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Polydimensional modelling of dendritic growth and microsegregation in multicomponent alloys

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Abstract

Various models for simulating dendritic solidification have been proposed in the past. However, those models based on cellular automata (adopting the virtual front-tracking (VFT) concept) are often only suitable for the consideration of one alloying element. As typical industrial alloys are constituted of numerous alloying elements, the application of these models to practical alloys is therefore rather limited. In order to overcome this drawback, a new, modified VFT model, which allows for the treatment of several alloying elements in the low Péclet number regime, is presented. By a new and effective approach, based on a functional extrapolation of the concentration gradient, we are able to study dendritic growth in multicomponent Fe–C–Si–Mn–P–S alloys. Comparisons with well-established analytical models confirm the correctness of the model; results for free and constrained dendritic growth effectively demonstrate the capabilities of this new model.

Keywords: Cellular automaton; Microsegregation; Multicomponent solidification

1. Introduction

The formation of microstructure during solidification can, generally speaking, be regarded as one of the most influential factors on material properties. In this context, two interrelated key issues can be identified: first, the topology of the microstructure itself (i.e. the formation of cells, dendrites, etc.) and secondly, its physical and chemical implications (in alloys most explicitly seen by solutal segregation). Since both subjects are always linked together, detailed, specific research on either phenomenon has helped to promote understanding of the topic as a whole.

1.1. Microstructure modelling

Microstructure description has attracted researchers for decades, and has thus answered fundamental questions regarding the formation mechanisms. In the past, the comprehension of microstructure development was mainly driven by experimental surveys and subsequent physical revelation. Based thereupon, analytical theories regarding dendrite tip formation, growth at marginal stability and the interrelations between heat transfer, solute diffusion and physical interfacial properties were deduced [1–5]. An excellent compendium on this subject was issued by Flemings [6]. Moreover, empirical relationships for different microstructural parameters (e.g. dendrite spacing) have been published (e.g. [4,7,8]). However, these theories could only partially account for the complex interactions, so a complete analysis of microstructure evolution was therefore not possible. The advances in computing have made it possible to approach this issue from the standpoint of

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pure physics by creating transient numerical simulation models for microstructure. In the literature three different approaches can be identified, which are explained below.

As solidification of metallic alloys is (under technically normal solidification conditions) mainly controlled by solute diffusion and interfacial curvature, the exact position of the solid–liquid interface is of key relevance. Front-tracking models [9–11], which are the first approach, can reproduce the interface precisely by a dynamically refined meshing in this region. Unfortunately, this method not only involves using algorithms of high complexity in order to account for the growing interface but is additionally limited to producing only simple solidification patterns. Consequently, the simulation of multidendritic microstructures can hardly be realized by such models.

Phase-field (PF) models deal with the solid–liquid interface by introducing a continuous transitional layer of finite thickness using an additional PF quantity, thus eliminating the problem of explicitly tracking the interface. Moreover, it is reported [12] that PF models are computationally less intensive than front-tracking models. Several reviews on the methodology and capabilities of the PF models are available [13–16], showing that the method has been successfully applied for simulating the dendritic solidification of binary alloys in two or three dimensions [17]. Lately, the effect of melt convection has been treated in numerical models [18]. Moreover, the method has recently been applied to multicomponent systems by coupling with the CALPHAD database [19].

The third possible approach is based on cellular automata (CA) modelling. The use of CA in microstructure modelling already dates back more than 15 years, when several research groups published first initiatives in this field – though with slightly different aims.

Regarding the topic of stochastic mesostructure simulations (i.e. simulating grain growth during solidification), the contributions by Rappaz, Gandin and their co-workers (e.g. [20,21]) illustrate the benefits of this method for deriving conclusions on a granular scale. The CA model, which was coupled with a finite element model and was hence termed CA–FE, was later successfully used for simulations in three dimensions [22,23] and for modelling macrosegregation [24].

Models of microstructural features during solidification with the CA technique also date back to the early 1990s: Spittle and Brown were the first to successfully apply this method in a still quite deterministic way for granular models [25] and for dendritic growth [26]. Dilthey et al. [27] developed models for thermal as well as solutal dendrites in binary systems, reproducing the typical dendritic features quite well. Although no quantitative comparison of the simulation results with micrographs was reported, the visual agreement justified the CA model assumptions. Due to the methodology of interface curvature computation, a strong, mesh-induced artificial anisotropy was observed (the dendrites were strongly aligned along certain directions). Moreover, the interaction between thermal and solutal aspects had not been considered. The latter drawback was resolved by a model by Nastac [28], who published results on constrained and unconstrained growth in binary systems as well as on columnar-to-equiaxed transitions. In Ref. [27] as well as in Ref. [28] the interfacial growth velocity is considered via a solute balance at the interface. Zhu, Hong and their co-authors (e.g. [29,30]) first addressed the influence of melt convection on dendritic solidification in their CA model, in which the growth velocity was calculated via the analytic models of [2,3]. However, all of the mentioned models still lacked an arbitrary dendrite growth direction due to the mesh anisotropy.

The problem of dendrite orientation was subsequently addressed by two models: Jacot and Rappaz [31] published a pseudo-front-tracking model based on a hexagonal grid, thus eliminating a certain anisotropy induced by regular, rectangular spacing. Moreover, the authors proposed to calculate the interfacial curvature, which greatly influences the interfacial temperature and thus the growth velocity, by computing the divergence of the surface gradient. Although the use of hexagonal meshing involves sophisticated mathematical methods, the results demonstrated that mesh-induced anisotropy was not observed. The concept of calculating the interface curvature was also used by Brackbill et al. [32] in developing a computational fluid dynamics tool for free surfaces. Beltran-Sanchez and Stefanescu [33,34] adopted this approach in an orthogonally meshed CA model for low Péclet numbers in binary systems. Furthermore, the results showed that an arbitrary dendrite orientation could be achieved by the virtual front-tracking (VFT) of the interface. Zhu et al. [12,35] used the VFT scheme by Beltran-Sanchez and Stefanescu in a model which was additionally used to study the effects of forced melt convection with the Lattice-Boltzmann method. The results, obtained for a binary Al–Cu system, show the significant effects of convective flow on unstable dendritic solidification.

However, except for the model in Ref. [31,36,37], which will be discussed in the next section, each of the models mentioned above was created for binary systems (mostly Al–Cu, Al–Si or Fe–C). Therefore, although yielding remarkable results with respect to dendrite morphology, and columnar and equiaxed solidification, their application to industrial materials is limited. Therefore, one aim of the present paper is to present a model based on the theory of CA which additionally allows consideration of the latter issue.

1.2. Microsegregation

Next to the fundamental question of overall microstructure formation during solidification, the effect of solute distribution and resulting segregation can be identified as the second key influence on all subsequent material properties. Microsegregation (MS), caused directly by the phase-dependent solubility of alloying elements, remains a predominant problem in nearly all technical solidification processes. Driven by its strong significance