A phase-field model investigating the role of elastic strain energy during the growth of closely spaced neighbouring interphase precipitates

Alireza Rahnama [a,*], Samuel Clark [a,b], Vit Janik [a,c], Seetharaman Sridhar [a,d]

[a] Advanced Steel Research Centre, University of Warwick, CV4 7AL, United Kingdom
[b] School of Materials, University of Manchester, Manchester M13 9PL, United Kingdom
[c] Faculty Research Centre for Manufacturing and Materials Engineering, Coventry University, Coventry CV1 5FB, United Kingdom
[d] George S. Ansell Department of Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO 80401, USA

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ABSTRACT

A multi-phase field method is developed to investigate the effects of transformation strain on the transformation kinetics, thermodynamic stability and pairing of interphase precipitates in micro-alloyed steels. The model conserves homogeneity of stress in the diffuse interface between elastically inhomogeneous phases and provides an explanation of the mechanism resulting in the pairing of two adjacent interphase precipitates. Several scenarios of inhomogeneous elastic conditions have been considered. The simulations for a situation where only the interfacial energy is considered to contribute to the transformation show that this energy can lead to the establishment of a neck between two neighbouring precipitates. However, if sufficient time is given, one of the precipitates will completely dissolve into its neighbouring particle. On the other hand, when both strain and interfacial energies act on the system, the bridge between the particles becomes stabilised leading to the pairing of the particles. This is a result of the particles tendency to minimise the strain energy due to the excessive strain field generated by the neck between the two particles.

1. Introduction

Interphase precipitation in steels is characterised by periodic parallel planes of randomly oriented carbide precipitates which form at the interphase between the austenite and ferrite as the former decomposes into the later [1]. Interphase precipitation is often found in ferritic steels when the steel is alloyed with one or several strong carbide forming elements such as V, Nb or Ti [2]. It has been found that a single-phase ferritic matrix in low carbon steels strengthened by periodic arrangement of interphase carbide precipitates offers a high strength, high formability, and low-cost structural material, suitable for large scale production of automotive sheet [3,4].

Interphase precipitates are found in allotriomorphic α ferrite which itself is considered to grow on either side of a prior γ austenite grain boundary, with at least one interphase boundary adopting a low energy, semi-coherent, orientation relationship [5], such as

the Kurdjumov-Sachs (KS) [6], or the Nishiyama-Wasserman (NW) [7,8] orientation relationships (OR). A growth ledge on a semi-coherent γ/α interphase boundary consists of a disordered, mobile riser and a comparatively coherent and immobile tread [9]. Typically, it is thought that the nucleation of interphase precipitates occurs on ledged γ/α interphase boundaries [1]. Although the high-energy interphase boundary of the riser would be favourable for the nucleation of precipitates through the formation of abutted spherical cap nuclei [10], and further eased by the segregation of substitutional solutes through the solute drag effect [11], interphase precipitates are however observed to have nucleated on the comparatively low energy γ/α tread [12]. This is thought to be because there would be an insufficient time for successful stable nuclei to form on the mobile riser. Further, implications of nucleation on the low energy tread are as follows:

- As the interfacial energy of the ledged interphase boundary tread is low, therefore a precipitate nuclei would subsequently be expected to be nearly spherical [10].

* Corresponding author.
    E-mail addresses: A.Rahnama@warwick.ac.uk (A. Rahnama), S.J.Clark@warwick.ac.uk (S. Clark), V.Janik@warwick.ac.uk (V. Janik), S.Seetharaman@warwick.ac.uk (S. Sridhar).

- The nucleation of interphase precipitates is not aided by the segregation of substitutional alloying elements as they are not thought to be able to readily segregate to the mobile, low energy tread of the semi-coherent γ/α interphase boundary [11].

In a single study, it has been observed using TEM that in some circumstances disc shaped interphase precipitates can join at the tips and form pairs of connected precipitates [13]. The reason for the paucity of TEM observations of connected precipitates is that unless the planes of interphase carbides are suitably spread it is impossible to tilt a specimen such that an individual plane can be imaged [14]. Re-examination of the images by Davenport and Honeycombe [14] does, however, confirm that individual carbide precipitates located on planar rows of interphase precipitates often interact with one another. It is hypothesized that the phenomenon of precipitate-precipitate interactions on the densely populated planes of interphase precipitates, may, in fact, be commonplace.

In our previous paper [15], a multi-component phase field method (PFM) model was derived which was coupled with a multi-component CALPHAD thermodynamic database using a four-sublattice model. Such models, including the phase-field method or other time-dependant Ginzburg-Landau methods, are a powerful means of encapsulating the complex interactions between atomistic mechanisms and macroscopic conditions on the mesoscopic scale [16]. In the phase-field method, the continuum field variables can be identified with the phase field (structural order parameter) ϕ_α with temperature T, concentration $\vec{c}$, total strain ϵ^{ij}, magnetisation m^i or other variables relevant to describe the system of interest.

The premise of this work is to extend our model [15,17,18] by investigating the effect of the previously neglected elastic transformation strain upon the transformation kinetics, thermodynamic stability, and pairing and necking of interphase precipitates in micro-alloyed steels. The elastic transformation strain associated with precipitation is known to have a potent influence upon the morphology of said precipitates. A coherent hard precipitate (nuclei) in an isotropic matrix would be expected to adopt the morphology of a sphere [19] to minimize the elastic strain energy whereas a soft coherent precipitate would result in an oblate spheroid. In contrast, Nabarro [20], mathematically explored the role of strain upon the morphology of incoherent precipitates within an isotropic matrix. The elastic strain associated with interphase precipitates is hypothesized to play an important role in the growth of individual precipitates and the interactions between neighbouring precipitates, explaining the complex, compound morphologies, and particularly the necking behaviour of interphase carbide precipitates.

