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Diffusion processes in a migrating interface: The thick-interface model

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Abstract

During a solid/solid diffusive phase transformation from a parent β-phase to a product α-phase, dissipative processes due to diffusion in the bulk phases as well as rearrangement of the crystal lattice and diffusion in the interfacial region occur. A model has been developed that accounts for all the above-mentioned dissipative processes. By means of this thick-interface model it is possible to assign a finite thickness and a finite mobility to the interface. The evolution of the mole fraction profiles of the components in the bulk phases and in the interface can be simulated from a given initial state until a steady state or equilibrium is attained. Based on this theoretical framework the kinetics of the γ/α phase transformation in the Fe-rich Fe–Cr–Ni system is simulated. Starting from a certain initial composition the transformation kinetics exhibits the features of a massive or a bulk diffusion controlled transformation depending on temperature.

Keywords: Modeling; Phase transformation; Diffusion; Interface migration; Thermodynamic extremal principle

1. Introduction and motivation

Rearrangement of atoms in the migrating interface, solute drag, trans-interface diffusion and spike formation are phenomena occurring to a smaller or larger extent in the interface and its nearest surroundings during diffusive and massive transformations. Several models of the interface were developed and have been used to describe the transformation kinetics. The task to model the kinetics of diffusive phase transformations becomes less complicated, if the dissipation of some of the above-mentioned processes is negligibly small compared to the remaining processes and can be neglected. Frequently it is assumed that the bulk phases are separated by an infinitely thin, i.e. sharp, interface. Diffusion processes in the interfacial region are then automatically out of the scope of these sharp interface models.

The simplest sharp interface model is used in the standard package DICTRA [1]. It is assumed that the transformation kinetics is controlled by diffusion processes in the bulk only and local equilibrium prevails at the interface. This implies that no Gibbs energy is dissipated due to lattice rearrangement. The simplifying assumption is equivalent to an infinite mobility of the interface. Such a model is suitable to describe the kinetics of bulk diffusion controlled diffusive phase transformations.

A sharp interface model, which considers the dissipation due to lattice rearrangement by a finite interface mobility, has been introduced by Svoboda et al. [2]. The evolution equations for the transformation kinetics are obtained by using the thermodynamic extremal principle (TEP), and the transformation kinetics can be simulated by means of this model in the full range – from bulk diffusion controlled to massive growth. In the frame of this model jumps at the interface of the chemical potentials of the interstitial components are zero and all of the substitutional components are equal [3]. It is evident that diffusion processes in the interface result in different contact conditions at the

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interface. As a consequence of these processes the jumps of the chemical potentials of the substitutional components need not be equal. This fact has been discussed, e.g. in Hillert's review paper [4] and by Hillert and Rettenmayr [5].

A completely different sharp interface model is presented by Larsson et al. [6], who considered trans-interface diffusion instead of atomic rearrangement and Kirkendall shift instead of the interface migration.

The trans-interface diffusion, solute drag as well as the atomic rearrangement in the migrating interface are also incorporated into the thick-interface model for the phase transformation by Odqvist et al. [7]. All mentioned processes are also treated by the thick-interface model for the phase transformation by Svoboda et al. [8]. This model was applied to the simulations of massive transformation in a ternary substitutional system yielding the steady state solution of the evolution equations. Both models [7,8] seem, however, to be far too complicated for practical applications.

From the cited papers it is evident that a robust and effective treatment of the coupled dissipative processes in the migrating interface is required. The motivation and goal of this paper are to present a thick-interface model for the phase transformation in substitutional alloys accounting for the rearrangement of atoms in the migrating interface, solute drag, trans-interface diffusion and spike formation. The mole fraction profile in the migrating interface is approximated by a parabola and, thus, described by a limited number of variables. The evolution equations for all variables describing the system are derived from the TEP (see Ref. [9]). The model is used for the simulation of phase transformation in the Fe–Cr–Ni system, and results of simulations are discussed.

