



# Analysis of elastic–plastic accommodation due to volume misfit upon solid-state phase transformation

S.J. Song<sup>a</sup>, F. Liu<sup>a,\*</sup>, Z.H. Zhang<sup>b</sup>

<sup>a</sup> State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, People's Republic of China

<sup>b</sup> Steel Tube Division, Baosteel Research Institute, Shanghai 201900, People's Republic of China

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## Abstract

During solid-state phase transformation, volume misfit between the parent and the product phases leads to strain energy and affects the transformation kinetics. Considering a misfitting spherical inclusion growing/shrinking in a finite elastic–perfectly plastic medium and recognizing the isolated product/present phase as the inclusion at different stages of transformation, complete solutions to the displacement, stress and strain fields for the purely elastic and elastic–plastic accommodations of the transformation misfit are obtained. Then, analytical expressions for the transformed fraction dependences of the total molar accommodation energy and the mechanical driving force at an interphase are presented and incorporated into the transformation kinetics. The present model is evaluated using the austenite-to-ferrite ( $\gamma \rightarrow \alpha$ ) transformation in pure iron with temperature-dependent material properties. During the elastic–plastic accommodation, the elastic strain energies in the matrix and inclusion are negligible compared to the plastic work in the matrix; and meanwhile, the total strain energy is relaxed to a lower value in contrast to the corresponding purely elastic accommodation. Furthermore, during almost the entire process of transformation, the matrix remains completely plastic. The mechanical driving force varies monotonously with the transformed fraction, which counteracts the transformation at the initial stage but favors the transformation at the later stage. Application of the present model in the non-isothermal  $\gamma \rightarrow \alpha$  transformation of pure iron conducted with a cooling rate of  $10 \text{ K min}^{-1}$  is performed, and the effect of the misfit accommodation on the metastable equilibrium temperature is demonstrated. As compared with the chemical driving force, the mechanical driving force is much smaller but has a significant effect on the transformation kinetics.

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## 1. Introduction

Solid–solid phase transformations are important means of adjusting the microstructure to attain the desired properties of materials, such as mechanical, electrical or magnetic properties, and therefore understanding and controlling the nucleation and growth processes involved in phase transformations are of great concern in the production of very many materials [1–3]. In order to follow the progress of the transformation, a global, macroscopic

parameter such as the transformed fraction  $f$  ( $0 \leq f \leq 1$ ) can be determined experimentally as a function of time and/or temperature. The theoretical aspect of the reaction kinetics is ascribed to the classical Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation, which provides an expression for  $f$  in terms of nucleation and growth rates [4–8]. Later, taking into account that the original JMAK theory has too many restrictive conditions, a generalized, modular transformation kinetic model incorporating the prevalent nucleation, growth and impingement modes as well as the arbitrary time–temperature dependencies has recently been developed [3,9]. In the case where the modular model describes the transformation kinetics correctly,

\* Corresponding author. Tel.: +86 29 88460374; fax: +86 29 88491484.  
E-mail address: [liufeng@nwpu.edu.cn](mailto:liufeng@nwpu.edu.cn) (F. Liu).

the operating mechanisms for the nucleation and growth of phase transformations can be derived from measuring only the fraction transformed as a function of time [3,10–13]. But, in practice, local variations in the microstructure may alter this simplified model of the transformation kinetics and more advanced measurements are required that probe the nucleation and growth kinetics simultaneously and in situ [14,15].

As indicated in Refs. [3,9], however, the modular kinetic model is mainly focused on the transformations under large undercooling or overheating, where both the nucleation and growth rates are only Arrhenius-type temperature dependent. In reality, for solid-state phase transformation involved in allotropic polycrystalline materials, e.g. austenite ( $\gamma$ ) to ferrite ( $\alpha$ ) transformation in iron-based alloys, the thermodynamic driving force frequently plays an important role during the nucleation and growth processes. Assuming interface-controlled growth, e.g. massive transformation, a modular model accounting for the isothermal transformation with the constant chemical driving force (i.e. the molar chemical Gibbs energy difference between the present and product phases) is available [3,9]; while, for non-isothermal transformation, an extended analytical model associated with the temperature-dependent chemical driving force has been developed on the basis of the discretized temperature integral [16]. It is well known, however, that the energies corresponding to the elastic and plastic deformations associated with the accommodation of volume misfit between the parent and product phases upon phase transformation depend on the transformation process and simultaneously, as part of the thermodynamic driving force for transformation, probably influence the interface-migration process. Whereas the allotropic phase transformations considering the temperature-dependent chemical driving force can be subjected to a formal or analytical treatment, the transformed fraction dependence of elastic–plastic accommodation energy and its effects on the kinetics of transformation are not yet fully understood. This is the motivation for the investigations presented here.

