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# Effect of thermal anisotropy on binary alloy dendrite growth

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ABSTRACT

A numerical model to study the effect of thermal anisotropy on binary alloy dendrite growth is presented. The model is based on the volume averaged enthalpy method with explicit surface tension anisotropy for crystal orientation. Thermal anisotropy is incorporated using anisotropic thermal conductivity in the energy equation. This is done by splitting the anisotropic conductivity into two parts, equivalent isotropic conductivity and anisotropic departure source term, enabling the use of a conventional isotropic solver to model anisotropic heat transfer. The proposed model is applied to study the effect of thermal anisotropy ratio on tip velocity, aspect ratio and equivalent radius of an equiaxed grain growing in an undercooled binary alloy melt. It is found that the thermal energy stored in the grain during solidification plays an important role in interface evolution, and thus anisotropic conductivity in the solid affects the grain morphology. There is a consistent increase in the aspect ratio of grains with increase in thermal anisotropy ratio, although the grain volume remains almost invariant. Due to unequal growth rates of the perpendicular arms, severe distortion of the solid crystal is seen at higher thermal anisotropy ratios. The model is further extended to study the growth of multiple dendrites in order to simulate microstructure evolution with thermal anisotropy. It is observed that thermal anisotropy significantly affects the grain morphology at low grain density but has a smaller influence at high grain density as compared to other governing factors such as solute transport.



## 1. Introduction

Modelling of microstructure evolution during alloy solidification can give critical insight into the various mechanisms governing grain morphology. There are several parameters such as surface tension, fluid flow, mass diffusion, thermal diffusion, magnetic susceptibility and degree of undercooling which control the dendritic growth during solidification of an alloy. A lot of studies individually and combining the above-mentioned parameters, have been undertaken to observe their effects on the formation and growth of dendrites during alloy solidification [1–5]. Thermal anisotropy is another major parameter that plays an important role in shaping dendrite morphology for some materials. Anisotropy can be present in several thermo-physical parameters, but in the current work, thermal conductivity is considered as the source of anisotropy. Generally it is seen that single solid crystal of gallium, indium and many other compounds behave in an anisotropic manner where the thermal conductivity is a function of direction [6–13]. This is attributed to the fact that, for crystals with close-packed structures (Simple Cubic, BCC, FCC and HCP), the packing fraction along each plane is different, which leads to variation in thermal conductivity along different planes. The thermal conductivity generally is highest in the plane where packing fraction is highest and minimum in the plane where the packing fraction is least. The aim of the present work is to study the effect of similar anisotropic conductivity on grain growth and morphology through the development of an enthalpy based model for simulating dendrite growth with thermal anisotropy.

For investigating and analysing the growth of an equiaxed crystal, tracking the evolution of solid-liquid interface is the most important step. A range of methods has been proposed to track the solid-liquid interface. The most commonly used models are based on phase-field and cellular automata methods. The phase-field method [14–21] uses a phase-field parameter to track the solid-liquid interface and employs energy-minimization techniques to calculate its evolution. Although it is computationally intensive, the phase field method is versatile and can handle complex microstructure evolution. On the other hand, the cellular automata method [22–25] simulates dendrite growth by explicitly calculating the interface velocity based on interface undercooling without solving the actual transport of energy at the interface. Due to its simplicity, it is suitable for simulating large scale grain

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**Nomenclature**

| | |
|---|---|
| $AR$ | thermal anisotropy ratio |
| $C$ | concentration |
| $c_p$ | specific heat (J/kg K) |
| $D$ | mass diffusivity ($m^2/s$) |
| $d_o$ | capillary length (m) |
| $f$ | phase fraction |
| $H$ | total enthalpy (Sensible and Latent) (J/kg) |
| $K$ | thermal conductivity (W/mK) |
| $k_p$ | partition coefficient |
| $L$ | dimension of cavity (m) |
| $L_f$ | latent heat of fusion (J/kg) |
| $Le$ | Lewis number ($\alpha_l/D_l$) |
| $M$ | dimensionless liquidus slope |
| $m$ | liquidus slope (K) |
| $T$ | temperature (K) |
| $T_m$ | melting temperature (K) |
| $S_D$ | departure source term |
| $t$ | time (s) |
| $V$ | concentration potential |
| $x, y$ | global coordinates |
| $X, Y$ | crystal coordinates |

*Greek symbols*

| | |
|---|---|
| $\alpha$ | thermal diffusivity ($m^2/s$) |
| $\rho$ | density ($kg/m^3$) |
| $\varepsilon$ | anisotropic strength |
| $\kappa$ | curvature (1/m) |
| $\gamma$ | surface tension (N/m) |
| $\theta$ | interface angle |

*Subscripts*

| | |
|---|---|
| $b$ | boundary |
| $eq$ | equivalent property |
| $l$ | liquid phase |
| $o$ | initial state |
| $s$ | solid phase |
| $Su$ | surface |

*Superscripts*

| | |
|---|---|
| $*$ | non-dimensional |
| $i$ | interface value |

structure evolution. Its main drawback is that it cannot resolve the tip growth kinetics accurately.

