Acta Materialia 108 (2016) 85–97

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Kinetic modeling of solid-state partitioning phase transformation with simultaneous misfit accommodation

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ARTICLE INFO

Article history:
Received 1 December 2015
Received in revised form
4 February 2016
Accepted 5 February 2016
Available online xxx

Keywords:
Misfit strain
Strain accommodation
Mixed-mode growth
Phase transformation kinetics
Theory and modeling

ABSTRACT

Considering a spherical misfitting precipitate growing into a finite elastic-perfectly plastic supersaturated matrix, a kinetic modeling for such solid-state partitioning phase transformation is presented, where the interactions of interface migration, solute diffusion and misfit accommodation are analyzed. The linkage between interface migration and solute diffusion proceeds through interfacial composition and interface velocity; their effects on misfit accommodation are mainly manifested in an effective transformation strain, which depends on instantaneous composition field and precipitate size. Taking γ to α transformation of a binary Fe-0.5 at.% C alloy under both isothermal and continuous cooling conditions as examples, the effects of misfit accommodation on the coupling interface migration and solute diffusion are well evaluated and discussed. For the isothermal transformation, a counterbalancing influence between mechanical and chemical driving forces is found so that the mixed-mode transformation kinetics is not sensitive with respect to the elastic–plastic accommodation of the effective misfit strain. Different from the isothermal process, during the continuous cooling condition, the effects of misfit accommodation on the kinetics of solid-state partitioning phase transformation are mainly manifested in the great decrease of the transformation starting temperature and the thermodynamic equilibrium composition. The present kinetic modeling was applied to predict the experimentally measured γ/α transformation of Fe-0.47 at.% C alloy conducted with a cooling rate of 10 K min^{-1} and a good agreement was achieved.

1. Introduction

Understanding the inherent mechanisms in solid-state phase transformations is essential to control the microstructure, and thus to tune the properties of materials. Therefore, over several decades since the advent of the pioneering theory of Johnson-Mehl-Avrami-Kolmogorov (JMAK) [1–5], extensive research efforts have been made to improve the kinetic modeling of transformations, see e.g. Refs. [6–8]. These kinetic models, along with thermodynamic calculations, constitute the theoretical cornerstone of solid-state phase transformations. In crystalline solids, however, the phase transformations are well known to be normally accompanied by the accommodation of misfit strain, which mainly arises from the lattice distortion in vicinity of coherent interface or the volume change between parent and product phases with incoherent interface, due to changes in lattice parameters [9]. However, the mismatch effects are often ignored during the conventional kinetic modeling, although the so-called stress-free transformation strain, as well as its accommodation, plays a crucial role in the aspect of transformation induced plasticity [10,11] and delayed hydride cracking [12,13]. And, it is evident that internal stresses or strain energies arising from the misfit strain may have significant influences on the kinetic process. Therefore, incorporation of the effects of misfit accommodation into the kinetic modeling of solid-state phase transformations not only allows for developing a fundamental understanding of the formation of microstructures, but also provides an opportunity to engineer new microstructures of salient features for novel applications [14–17].

Starting with the pioneering work of Eshelby [18], a vast amount of literature has thus appeared for calculating stresses and strain energies involved in the solid-state phase transformations [19–23]. But these works focus only on the transformation condition and are rarely concerned with the kinetic process. Concerning interface-controlled phase transformation (e.g. the austenite-to-ferrite ($\gamma \rightarrow \alpha$) transformation of pure iron or the massive

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http://dx.doi.org/10.1016/j.actamat.2016.02.010
1359-6454/

transformation), for an infinite elastic–plastic matrix surrounding a growing spherical precipitate, the mechanical contribution of inelastic misfit strain to the precipitation driving force has been modeled by Fischer and Oberaigner [24]. On this basis, for a misfitting spherical precipitate growing or shrinking in a finite elastic–plastic matrix, closed-form analytical expressions, to describe the transformed fraction-dependences of misfit strain energy and mechanical driving force, have been presented in our recent paper [25]; and therein, significant effects of the misfit accommodation on the transformation kinetics and metastable equilibrium have been demonstrated.

It should be noted that, however, the interface-controlled transformation is only a limiting case in the field of diffusive solid-sate transformations. In that case, the short-range transfer of atoms across the parent/product phase interface (related to the interface mobility) is rate-controlling; the diffusion processes are only localized to the interface and its nearest surroundings, thus the parent and product phases have the same compositions [26]; the interface migration velocity is the product of overall driving force and interface mobility [27]. For diffusive transformations involving solute partitioning, the other limiting case, termed as diffusion-controlled transformation, indicates that the long-range diffusion of solute components[1] is the only rate-controlling process. For this case, a rather popular assumption is the local equilibrium concept, and its classical kinetics is ascribed to Zener [29]. In general cases, however, phase transformation should, actually, occur under simultaneous control of both the rate-controlling processes above. The two processes are in series so that interface velocity as calculated from the interface migration always equals that computed from the solute diffusion ahead of interface [28,30]. Such transformation is denoted as mixed-mode transformation, whose nature and phenomenologically kinetic description have been well developed, recently [31–34].