2. Model

2.1. State and kinetic variables of the system

Let us assume a one-dimensional (1-D) system of a unit cross-section area composed of two phases (product phase α and parent phase β) separated by a thick interface. Both phases are represented by substitutional alloys with s components. The site fraction profile of each component i is approximated by a profile determined by a limited number of variables as depicted in Fig. 1. The thick interface and its nearest surroundings consist of two α-phase regions left to the interface characterized by their thicknesses Δ_{n-1} and Δ_n, two β-phase regions Δ_{n+1} and Δ_{n+2} right to the interface, and the interfacial region of width h. The system moves from the right to the left with a velocity v. The centre of the interface coincides with the origin of the spatially fixed coordinate system. Moreover we assume that the partial molar volumes Ω of all components are the same, and no sources and sinks for vacancies act in the system (no Kirkendall effect). Then the total length of the system $\sum_{k=1}^{m}\Delta_k + h$ remains constant. Furthermore, we assume that the regions, characterized by Δ_k ($k = 1,\ldots, n-1, n+2, \ldots, m$), move with a velocity v from the right to the left in the case that a transformation from the parent β-phase to the product α-phase occurs. The region Δ_{n+1} shrinks ($\dot{\Delta}_{n+1} = -v$) and the region Δ_n grows with the rate $\dot{\Delta}_n = v$. The values of Δ_k ($k = 1, \ldots, n-1, n+2, \ldots, m$) and the thickness h of the interface are kept constant as well as the sum Δ as

$$\Delta = \Delta_n + \Delta_{n+1}. \tag{1}$$

The mole fractions x_{ik}, the fluxes j_{ik} and the chemical potentials μ_{ik} are defined by the two subscripts i ($i = 1, \ldots, s$) and k ($k = 1, \ldots, m$), indicating the component and the location, respectively. The chemical composition of the interface is given by the local mole fractions of $x_{iL} \equiv x_{in}$, x_{iC} and $x_{iR} \equiv x_{in+1}$, with a parabolic profile in the interface. As a closed system is investigated, the fluxes at the boundaries of the system are zero:

$$j_{i0} = 0, \quad j_{im} = 0. \tag{2}$$

For no sources and sinks for vacancies in the system, the vacancy fluxes can be neglected at every point in the system, leading to the constraint

$$\sum_{i=1}^{s} j_{ik} = 0. \tag{3}$$

2.2. Mass balances

The mole fractions x_{ik} are constrained by

$$\sum_{i=1}^{s} x_{ik} = 1 \ \ (k = 1, \ldots, m), \quad \sum_{i=1}^{s} x_{iC} = 1, \tag{4}$$

and thus the total time derivatives are related by

$$\sum_{i=1}^{s} \dot{x}_{ik} = 0 \ \ (k = 1, \ldots, m), \quad \sum_{i=1}^{s} \dot{x}_{iC} = 0. \tag{5}$$

The mass conservation relations hold in the individual regions characterized by Δ_k as

$$\begin{aligned} &\Delta_k \dot{x}_{ik} = \Omega(j_{ik-1} - j_{ik}) \ \ \text{for } k = 1, \ldots, n-1, n+2, \ldots, m, \\ &\Delta_n \dot{x}_{iL} = \Omega(j_{in-1} - j_{iL}), \quad \Delta_{n+1} \dot{x}_{iR} = \Omega(j_{iR} - j_{in+1}) \end{aligned} \tag{6}$$

with the total time derivatives $\dot{x}_{iL} \equiv \frac{dx_{iL}}{dt}$, $\dot{x}_{iC} \equiv \frac{dx_{iC}}{dt}$ and $\dot{x}_{iR} \equiv \frac{dx_{iR}}{dt}$, since the variables x_{iL}, x_{iC} and x_{iR} are considered to be dependent only on time t (see Fig. 1 for introduction of the variables).

The parabolic mole fraction profile $x_i(z, t)$ in the interface is expressed as

$$x_i = x_{iC} - (x_{iL} - x_{iR})\frac{z}{h} + 2(x_{iL} - 2x_{iC} + x_{iR})\left(\frac{z}{h}\right)^2. \tag{7}$$

The material time derivative, being the rate of a quantity in a material point fixed to the lattice and moving with the velocity v from the right to the left, is given by

$$\dot{x}_i = \frac{\partial x_i}{\partial t} - v\frac{\partial x_i}{\partial z} \tag{8}$$