The enthalpy method [26–43] has gained a lot of popularity in simulating macro and micro-scale solidification due to its ease and simplicity of implementation. The enthalpy method uses a single domain approach where the solidification is simulated by solving the volume averaged energy and species concentration equations. The enthalpy at each discretized node is used to calculate the position of the solid-liquid interface [26]. The enthalpy method has been used extensively for simulating macro-scale solidification of binary alloys by Incropera [27–30], Voller [26,31–37], Chakraborty [38–41] and their co-authors. Subsequently, it has been modified for simulating micro-scale solidification and grain structure evolution. The first approach in this area was carried out by Tacke and co-authors [44,45] in which they simulated the growth of an equiaxed crystal in a 2D domain maintained at uniform undercooled temperature. Pal et al. [46] extended the study by analyzing the effect of pure material crystal growth in the presence of fluid flow. Chatterjee and Chakraborty [47] used a combination of enthalpy method and Lattice Boltzmann method to simulate equiaxed crystal growth using an implicit approach. Subsequently, Voller [48] developed an enthalpy-based model for simulating binary alloy diffusion-driven dendrite growth. The model used explicit surface tension anisotropy and accurate interface curvature calculation and the simulation results were in good agreement with other models such as phase-field. Kao et al. [49–52] have used similar models for studying the effect of magneto-hydrodynamic flow on crystal growth. Later, Bhattacharya and co-workers [53–55] have extended this model and performed extensive numerical work to study the effect of flow field on binary alloy micro-scale solidification. Multiple parametric studies have also been performed by Bhattacharya et al. [56,57] to analyse the effect of flow on binary alloy crystal growth.

In our present work, a numerical model has been developed to simulate crystal growth in presence of thermal anisotropy in the solid phase. The current work is an extension of the work carried out by Bhattacharya and Dutta [53], where they have studied the growth of a thermally isotropic crystal. The main motivation for this work is that there has not been any significant study to simulate the effect of thermal anisotropy on crystal growth. Some experimental results are available involving the effect of thermal anisotropy [7]. However, no work has been done for predicting the effect of thermal anisotropy on binary equiaxed crystal growth as per the authors' knowledge. Using the developed model, an extensive parametric study has been undertaken to observe the effect of thermal anisotropy on dendrite tip velocity, grain equivalent radius and grain aspect ratio. The study has been extended to the growth of multiple nuclei with random location and orientation where the anisotropy of conductivity is aligned with the crystal axes.

## 2. The thermal anisotropic crystal growth model

In the present study, an investigation of dendritic solidification of a binary alloy is performed to observe the change in morphology and growth of equiaxed grains due to anisotropic thermal conductivity in the solid phase. A two-dimensional domain is considered, as shown by the schematic diagram in Fig. 1, initially filled with undercooled liquid with random nuclei locations. Each nucleus is assigned a random orientation to account for crystallographic anisotropy. The x and y axes are the global coordinate axes which are aligned with the domain boundaries, whereas X and Y are crystal coordinate axes which are aligned with the crystal axes. All the four boundaries of the domain have zero heat flux and zero solute flux conditions. Fluid flow due to forced and natural convection is neglected. The thermal conductivity is assumed to be anisotropic in the solid phase with variation in thermal conductivity along one of the crystal axes while keeping that along the other axis invariant. Anisotropic strength is measured by defining a thermal anisotropy ratio which is equal to the ratio of thermal conductivity along the $X$ crystal axis to that along the $Y$ crystal axis. The thermal conductivity of the liquid is assumed to be isotropic. Initial test cases are run for the growth of a single grain nucleating at the centre of the domain and aligned with the domain axes. This is done to observe the effect of thermal anisotropy on dendrite tip growth rate, grain size and morphology directly. Subsequently, growth of multiple nuclei with random orientation is simulated.

Evolution of a grain depends on the undercooling at the solid-liquid interface which in turn depends on the thermal and solutal transport in the vicinity of the interface. To capture the interface