A new question then arises, i.e. how the simultaneous misfit accommodation affects the solid state partitioning phase transformation. As far as diffusion in solids is concerned, the question will become much more difficult, since the self-stress owing to compositional inhomogeneity has to be considered. Study about the effect of elastic self-stresses on solute diffusion in a single-phase crystalline solid can be found in a classical overview of Larché and Cahn [35]. It is mainly manifested in the effect on diffusional mobility and boundary conditions, which can be neglected due to a small stress magnitude, and in the effect on thermodynamic diffusion potentials, which causes local diffusion fluxes becoming a function of both gradients in composition and stress. Since the self-stress that influences the flux instead of being an explicit factor will be expressed in terms of compositional inhomogeneity, the evoked long ranged elastic interactions give rise to significant non-local contributions to flux, which is considered to be a failure of Fick's law [35]. Accordingly, the self-stress effect must be incorporated into the governing equations for diffusion. Concerning the diffusion-controlled growth of a misfitting precipitate in a supersaturated matrix, the internal stresses can be generated, not only by the intrinsic dilatational misfit of precipitate similar to the interface-controlled mode, but also by the non-uniform matrix composition field. Incorporating the both stress effects on the diffusion flux and the equilibrium interfacial compositions, a kinetic modeling of this issue in infinite matrix has been already addressed by Laraia, Johnson and Voorhees (LJV) [36]. The main results are that, the classical parabolic growth law continues to be valid, but the magnitude of growth coefficient is altered by the elastic effects; these effects shift the equilibrium interfacial composition of matrix in the direction of far-field composition, reducing the effective driving force for growth, while the appearance of compositionally stress increases the flux, tending to increase the growth rate [36]. Using the phase field simulations, Mukherjee et al. [37] studied the effect of misfit on diffusion-controlled growth of an isolated precipitate and validated the results of LJV theory.

Unfortunately, on the one hand, both the diffusion kinetics subjected to self-stress and the LJV kinetic theories for diffusional growth of precipitate with misfit are merely restricted to the case of linear elasticity. In many instances, the transformation stress and the strain energy associated with the formation and the growth of misfitting precipitates can be subjected to a plastic relaxation [19,20,38]. On the other hand, both interface-controlled and diffusion-controlled modes must be regarded as the extreme possibilities for actual kinetics in the case of partitioning diffusive transformation. In general, the diffusive phase transformation will be of a mixed-mode character. As such, the question mentioned above will change to the more specific one: How does the concurrent elastic–plastic accommodation of the misfit strain and the composition strain affect the coupled kinetic processes of solute diffusion and interface migration? This is important to deserve an in-depth investigation in order to obtain further insights into the formation of desired microstructures. To the authors' knowledge, however, there has been no obvious answer for now, except several preliminary attempts, e.g. the works of Ammar et al. [39], Svoboda et al. [28] and Gamsjäger et al. [40]. This may be attributed to the troublesome treatment of complex interaction of the three concurring process: interface migration, solution long-range diffusion, and misfit accommodation. As stated in Ref. [39], the main difficulty lies in the multiple free boundary problems, i.e. tight couplings between the interface evolution and the two fields of solute diffusion and internal stress. By considering a spherical misfitting precipitate growing into a supersaturated elastic-perfectly plastic finite matrix, the present work is devoted to modeling the kinetics of solid-state partitioning phase transformation with simultaneous misfit accommodation, and then to accounting for the above interactive problem.

2. Theory

2.1. Problem analysis and description

The phase transformation of austenite (γ) to ferrite (α) in a binary hypo-eutectoid Fe–C alloy, as the most important and typical representative of solid-state partitioning phase transformations, is selected for the present kinetic modeling. Based on the analysis approach of our previous paper [25], consider a spherical misfitting α inclusion growing in a finite, concentric, spherical, and elastic-perfectly plastic supersaturated γ matrix which is stress-free at the external surface, as sketched in Fig. 1a. The spherical hypothesis is very often used in these diffusional transformations, for example, the classic work of Vandermeer [41]. It should be borne in mind that, however, ferrite will not preserve its spherical shape during growth and will change into the form of thickening plates at rather small transformed fraction; see Ref. [42]. In present investigation, there are three aspects concerning the spherical hypothesis: (a) under this hypothesis, governing equations for solute diffusion field and stress field can be greatly simplified; (b) as far as a sphere is concerned, there is no distinction between coherent and incoherent precipitates if only a pure dilatational transformation strain is considered, as indicated by Christian [27,43]; and (c) the overall transformation kinetics is based on JMAK model which is of a statistical average theory, and thus the spherical hypothesis seems to

[1] Taking sharp interface and interstitial components into consideration, the trans-interface diffusion can be neglected [28].