Available online at www.sciencedirect.com
ScienceDirect
Acta Materialia 55 (2007) 1523–1532
Acta MATERIALIA
www.actamat-journals.com

Two-dimensional modelling and experimental study on microsegregation during solidification of an Al–Cu binary alloy

Q. Du [a,*], D.G. Eskin [a], A. Jacot [b,c], L. Katgerman [d]

[a] Netherlands Institute for Metals Research, Mekelweg 2, 2628CD Delft, The Netherlands
[b] Laboratoire de Simulation des Matériaux, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
[c] Calcom-ESI SA, Parc Scientifique, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
[d] Delft University of Technology, Mekelweg 2, 2628CD Delft, The Netherlands

Received 21 April 2006; received in revised form 9 October 2006; accepted 9 October 2006
Available online 20 December 2006

Abstract

To explain the experimentally observed relation between the cooling rate and the non-equilibrium eutectic fraction obtained during solidification experiments of Al–Cu binary alloys [Eskin DG, Du Q, Ruvalcaba D, Katgerman L. Mater Sci Eng A 2005;405:1–10], a two-dimensional (2-D) microsegregation model, the pseudo-front tracking (PFT) method [Jacot A, Rappaz M. Acta Mater 2002;50:1909–26, Jacot A, Rappaz M. Acta Mater 2002;50:3971, Du Q, Jacot A. Acta Mater 2005;53:3479–93], is employed. The analysis of simulated solidification kinetics, including the grain morphology evolution, coarsening and back diffusion, reveals the pronounced effect of dendrite coarsening on the final non-equilibrium eutectic fraction. Because the 2-D modelling can describe rigorously how the important microstructure feature – dendrite arm spacing – evolves, its predictions are in good agreement with the trend observed in the experiments, which both the classic Brody–Flemings model and the 1-D PFT model have failed to explain.
© 2006 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Modelling; Microsegregation; Coarsening; Aluminium alloys; Dendritic growth

1. Introduction

Microsegregation is the chemical inhomogeneity at the scale of a grain size or a dendrite arm, and is a result of non-equilibrium solidification of alloys. It is a hot research topic and both experimental and modelling approaches are employed to investigate the concentration profile along dendrite arms and the type and fractions of the interdendritic phases, because of their great importance for downstream processing and for mechanical properties [1–11]. It is clear that back diffusion in the solid is important in the formation of microsegregation, and the diffusion in the liquid is insignificant upon normal casting conditions. The other important factor is dendrite coarsening during solidification. Coarsening in Al–Cu alloys is a result of the flux of Cu from coarse arms towards fine arms coming from the Gibbs–Thomson effect. During coarsening, highly curved solids (fine arms) are dissolved while regions of low or negative curvature (coarse arms) continue to grow. Although the coarsening is expected to reduce microsegregation [5,6], the extent of this effect is unclear (see Ref. [7] for a debate on this topic). It appears that, depending on the cooling rate, the shape of the cooling curve and the phase diagram, the influence of coarsening could be negligible on the solute distribution in the primary phase, but significant on the eutectic fraction formed [7]. Voller and Beckermann proposed an approximate model of microsegregation with coarsening, in which the effect of coarsening on microsegregation measured by the fraction of non-equilibrium eutectic was estimated [8]. They showed that, depending on the Fourier number (defined as a dimensionless solid-state back diffusion parameter calculated by the product of a constant solid diffusion coefficient and the local solidification time divided by the square of the

* Corresponding author. Tel.: +31 15 2782263.
E-mail address: q.du@nimr.nl (Q. Du).

1359-6454/$30.00 © 2006 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.actamat.2006.10.035

characteristic solidification length), the final eutectic fraction could significantly deviate from the one obtained when coarsening was not taken into account. In contrast, Flemings concluded that the effect of coarsening on microsegregation is small, and certainly less than the effect of back-diffusion in the solid [9].

There are some one-dimensional (1-D) models available [10] in which the coarsening process of dendrite arms is described as a function of local solidification time. Yan et al. [11] demonstrated that the proper description of dendrite grain morphology is very important in modelling microsegregation, though, owing to their intrinsic geometrical assumptions, 1-D models cannot do this in a direct way. Certainly 2-D or 3-D direct simulations of complex grain morphology evolution would be more appropriate. Recently, a 2-D pseudo-front tracking (PFT) model has been developed by Jacot, Rappaz and Du [2–4] for normal casting conditions to predict the final concentration profile and the types and fractions of secondary phases formed, in which the evolution of dendrite arms can be explicitly tracked in a physical manner, and ripening as well as coalescence can be described based on their controlling factors, i.e. the combination of curvature effect and diffusion in the liquid, as well as the possible influence of the grain boundary energy [4].

