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Front tracking method in modeling transport phenomena accompanying liquid–solid phase transition in binary alloys and semitransparent media

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ABSTRACT

The paper presents the potential of an efficient front tracking method on a fixed control-volume grid in micro–macroscopic numerical modeling of both binary alloy solidification and a solid–liquid phase transition of single-component or doped optically functioning materials. In the former case, the method, basing on the assumption that an envelope of columnar dendrite tips moves locally according to a single crystal growth law, allows more precise identification of zones of different dendritic structures developing within the two-phase region, and thus more detailed analysis of some closing models. It is shown, by exploiting the commonly used benchmark problem that a porous medium model of the columnar mush must be carefully chosen since it strongly affects the predicted macro-segregation pattern. In the case of solidification of a single-component or doped semi-transparent material the combination of the front tracking method with the immersed boundary technique provides a new simulation method, which can handle different thermo-physical and optical properties of liquid and solid phases, processes of emission, absorption, reflection and refraction or transmission of thermal radiation at a diffusive or specular distinct solid–liquid interface detected by the front tracking technique. The method has been used in a detailed parametric analysis where the impact of different optical configurations of both phases and their various optical properties as well as variable transmissivity of solid–liquid interface on the phase change process development has been addressed.

1. Introduction

Solidification of a binary alloy is a phase change process involving complex transport phenomena in two phase regions of different grain structures and at a solid–liquid interface (SLI). The SLI develops into complex shapes due to thermo-solutal instability at the interface and capillary forces. Different solubility of constituents in the solid and liquid leads to segregation of solute at the scale of a single dendrite arm, the process called micro-segregation [1]. Moreover, buoyancy induced convective flow between dendritic crystals transports enriched alloy into a bulk liquid, being a main source of compositional heterogeneity in a cast – known as macro-segregation. Within the two-phase region (called a *mushy zone*) different grain structures grow creating macroscopic zones of columnar and equiaxed crystals, where different liquid flow conditions occur.

The phase change process in semi-transparent materials, such as melting or solidification, may occur with either discrete SLI [2,3] or with an isothermal two-phase zone developing between pure liquid and pure solid phases and induced by volumetric thermal radiation [4–7]. In pure or doped semi-transparent materials under strictly controlled conditions (e.g. during single crystal growth process) a distinct SLI, separating liquid and solid phases, can be observed [2,3]. Its shape and motion are affected by thermo-physical and optical properties of both phases, convection in the melt, thermal radiation and phenomena that occur at the SLI. In the case of solidification of partially (one phase either solid or liquid) or fully (both phases) semi-transparent materials specular and/or diffusive optical properties of the SLI as well as absorption, emission, reflection and refraction/transmission of thermal radiation at the SLI should be considered along with thermal radiation transport across the phases [2].

Therefore, it becomes obvious that for reliable macroscopic modeling of both the above discussed types of liquid–solid phase transition there is a need for efficient techniques of precise identification and tracking the SLI during the phase change process. In the case of binary alloy solidification such technique has been proposed in [8] and further developed in [9–11]. It is based on the

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computationally effective single domain solution of macroscopic conservation equations (Eulerian representation) coupled with a special technique of tracking the interface between macroscopic regions of columnar and equiaxed grains (developing within the *mushy zone*), through the use of mass-less marker particles (Lagrangian method). This allows using different macroscopic models of fluid flow resistance within distinct, thus recognized, dendritic zones. Similar approach of tracking the SLI during solidification of semi-transparent medium has been developed in [12–15] providing the possibility of analyzing the role of SLI optical properties on solidification of an optically functional material.

The present paper shows, using two carefully selected example problems, the potential of this front tracking approach (FTA) when applied to efficient macroscopic modeling of transport phenomena during solidification of single component and binary materials.

2. Front tracking procedure

The concept of tracking a front moving across a stationary control-volume grid is necessary for distinguishing different phase structures forming during phase transition in the whole analyzed domain, where various transport models are defined. Although different processes of binary alloy solidification and phase change in single component semitransparent media are considered, geometrical representation of the interface is the same. The interface is represented by a set of mass-less markers connected with linear segments (solid line in Fig. 1). At the nodes, shown as dots in Fig. 1, temperature is determined and, based on an appropriate crystal growth law, the markers are shifted towards a cooler region along the normal vector to the interface. Their new positions and a new shape of the interface are marked in Fig. 1 with squares and a dashed line, respectively. Simple formula describing a new position of the marker takes the general form:

$$\mathbf{X}_{i,n} = \mathbf{X}_{i,0} + \mathbf{n}_i \cdot w_i \cdot \Delta t \tag{1}$$

where: $\mathbf{X}_{i,0}$ is the ith marker position in the previous time step, $\mathbf{X}_{i,n}$ is the ith marker position in the current time step, $\mathbf{n}_i$ and w_i, respectively, stand for the vector normal to the front and the interface growth rate determined in the ith marker, according to the chosen law of crystal growth, and Δt is the time step.

