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Numerical Simulation of Solute Trapping using Phase-Field Model for Dilute Binary Alloys Solidification

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Abstract - Solute trapping in solid phase due to increase of solidification velocity was predicted using isothermal phase-field model for dilute binary alloys [2,3]. Semi-empirical models [5-7], adjusted by the present phase-field numerical results, reproduced with reasonable agreement the experimental data [4] for Si-As and Si-Bi alloys. These results support the applicability of phase-field models as useful tools in designing experiments of rapid solidification, proper to obtain fine structured materials with very low or even without solute segregation.

Fast solidification may lead to the solid-liquid interface to deviate from local equilibrium, producing solute trapping in solid phase [1]. This phenomenon increases the solute concentration in solid phase and reduces the segregations in the liquid side of interface. In the limit of partition-less solidification, the solute concentration in both phases are equal. This process is useful to obtain very fine structure with uniform properties. In the present work, numerical simulations of fast solidification process have been performed. A phase filed model has been used. In our model, the phase field variable, which tracks the solidification progress and varies within an solid-liquid interface of finite thickness, was defined ranging from +1 (solid phase) to 0 (liquid phase). Based on that, two diffusion equations (phase field variable and solute concentration) were developed via linear expansion of equilibrium conditions [2,3]. Numerical results of solidification velocity and solute concentration profile were validated against analytical solution for a Ni-Cu alloy (figure 1), as well as against experimental data [4] for Si-As alloy (figure 2). Different semi-empirical modes [5-7] adjusted by those numerical results reproduced with reasonable agreement the experimental data for Si-Bi alloy (figure 3). Therefore, one can conclude that phase-field model can be a useful tool in designing rapid solidification experiments, that are proper to obtain fine structured materials with very low or even without solute segregation.

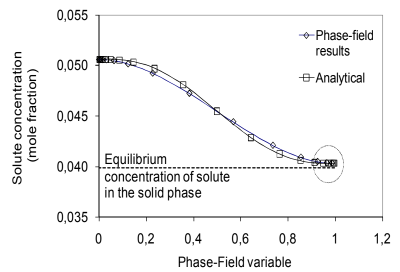

Figure 1: Solute concentration profile of Ni-Cu alloy along the interface, from solid side (+1) to liquid side (0) at very low solidification velocity: analytical results are from [2].

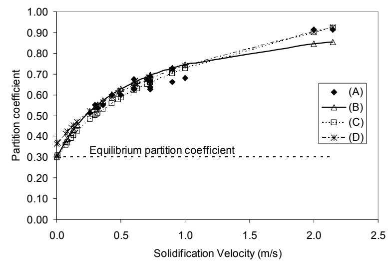

Figure 2: The effect of solidification velocity on As partition coefficient in Si-As alloy: (A) experimental [4]; (B) present phase-field results; (C) and (D) Semi-empirical formulas [5-7].

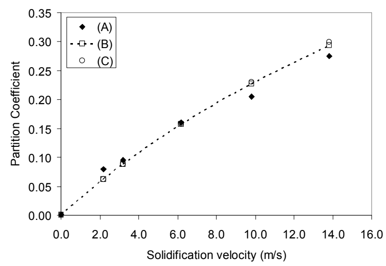

Figure 3: The effect of solidification velocity on Bi partition coefficient in Si-Bi alloy: (A) experimental [4]; (B) and (C) semi-empirical formulas [5-7].

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