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Application of the thermodynamic extremal principle to diffusion-controlled phase-transformations in multi-component substitutional alloys: Modeling and applications

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ABSTRACT

The thermodynamic extremal principle was applied to model of diffusion-controlled phase-transformations in multi-component substitutional alloys, in which dissipations by interface migration and trans-interface diffusion were integrated for a sharp interface. In the modeling, a new concept of trans-interface diffusion in two-steps, i.e. from the product phase to the interface and from the interface to the parent phase, was introduced, ascribing to which the model follows the Onsager's reciprocal relation. In contrast to the work of Svoboda et al. (2004) that considers only the interfacial dissipation by interface migration, non-equal jumps of chemical potentials across the interface are herein allowed. Applications to the Fe–Cr–Ni and Fe–Ni alloys showed that the model is able to describe accurately not only the kinetic processes of massive transformation and diffusive transformation but also the critical limit between them. Since the transformation direction is not a priori condition for model calculations, the model is of potential value in applications to the cases in which the migrating direction changes, e.g. cycle phase-transformations etc.

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1. Introduction

Diffusion-controlled phase-transformations (e.g. the austenite-ferrite (γ-α) transformation [1,2], precipitation [3] and eutectoid transformation [4] in steels) have been studied extensively due to their technological importance in determining the microstructure features and the mechanical properties of materials [5]. For diffusion-controlled phase-transformations, two kinds of dissipation processes happen at the interface, i.e. interface migration and trans-interface diffusion [6–9]. Although the dissipation processes exist in both the diffusive transformation (DT) and the massive transformation (MT), their transformation characteristics are significantly different [10–14].[1] The critical limit between DT and MT was debated in the past and its location is now regarded to be in the two-phase field [14,15]. The model for diffusion-controlled phase-transformations therefore should be able to describe not only the kinetic processes of DT and MT but also the critical limit between them.

One kind of the most widely used models is the solute-drag model with a thick interface [16–23]. Based on the description of binding forces between solute atoms with the migrating boundary, Cahn [16] did the pioneering work. Hillert and Sundman [17] then introduced the concept of Gibbs free energy dissipation, according to which they derived the dissipations by interface migration and trans-interface diffusion. After that, Odqvist et al. [18,19] proposed a continuum model in which the interface conditions are determined by balancing the total driving free energy with the dissipations by interface migration and trans-interface diffusion. Such a Gibbs free energy balance approach [18,19] was applied recently to the transition between equiaxed ferrite and bainite ferrite in the Fe–C–Mo and Fe–C–Mn alloys [20]. Following a similar idea, Zurob et al. [21] developed the model with a discrete interface in which trans-interface diffusion is consist of three-steps, i.e. from the product phase to the interface, within the interface and from the interface to the parent phase. Such a model predicted well the kinetics of ferrite precipitation

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[1] MT according to Massalski [11] is a composition invariant and interface-controlled phase transformation, whereas, DT with a much slow and gradually decrease velocity is controlled by bulk diffusion [13].

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and decarburization in the Fe–C–Ni, Fe–C–Mn, Fe–C–Mo, Fe–C–Co and Fe–C–Si alloys [21,22]. Despite of its successful applications, the solute-drag model depends strongly on the assumptions of interface properties and its applicability to the practical multi-component alloys is limited [1].

Another choice for modeling of diffusion-controlled phase-transformations is the sharp interface model. Based on the Gibbs free energy diagram, Hillert et al. [6–9] discussed the case of a binary alloy in which two independent dissipation processes happen, i.e. interface migration and trans-interface diffusion. If only diffusion in the parent phase is considered, the solute molar fraction transferred across the interface is the same as that of the product phase at the interface [6,9]. If diffusion in both phases is considered, the solute molar fraction transferred across the interface is dependent on other interfacial variables, e.g. the growth velocity and the solute flux of product phase [7,8]. The total molar driving free energy and the dissipation by trans-interface diffusion for the two cases are different but not the dissipation by interface migration [7,8]. The flux of trans-interface diffusion in both cases is equal to the solute flux of parent phase at the interface [8,24]; see Appendix A. Another work one should pay attention to is from Aziz et al. [25,26], which aims to model of rapid solidification by the absolute chemical reaction theory. In the case of linear thermodynamics and with only diffusion in the parent phase, the model of Aziz et al. [25,26] is comparable with that of Hillert et al. [6–9]. Although the sharp interface model [6–9,24,25] is independent of the assumptions of interface properties, the interface conditions are determined by the evolution equations that relate the fluxes and their conjugate driving forces in a phenomenological way [27,28] and it is not convenient to be extended to multi-component alloys with complex additional constraints.

