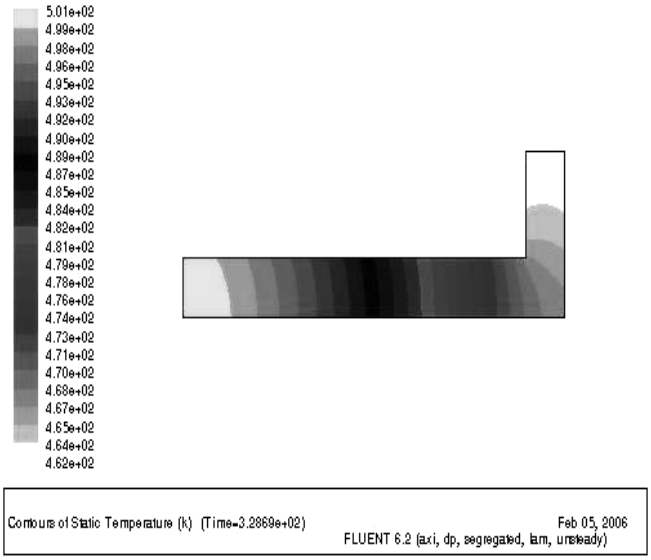



**Figure 3.** Temperature Profile of the casting after complete solidification at t = 328.69s

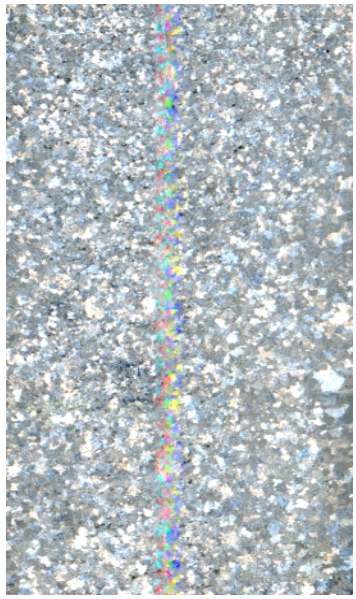


**Figure 4**. Macrostructure of Al-20Sn

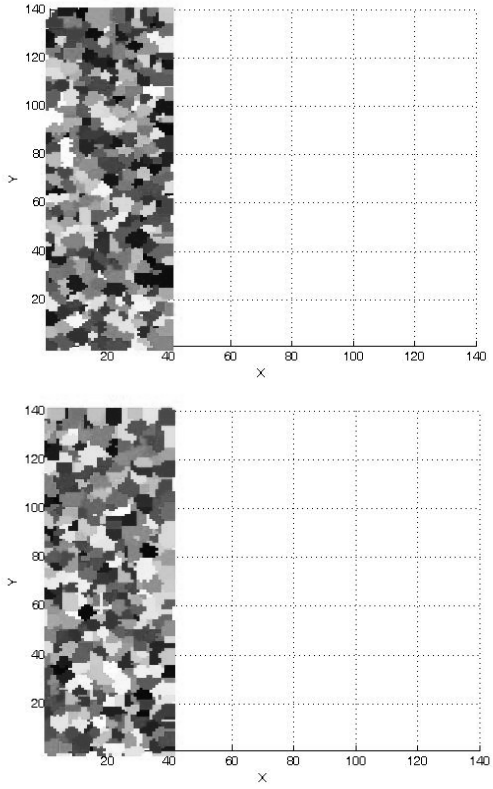



**Figure 5.** Simulated macrostructure of the casting (a) with Brownian motion, (b) without Brownian motion

## Conclusion

(a) As per prediction, the observed macrostructure is showing more uniform macrostructure through the casting, very few columnar grains, absence of sharp columnar to equiaxed transition and larger grains at midway distance from centre to the outer surface.

(b) Incorporation of Brownian motion gave locally a more uniform macrostructure as observed in the experimental macrograph.

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