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Computer Simulations of the Dynamics of Spinodal Decomposition in Alloys

Based on a numerical version of the Fourier transformation approach to the nonlinear Cahn-Hilliard diffusion equation, computer simulations of the dynamics of spinodal decomposition for a model alloy are carried out. The present simulations start from fluctuations in composition with small amplitudes and wavelengths (a few lattice spacings). This version predicts that the Cahn-Hilliard equation has only weak nonlinear character. The evolution of the composition profile and the dynamical wave-number selection of the modulated structure are studied. The wavelength modulation of the composition profile occurs strongly in the early stage and becomes much weaker in the later stage. This selection has a strong dependence on both the mobility of solute atoms and the coefficient of the gradient energy. The kinetic evolution of the modulated structure with time is investigated as a function of the composition, the mobility of solute atoms and the coefficient of the gradient energy. A critical comparison of the simulated results with predictions of the linearized Cahn-Hilliard theory is presented.

Computer-Simulationen der Dynamik der spinodalen Entmischung von Legierungen


1 Introduction

When a solid solution is quenched into the unstable region of the phase diagram (bounded by the absolute instability limits), any fluctuation of composition grows initially, and the solid solution decomposes into a two-phase modulated structure. This process is named spinodal decomposition, and is of extreme importance both as a fundamental concept of thermodynamics and as one of the two mechanisms for a first-order transformation in solid solutions [1 to 7].

Up to now, there have been several theoretical proposals about this problem [1, 8 to 11]. An analytic description requires solving the diffusion equation in the supersaturated solution, which includes nonlinear terms essential for modulating the structure [2]. Hillert [12] first tried to explain the formation of the modulated structure using the concept of a negative diffusion coefficient based on a nonlinear flux equation for a one-dimensional system. Introducing the interfacial energy term and the elastic strain energy term, Cahn [1, 13] developed a classic continuum theory for the decomposition of alloys. This theory successfully predicted the intermediate stage of the phase transformation, but seemed to lose its validity for the early stage because it only was a linearized approach of the diffusion equation and for the late stage did not describe coarsening of the decomposed structure. Some of the theoretical approaches to the late stages [1, 11, 14] seem to be not valid. These introduced serious assumptions due to the difficulty of solving the nonlinear diffusion equation.

Experimentally, there are a lot of alloy systems showing spinodal features during a phase transformation [15 to 21]. But these systems have components too numerous for an exact determination of their thermodynamic parameters. Moreover, experiments focusing on the early stage of phase transformation are difficult. Thus experimental data are not sufficient to compare the results with the theories.

A computer simulation of the spinodal decomposition seems to be a possible and illuminating technique for a better understanding of this process. Recently, Miyazaki et al. [22] developed a numerical version of the Fourier transformation solution of the Cahn-Hilliard diffusion equation. They predicted the time evolution of the modulated structure, and also described some kinetic behaviour of the nucleation-and-growth mechanism. However, some errors seem to exist in their simulations. First, a probably wrong diffusion coefficient $D$, as a function of the alloy composition was presented in Fig. 1 of their paper; secondly, their simulations showed strong nonlinear effects of the higher order diffusion coefficients, which are not reproduced in the present simulation. The amplitude of the Fourier wave with the highest growth rate always increased with time and finally lost its physical meaning. An interesting but probably unreasonable conclusion in their simulations is that nucleation and growth kinetics initiated from mini-fluctuations and did not need to overcome any potential barrier. The assumed initial composition profile with a wavelength comparable to the modulating one seemed not to be realistic. The authors argued that this was attributed to thermal fluctuations. In fact, thermal noise should be a stochastic property, and so initially, the composition fluctuations in the super-saturated solution should be localized within a few lattice spacings. The assumed initial fluctuations, no doubt, produced artificial effects on the actual evolution

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