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Numerical simulation of Bridgman solidification of binary alloys

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ABSTRACT

A transient 2D axisymmetric numerical model for the Bridgman solidification process for a stationary furnace and moving sample is presented. The model is able to predict the evolution of temperature and solid fraction of binary alloys in cases where buoyancy induced convection is negligible, such as in microgravity conditions. A dimensionless form of the governing equations was derived in order to identify the dimensionless parameters that characterise the process, those being the Stefan, Péclet, and Biot numbers. The problem was solved using a finite volume method and an explicit time stepping scheme. To test the efficacy of the model, simulated results were compared with experimental data from the literature and acceptable agreement was obtained. Finally, a parametric analysis was performed for understanding the influence of the process parameters on solidification. One key feature of this study was the inclusion of a term describing the advection of latent heat due to the translation of the mushy zone with varying solid fraction. This thermal transport mechanism was shown to be significant, since its magnitude was comparable to the advection of sensible heat. It was also found that when small Biot numbers were due to low values of the heat transfer coefficients at the surface of the sample, rather than to small sample radii, advective mechanisms were enhanced resulting in more convex shapes of the liquidus isotherm. This highlighted the importance of considering both axial and radial heat fluxes when describing the process.

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1. Introduction

The Bridgman–Stockbarger solidification process, originally developed to produce single crystals [1,2], allows for control of directional solidification. Fig. 1 shows a simple schematic of a Bridgman furnace where a cylindrical sample is held inside a long and slender crucible. Using a series of controlled coaxial heaters and an adiabatic baffle zone, the material is subjected to a thermal gradient along its length such that the material is fully molten at the hotter end and fully solid at the colder end. As Fig. 1 shows, when samples of binary or multicomponent alloys are considered, a mushy zone (where solid and liquid phases coexist) develops. A relative axial translation, identified as the pulling speed u, is imposed between the sample and the furnace either by pulling the crucible from the hot to the cold regions while keeping the furnace stationary or by moving the furnace and keeping the crucible stationary. For typical constant pulling speed operation, steady-state conditions are reached and the solidification process keeps pace with the relative translation speed of the sample. However, the sample will experience initial transient conditions during start-up and stopping periods.

In steady state operation, the cooling rate of the solidification process can be roughly estimated as the product of the temperature gradient in the axial direction, G, and pulling speed, u. Accurate information about the temperature gradient may be lacking because the temperature distribution, and hence temperature gradients, change along the length of the sample. In addition, width, shape and position of the mushy zone during the solidification process depend on the temperature distribution to which the sample is subjected. In some processes, much attention is paid to the morphology of the solid–liquid interface. For example, radial temperature gradients can cause a deviation from a planar interface to either a concave or convex ones [3].

In some cases the Bridgman furnace is used in a transient mode of operation. For example, when a phenomenon such as the Columnar to Equiaxed Transition (CET) is investigated, it is necessary to establish transient conditions during the solidification process [4]. In this case, a step change in pulling rate (known as a velocity jump) can cause a CET. In other modes of operation, the Bridgman may use a combination of velocity jump and controlled power down of the heaters to provide the desired transient conditions in the sample [5].

In metallurgical studies, a Bridgman furnace under steady-state operation may be used to determine which conditions are favourable for the formation of different microstructural features in the

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Nomenclature

A	area
Bi	Biot number
c_p	specific heat capacity
g_E	solid fraction at eutectic temperature
g_s	solid fraction
h	heat transfer coefficient
H	enthalpy
k	thermal conductivity
k_{part}	partition coefficient
L	latent heat of fusion
P	general thermophysical property
Pe	Péclet number
q	heat flux
r	radial coordinate
R	non dimensional radial coordinate
Ste	Stefan number
t	time
T	temperature
T_E	eutectic temperature
T_L	liquidus temperature
T_M	melting temperature
u	pulling velocity
V	volume
$\mathbf{V}$	velocity vector
x	axial coordinate
X	non dimensional axial coordinate
α	thermal diffusivity
θ	non dimensional temperature
ρ	density
τ	non dimensional time