Recently, the thermodynamic extremal principle (TEP) [29,30] has been developed to be a handy tool for modeling of complex thermodynamic systems with complex additional constraints. So far, it has been successfully applied to diffusion and creep [31–33], precipitation [34,35], grain growth and coarsening [36–39], rapid solidification [24,40] etc. Since TEP is able to solve the complex additional constraints and derive the evolution equations in a strict mathematical and physical way, it should be a good choice for modeling of diffusion-controlled phase-transformations in multi-component alloys. Regarding it, Svoboda et al. [41–44] carried out a series of work. In their sharp interface model [41], only the dissipation by interface migration was considered for the interface and the condition of equal jumps of chemical potentials across the interface was re-derived. Because the dissipation by trans-interface diffusion is not considered, MT can be only found in the one-phase field [44]. In their solute-drag model with a thick interface [42,43], both interface migration and trans-interface diffusion are considered within the interface and the jumps of chemical potentials across the interface are not equal, thus allowing MT occur in the two-phase field [43]. Integrating the work of Hillert et al. [6–9] and Svoboda et al. [41–43], one may speculate that the sharp interface model of Svoboda et al. [41] is also able to predict the occurrence of MT in the two-phase field if both dissipations by interface migration and trans-interface diffusion are considered.

Following Svoboda et al. [41], a model for diffusion-controlled phase-transformations in multi-component substitutional alloys is derived by TEP in which the dissipations by interface migration and trans-interface diffusion are integrated for a sharp interface (Sec. 2). Following Zurob et al. [45,46], a new concept of trans-interface diffusion in two-steps, i.e. from the product phase to the interface and from the interface to the parent phase,[2] is introduced. Consequently, the model follows the Onsager's reciprocal relation and does not need to distinguish the migrating direction during calculations, indicating that it should be preferred for the cases in which the migrating direction changes upon transformations, e.g. cycle phase-transformations [47–49]. In Sec. 3, the model is applied to the Fe–Cr–Ni alloy and the different transformation characteristics of DT and MT are shown. Since the jumps of chemical potentials across the interface are allowed to be unequal, the location of the critical limit between DT and MT is found in the two-phase field. Adopting an appropriate parameter for trans-interface diffusion, the experimental results in the Fe–Ni alloy [15] are well predicted (Sec. 4). Finally, the current work is summarized in Sec. 5.

2. Model derivation

2.1. Problem descriptions

A closed system is set for the $\gamma \rightarrow \alpha$ diffusion-controlled phase-transformation. The position of the assumed planar interface is Z_I. The coordinate of the boundary between the α (γ) phase and the surroundings is Z_L (Z_R). The growth velocity of the migrating interface is V. At each side of the interface, there are $n+1$ substitutional components. The superscript "0" ("i" ($i = 1,2,\ldots,n$)) in the following section stands for the solvent (solute) and the superscript "*" stands for the variables at the interface. The mass conservation law at the interface is:

$$J_\gamma^{i*} - J_\alpha^{i*} = \frac{V}{V_m}\left(C_\gamma^{i*} - C_\alpha^{i*}\right), (i = 1, 2, \ldots, n), \tag{1}$$

where J_α^{i*} and J_γ^{i*} are the solute fluxes, C_α^{i*} and C_γ^{i*} are the solute molar fractions, and V_m the molar volume is assumed to be same for all the substitutional components in the system. The molar Gibbs free energy of the phase is:

$$g_p = \sum_{i=0}^{n} C_p^i \mu_p^i, (p = \alpha, \gamma), \tag{2}$$

where C_p^i and μ_p^i are the solute molar fraction and the chemical potential, respectively.

2.2. Total Gibbs free energy and its rate

The total Gibbs free energy of the system is given as:

$$G = \frac{1}{V_m}\left(\int_{Z_L}^{Z_I} g_\alpha \mathrm{d}Z + \int_{Z_I}^{Z_R} g_\gamma \mathrm{d}Z\right) = \frac{1}{V_m}\left(\int_{Z_L}^{Z_I} \sum_{i=0}^{n} C_\alpha^i \mu_\alpha^i \mathrm{d}Z + \int_{Z_I}^{Z_R} \sum_{i=0}^{n} C_\gamma^i \mu_\gamma^i \mathrm{d}Z\right). \tag{3}$$

It should be noted that there is no contribution from the interface energy due to the assumption of a planar interface, which means that the total interface energy is constant and does not influence the change rate of total Gibbs free energy. The local mass conservation in the bulk phases is:

$$\frac{\partial C_p^i}{\partial t} = -V_m \nabla J_p^i, (p = \alpha, \gamma, \quad i = 1, 2, \ldots, n). \tag{4}$$

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[2] In the case of a sharp interface, there is no diffusion within the interface as well as its dissipation.

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