Extensive studies have been devoted to the elastic–plastic accommodation energy due to the transformation misfit strain, since Eshelby reported his pioneering work [17]. However, Eshelby's theory is restricted to the case of linear, isotropic or anisotropic elasticity. For the more complex elastic–plastic case, Lee et al. [18] have derived an analytical expression for the misfit accommodation energy, provided that a spherical inclusion, with fixed radius  $R$  subjected to uniform sudden dilatational eigenstrain, is embedded in an infinite elastic–perfectly plastic material. Taking into account a general anisotropic (non-spherical) inclusion and/or a finite elastic–plastic matrix, analytical solutions for the stress and strain and the total accommodation energy are often intractable or even impossible, and hence the finite element method is preferable [19–24]. However, these works cited above focus only on calculations of the transformation strain energy for

an inclusion with fixed radius, in order to determine its nucleation condition or transformation condition or to describe the measured lattice parameter shifts of the precipitate phase [25–27], but are rarely concerned with the kinetic process of a misfitting precipitate growing in an elastic–plastic matrix. So far, there have been a few studies [28–35] dedicated to modeling the elastic–plastic misfit accommodation incorporated with the solid-state phase transformation kinetics. Some of these instances are outlined in the following.

Based on an incremental concept with respect to the development of plastic strain and plastic work, Fischer and Oberaigner [30] dealt with the dilatational growth of a spherical inclusion, instead of a fixed spherical inclusion, in an infinite elastic–plastic material; and then, the dissipated plastic work as well as the mechanical driving force on the transformation front (i.e. the normal component of the Eshelby energy momentum tensor [31]) were presented analytically. Subsequently, by deriving a micromechanics framework and using the concept of non-equilibrium thermodynamics, Fischer et al. [32] studied the kinetics of diffusional transformation due to interface migration into a multicomponent elastic–plastic material; and by combining the chemical and mechanical parts of thermodynamic driving force acting on the interface, a kinetic equation for the volume fraction of transformed phase was obtained. Nevertheless, due to the hypothesis that the isolated interface migrates into an effectively infinite materials, the former model [30] cannot provide the overall transformation kinetics involving the transformation-dependent elastic–plastic accommodation; due to the micromechanics arguments, the latter model [32] can only be performed by computational mechanics.

In the framework of the elastic–plastic model of a spherical inclusion, Zisman and Vasilyev [33] analyzed the evolution of phase stresses induced by the  $\gamma \rightarrow \alpha$  transformation in polycrystalline iron alloys. Considering the finite matrix, the isolated regions of  $\alpha$  phase and  $\gamma$  phase were treated as inclusions at the initial and the later stages of the transformation, respectively. Then, the phase stresses at the  $\gamma/\alpha$  interface can be expressed as functions of the volume fraction of ferrite. However, the elastic–plastic molar accommodation energy was simply regarded as the work due to the hydrostatic stresses in the  $\gamma$  phase adjacent to the interface with the volume eigenstrain.

Using the proposed non-linear elastic–plastic phase field model, Ammar et al. [34,35] investigated the effect of plastic accommodation on the diffusion-controlled growth of an elastic spherical misfitting precipitate into an infinite supersaturated elastic–plastic matrix, and addressed the elastic–plastic strain energy effect on the transformation kinetics in comparison with the corresponding purely elastic state and purely chemical transformation. Although the phase field model can be involved in finite size specimens, the exact analytical solution used to validate the proposed numerical model is derived from the above-mentioned work by Lee et al. [18,35]; this solution takes into account the growth

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