Subscripts

$cold$	cold heater
cv	control volume
E	east face of a cv
hot	hot heater
l	liquid
N	north face of a cv
s	solid
S	south face of a cv
W	west face of a cv

final casting. For instance, specific steady-state conditions can be related to microstructural characteristics such as primary and secondary arm spacing in dendritic growth [6]. In most cases, due to the opaque nature of metal alloys, only a post mortem analysis is possible, whereby the samples are cut, polished, and etched after solidification and then observed by optical or electron microscopy techniques. These types of procedures allow for the direct observation of relevant details, like the final grain structure and size, or the dendritic arm spacing [7–10]. Nevertheless, the observation of some features may still be difficult, as in the case of alloys that experience solid-state phase transformations that may alter or completely remove the initial solidification microstructure [11]. The main disadvantage of post mortem analysis is the lack of time resolved information during the solidification process.

Additional methods may be employed to investigate the solidification phenomenon in real time. X-ray radiographic imaging has been used in some alloy systems to monitor the real-time evolution of the microstructure. However, the applicability of this technique is limited by strict requirements on the sample geometry (thin samples only) and segregation of solute species [12–15]. For example, Reinhart et al. [16] observed CET in a Bridgman furnace in real-time after a velocity jump was imposed on the sample.

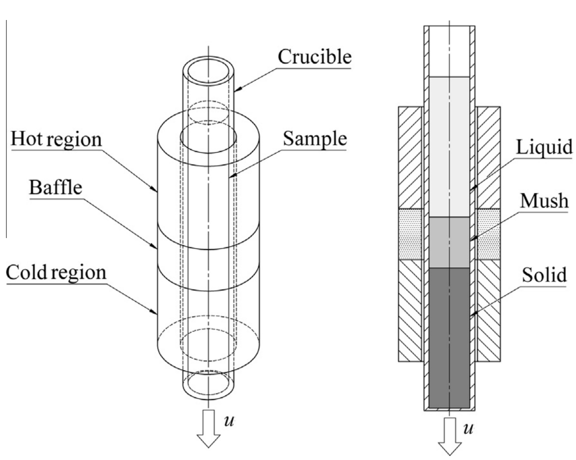

Fig. 1. Schematic of a Bridgman furnace.

Another approach for gathering real-time information during Bridgman solidification is the use of the ultrasonic pulse-echo technique. In this case the time-of-flight of an ultrasonic signal reflected by the solid–liquid interface was measured and used to estimate the velocity of the solidification front [17,18].

For the purpose of gaining accurate insight into the process, practitioners cannot always rely exclusively on experimental results. Therefore, reliable numerical models are valuable, and sometimes necessary tools for analysing alloy solidification. Simulations performed prior to physical experiments may be useful to predict the conditions that the material is likely to encounter during the process. In addition, computational models can be employed during or after the process to extract key information which would be difficult or impossible to observe or measure experimentally.

Nevertheless, it is crucial to highlight that the benefits of adopting numerical methods are highly dependent on the accuracy of the input data, the validity of initial modelling assumptions, and above all, the correctness of the model and solution technique themselves. Hence, when possible, verification and validation of the model are essential steps in establishing the efficacy of the model predictions [19].

Several models for the investigation of the Bridgman solidification process of alloys have been developed in recent years. Timchenko et al. [20,21] implemented a method, based on a single domain enthalpy approach, to study the evolution of temperature, solute concentration and solid–liquid interface during Bridgman solidification of Bi-1at%Sn. This model assumed furnace configurations with low growth speeds and high thermal gradients, allowing the model to treat the phase change as isothermal and without the formation of any mushy zone between solid and liquid. The simulated solutions showed good agreement with measured experimental results.

Mirihanage et al. [8] employed a front tracking method to simulate the advance of the columnar dendritic front and development of the undercooled region in Al-7wt.%Si samples during Bridgman solidification in microgravity. The purpose of this study was to estimate the conditions for CET. Thermal data collected during experiments were used as inputs for the thermal boundary conditions. In the aforementioned models, the relative translation of sample and furnace was treated as a moving boundary condition.

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