Typically, during non-eutectic binary alloy solidification tiny columnar dendrites start to grow from cooled walls and continue their development towards a mold center. In this case the tracking front is not a SLI, which is very complicated in fact, but rather a virtual surface (line for 2D geometry) representing the envelope of columnar dendrite tips. Such interface divides the two-phase zone in the slurry region (before the front) and the porous region (behind the front) (case 1 in Fig. 1). The columnar dendrite growth rate w_i is determined with the formula, taken from the microscale analysis, e.g. [16], and it can be expressed by a polynomial function of undercooling. In this approach control-volume shapes are not modified, but rather a pointing function is introduced in each cell, called the *switching function* (e.g. [9–11]), which carries information about the fraction of the cell behind the interface. It takes values between 0 for a slurry region and 1 for a porous region. This function is used to switch on or off appropriate source terms of the momentum balance equation (Eq. (2)), which imitate the flow resistance in the slurry and porous zones. More details concerning this procedure are available in Section 3.3 and in [9–11].

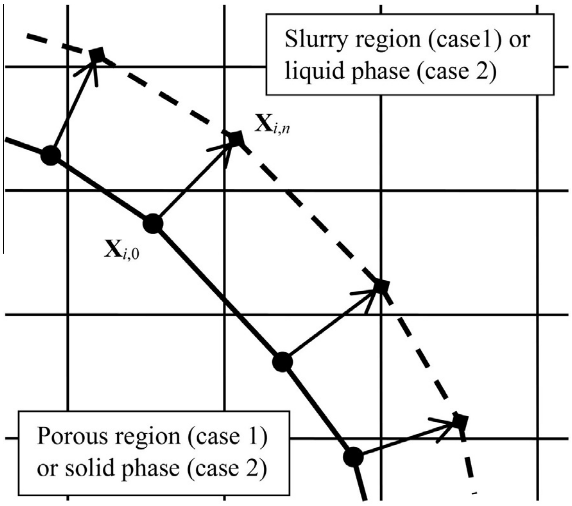

Fig. 1. Representation of the interface for binary alloys and solidification of semi-transparent materials.

In the second considered case of solidification of a pure semi-transparent medium, the interface coincides with the distinct SLI and its grow rate is described with the modified Stefan condition, which takes into account the incident and emitted radiative heat fluxes (case 2 in Fig. 1). The interface separates regions of various optical properties and has various optical transmissivity. In this case FTA is combined with the modification of control volumes sizes, such as their small parts cut off by the interface are merged to adjacent cells in the bulk solid or liquid zones. Fragments of boundaries of thus modified control volumes coincide with the SLI. More details are given in Section 4.1 and in [12–15].

3. Modeling binary alloy solidification

Binary alloy solidification and accompanying conjugate transport phenomena of mass, momentum, energy and solute develop at different length and time scales. Unfortunately, full computational simulation of metal alloy solidification which encompasses all these scales (from an atomistic level through an individual crystal scale to a macroscopic one), although highly desirable, is still not possible because of even now restricted computer capabilities. Therefore *micro–macroscopic* modeling has been developed, where various averaging techniques are used to obtain macroscopic transport equations from the corresponding microscopic ones. Information about the kinetics of crystal growth, solute micro-diffusion, inter-dendritic flow resistance in the *mushy zone*, and evolving different dendritic microstructures are accounted for through effective properties of the two-phase mixture and source terms of macroscopic conservation equations.

3.1. Modeling momentum transport in a slurry and stationary porous zones

One of the main difficulties in the micro–macroscopic modeling of metal alloy solidification involves proper description of transport phenomena within the *mushy zone*. Considering the developing solid phase morphology, two regions can be identified. In the first one the solid forms a matrix of motionless columnar dendrites immersed in the liquid phase. In the second region equiaxed grains immersed in the under-cooled liquid constitute the slurry medium. Due to different transport mechanisms in these two diverse dendritic structures, the recognition of zones occupied by each of them is vital to properly describe convective–diffusive transfer of momentum. In extensively used single component models a virtual interface between the columnar dendrite region, growing from the cooled walls into the superheated melt and the equiaxed grain region, developing in the under-cooled and solute reach liquid, is not directly tracked. These two distinct dendritic structures are not distinguished and the whole *mushy zone* is treated as a porous