2. Model

The model considers the growth and interaction between precipitates in-terms of transformation strain upon low energy γ/α ledged interphase boundary treads. In 3D space, for the problem with total strain ϵ^{ij} in the two directions i, j in terms of the phase strain ϵ^{ij}_α in each individual phase (α), we have:

$$\epsilon^{ij} = \sum_\alpha \phi_\alpha h_\alpha(\epsilon^{ij}_\alpha) \tag{1}$$

h_α is dependant on the elastic properties of each individual phase and ϕ_α is the field variable for phase α. Eq. (1) calculates the total strain as a linear summation of the strains of the individual phases α weighted by the phase densities ϕ_α. In other words, this equation is a direct extension of original multi phase function for diffusive

phase transformations [16]. To correlate the strain fields in the different phases equal elastic stresses in the interface are assumed.

2.1. The mechanical multi-phase model

The free energy can be defined as an integral of the density functional over the domain Ω. The density functional consists of the grain boundary energy density f^{gb}, the chemical free energy density f^{ch}, and the elastic energy density f^{el}. we have:

$$F = \int_\Omega f^{gb} + f^{ch} + f^{el} \tag{2}$$

where,

$$f^{gb} = \sum_{\alpha,\beta=1}^N \frac{4\alpha_{\alpha\beta}}{\gamma_{\alpha\beta}} \left\{ \frac{\gamma_{\alpha\beta}^2}{\pi^2} |\nabla\phi_\alpha.\nabla\phi_\beta| + w_{\alpha\beta} \right\} \tag{3}$$

where $\alpha_{\alpha\beta}$ refers to the grain boundary energy between different phases. Subscript α and β refers to the relevant pair from ferrite, austenite or precipitate. $\gamma_{\alpha\beta}$ refers to the interface width and $w_{\alpha\beta}$ is the dimensionless repulsive potential function that keeps the interface upright [21]. $w_{\alpha\beta} = \phi_\alpha\phi_\beta$ when $0 < \phi_{\alpha/\beta} < 1$ and ∞ elsewhere. This specific form of Eq. (3) follows the scaling invariance of the total interface energy as an integral over f^{gb} with respect to the interface width $\gamma_{\alpha\beta}$.

f^{ch} is expressed as:

$$f^{ch} = \sum_{\alpha=1}^N \phi_\alpha f_\alpha(\vec{c}_\alpha) + \vec{\mu}\left(\vec{c} - \sum_{\alpha=1}^N \phi_\alpha\vec{c}_\alpha\right) \tag{4}$$

$f_\alpha(\vec{c}_\alpha)$ is the bulk free energy of each individual phase, which depends on the phase concentrations $\vec{c}_\alpha$. $\vec{\mu}$ refers to the chemical potential vector. This vector is defined as a Lagrange multiplier to account for the mass balance between the neighbouring phases. This was achieved by defining the mixture concentration $\vec{c}$, which is continuous over the interface as $\vec{c} = \sum_\alpha \phi_\alpha\vec{c}_\alpha$.

Similarly, f^{el} is defined as:

$$f^{el} = \frac{1}{2}\left\{ \sum_{\alpha=1}^N \phi_\alpha(\epsilon^{ij}_\alpha - \epsilon^{*ij}_\alpha)C^{ijkl}_\alpha(\epsilon^{kl}_\alpha - \epsilon^{*kl}_\alpha) \right\} \tag{5}$$

where ϵ^{ij}_α is the total strain in individual phases, ϵ^{*ij}_α is the eigenstrain and C^{ijkl}_α is the Hook's matrix (Young's modulus). It is noted that ϵ^{*ij}_α and C^{ijkl}_α are concentration and temperature-dependant, however in the present work, it is assumed that these quantities are constant with both concentration and temperature but vary from phase to phase. To correlate the strain fields in the different phases, it is required to define an additional condition. Since $\vec{\mu} = \frac{\partial f^{ch}}{\partial \vec{c}}$, from analogy we can define the elastic stresses as $\sigma^{ij}_\alpha = \frac{1}{\phi_\alpha}\frac{\partial f^{el}}{\partial \epsilon^{ij}_\alpha}$. To define the additional condition, mechanical equilibrium is assumed between phases in the strong form, i.e. to solve the equations of elasticity it is required to define a domain for finding an equilibrium configuration of a deformable elastic body which is in the present case the precipitates' body. It is also assumed that a continuity of all stress components σ^{ij} exists in the interface. Thus, in the mathematical form for all α and β we have:

$$\sigma^{ij}_\alpha = \sigma^{ij}_\beta = \sigma^{ij} \tag{6}$$

Thus we have:

$$(\epsilon^{ij}_\alpha - \epsilon^{*ij}_\alpha)C^{ijkl}_\alpha = (\epsilon^{ij}_\beta - \epsilon^{*ij}_\beta)C^{ijkl}_\beta = (\epsilon^{ij} - \epsilon^{*ij})C^{ijkl} \tag{7}$$

and