The direct motivation to perform 2-D microsegregation modelling for the solidification of an Al–Cu alloy has been the interpretation of our earlier experimental results showing an unconventional relationship between cooling rate and non-equilibrium eutectic fraction, which initially increases in the range of slow cooling (<1 K/s) and then gradually decreases in the range of 1–20 K/s [1]. Similar experimental results had been reported by other authors, e.g. Novikov and Zolotorevsky [12]. Coarsening, undercooling of the eutectic reaction and efficient back diffusion due to structural refinement at a faster cooling rate were all suggested as potential causes of the observed behaviour. The diffusion in the solid (back diffusion) directly influences the prediction of the final eutectic fraction. The amount of solute transferred by back diffusion is proportional to the local concentration gradient at the periphery of a growing grain, the interfacial area and the solidification time. Obviously, the longer the solidification time, the more solute can diffuse into the solid phase. At the same time, the slower cooling rate accompanied by longer solidification time favors the formation of coarse dendrite arms. Therefore, the back diffusion in the coarse structure will be hindered by the reduced interfacial area and a lower local average concentration gradient. As a result of the opposite effects of the solidification time and the coarse structure, the final eutectic fraction is difficult to predict. Although the 1-D microsegregation models could predict the fraction of non-equilibrium phases, their average nature and the simplified grain morphology assumption make it impossible to describe how the interface dynamics and the spatial distribution of grain morphology affects the non-equilibrium phase formation. Two-dimensional calculations could shed some light on the effects of coarsening and structure refinement on the formation of non-equilibrium eutectics. The results of such calculations are presented here below after a brief description of the model and the experimental procedure.

2. Model description

The model combines a direct simulation of the primary phase formation based on the PFT method [2,3] and a mixture approach for the description of the formation of secondary phases [4]. In the 1-D PFT model, the solidified microstructure is assumed to consist of plate-like dendrite arms, the spacing of which is determined from the experimental secondary arm spacing; the diffusion in the liquid and solid can be taken into account, but the curvature undercooling is neglected; the calculation domain is half of the experimental measured value. The 2-D PFT model takes into account both diffusion in the liquid and solid phases and curvature undercooling, which together determine the velocity of the solid–liquid interface. Therefore, this model can explicitly track how the grain morphology evolves. The curvature of solid–liquid interface is calculated with the piecewise linear interface calculation technique [13]. As soon as the liquid becomes undercooled for a secondary solid phase, the calculation enters a second stage in which the mixture approach is invoked and aimed at predicting the formation of secondary phases in the remaining interdendritic regions. In this approach, the interdendritic regions are considered as a mixture of liquid and solid phases. The model provides the evolution of the interdendritic mixture as solidification proceeds, taking into account the effects of back diffusion, which continuously modifies the composition and the volume of the interdendritic regions. See Refs. [2–4] for more details about this model.

The effect of the eutectic reaction undercooling can only be taken into account by imposing a pre-described undercooling value, since no rigorous description of the eutectic reaction is included in the 2-D PFT model. This choice is dictated by the numerical difficulty to resolve spatially both the grains of the primary dendritic phase, which are on a scale of 100 μm, and the interdendritic eutectic phases which are on a scale of several microns. In this paper, the effect of the eutectic undercooling is neglected. The possible implications of the eutectic reaction undercooling on the eutectic fraction in our experiments are discussed elsewhere [1].

Due to the 2-D nature of the model, some input parameters, such as the surface energy, have to be tuned to reproduce the appropriate average dendrite arm spacing (DAS) observed upon the metallographic examination. When the calculated DAS is close to the measured value, the effect of grain morphology on the eutectic fraction is considered to be properly taken into account. With this idea, simulations of solidification experiments with cooling rates of 0.8 and 16 K/s were performed (for the choice of the

Download English Version:

https://daneshyari.com/en/article/1450861

Download Persian Version:

https://daneshyari.com/article/1450861

Daneshyari.com