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Predicting equilibrium shape of precipitates as function of coherency state

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Abstract

A general approach is proposed to predict the equilibrium shapes of precipitates in crystalline solids as function of size and coherency state. The model incorporates effects of interfacial defects such as misfit dislocations and structural ledges on transformation strain and on interfacial energy. Using α precipitation in α/β titanium alloys as an example, various possible equilibrium shapes of precipitates having different defect contents at interfaces are obtained by phase-field simulations. The simulation results agree with experimental observations in terms of both precipitate habit plane orientation and defect content at the interface. In combination with crystallographic theories of interfaces and experimental characterization of habit plane of finite precipitates, this approach has the ability to predict the coherency state (i.e. defect structures at interfaces) and equilibrium shape of finite precipitates.

Keywords: Precipitation; Misfit dislocations; Structural ledges; Phase field; Titanium alloy

1. Introduction

Most engineering alloys are strengthened by second-phase particles, and the quantity, size, shape, orientation, coherency state and spatial distribution of these particles determine the deformation mechanism and mechanical behavior of the alloys [1,2]. Classical examples include Al-, Ti- and Mg-based light alloys [3–6] and high-temperature Ni-base superalloys [7], to name a few. To assist in alloy design, it is essential to develop modeling capabilities to predict these key microstructural features. However these features are determined by the interplay between interfacial and elastic strain energy minimization during precipitation, which is difficult to quantify theoretically or by experiment.

New phases formed during precipitation reactions in solids usually have different compositions and structures from those of the parent phase. During nucleation and in the early stages of growth, precipitates tend to be coherent with the matrix, which minimizes the interfacial energy [8,9]. They may lose coherency during continued growth when the elastic strain energy contribution to the total free energy of the system becomes dominant. Formation of line defects such as misfit dislocations within the interface relieves misfit stress at the expense of increasing interfacial energy. In addition to misfit dislocations, another type of line defect, structure ledges [10], which exhibit step character as well as dislocation properties [11,12], are also frequently observed at interphase interfaces. They are also referred to as transformation dislocations or disconnections to distinguish themselves from defects without the step character in the topological model for structural phase transformations [11]. In contrast to misfit dislocations, it is well recognized that the existence of structure ledges increases the degree of coherency of a heterophase interface and hence lowers the interfacial energy [13]. Examples of these line defects at a body-centered cubic (bcc)–hexagonal close-packed (hcp) interface are shown schematically in Fig. 1a.

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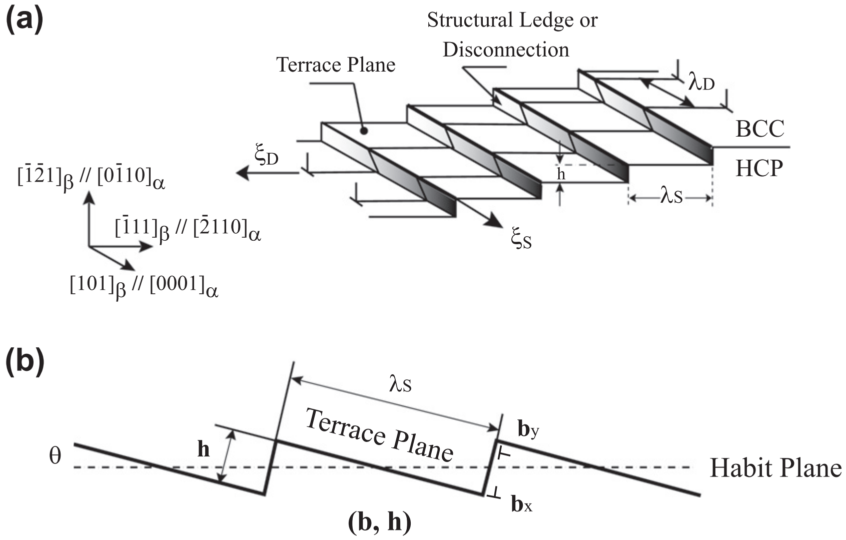

Fig. 1. (a) Schematic illustration of an interphase interface between bcc and hcp, exhibiting both structural ledges (disconnections) [12] and misfit dislocation arrays. The interface is decorated by arrays of structural ledges (**b**, *h*) with height *h* and spacing λ_S and misfit dislocations with spacing λ_D. The terrace coordinate frames, the line direction of the ledges, ξ_S, and dislocations, ξ_D, are also shown. (b) Schematic illustration of the dislocation properties associated with structure ledges (disconnections) with Burgers vector resolved in the terrace plane. The terrace plane (bold) is inclined at an angle θ to the habit plane (dashed).

Since misfit dislocations and structure ledges not only alter the coherency stress and change the interfacial energy and its anisotropy, but also introduce growth anisotropy, they impact all the key microstructural features mentioned above. In addition, the structural defects at interfaces may alter the nature of precipitate–dislocation interactions and change the deformation mechanisms (e.g. cutting vs. looping), as well as the nature of precipitate–martensite interactions and change the transformation paths [14,15]. Therefore, in order to predict the key microstructural features of precipitates and how they interact with dislocations and other types of precipitates, the interfacial defect structure as a function of precipitate size has first to be determined. With the advances in high-resolution electron microscopy, defect structures at many heterophase interfaces have been characterized. However, it is difficult to determine how the defect structure changes when particle size changes. Models accounting for misfit dislocations and structural ledges in an integrated manner, in terms of their effect on coherency elastic strain energy, interfacial energy and final equilibrium shape of finite precipitates, are still lacking. Existing crystallographic theories, such as the invariant line model [16,17], structure ledge model [18], edge-to-edge matching model [19], O-lattice model [20,21] and topological model [11,12], have been successful in predicting some of the major crystallographic features of heterophase interfaces in infinite systems, including orientation relationship (OR), habit plane orientation and defect structure within interfaces. Nevertheless, it is difficult to predict the shape and interfacial defect structure of a finite precipitate, which is a typical variational problem where the sum of the interfacial and elastic strain energies as a functional of interfacial defect structure is minimized.

Most of the existing models for microstructural evolution during precipitation consider either coherent [22–24] or incoherent precipitates and ignore interfacial defects. In this paper, we propose a general approach that incorporates interfacial defects in a phase-field model. Using precipitation reaction in a near-α-Ti alloy as an example, we show how different types of interfacial defects relieve the coherency elastic strain, change the interfacial energy and its anisotropy, and affect the habit plane orientation and equilibrium shape of precipitates. We also discuss how to predict interfacial defect structures and the critical information required.

2. Elastic strain energy of coherent and semicoherent precipitates

As mentioned above, a precipitate phase is usually different from the matrix in terms of composition, crystal structure and orientation, which results in lattice misfit across the precipitate–matrix interface. The elastic deformation that accommodates the misfit in the crystal lattices of adjoining phases to form coherent or semicoherent interphase boundaries, known as coherency strain, usually plays a significant role in solid-state phase transformations [22–26]. Being both volume- and morphology-dependent, the coherency elastic strain energy affects precipitate shape, spatial arrangement, as well as the overall driving force for the transformation. In addition, as a nucleating phase may possibly adopt a metastable structure with low-energy coherent interfaces with the parent matrix, the final transition to the stable phase structure is controlled by the coherency strain energy and its interplay with the interfacial energy.