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An atomistic simulation study of the migration of an austenite–ferrite interface in pure Fe

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Abstract

Molecular dynamics (MD) simulations using an embedded atom method potential for pure Fe were performed to determine the atomic mechanisms taking place during the migration of a face-centered-cubic–body-centered-cubic (fcc–bcc) interface. A centro-symmetry parameter (CSP) has been utilized to discriminate between atoms of the fcc and bcc phases. It is shown from both simulation and disconnection theory that the primary structural disconnections formed when creating the fcc–bcc bicrystal do not move laterally across the boundary as the transformation proceeds. However, it is observed that a second set of glissile disconnections forms on the terraces and the interface migrates by the rapid advance of these mobile defects. The rate-limiting step of the interface propagation process is the nucleation of new bcc islands on the terraces and it is shown that the nucleation event is heterogeneous, with the primary disconnections acting as the preferred nucleation sites. The nucleation and growth mechanisms identified here may provide important insights into the mobility of more general incoherent interphase boundaries.

Keywords: Interface dynamics; Grain boundary defects; Molecular dynamics; Interface structure; Interface migration

1. Introduction

From as early as 1960 it has been recognized that, in many examples of crystalline phase transformations, the migration of interphase boundaries occurs by the lateral motion of interface steps [1], a process analogous to the terrace-ledge-kink mechanism in the growth of surfaces. It is also well established that strain mismatch between two phases is often accommodated by an array of misfit dislocations at the boundary. The seemingly distinct roles of strain relief by misfit dislocations and mass transfer during growth via step motion were unified in the seminal work of Hirth and Pond [2,3]. These authors defined a defect known as a disconnection, which exhibits both dislocation and step character, and elucidated the role of these defects in solid–solid phase transformations.

The concept of a disconnection has lead to an improved understanding of the crystallography of interfaces and several examples of the application of disconnection theory exist for both martensitic and diffusional transformations [4]. Using high resolution transmission electron microscopy (HRTEM) Chai et al. [5] were able to show that the habit plane in the body-centered-cubic (bcc) (β)–orthorhombic (α) martensite transformation in Ti–Nb consists of an array of disconnections and the observed structure is in excellent agreement with theory. Ma and Pond [6] theoretically determined the disconnection structure and habit planes for a range of orientation relationships in steels and were able to predict the existence of experimentally observed habits such as {5 7 5} and {2 9 5}. The disconnection structure of lath martensite has been studied using HRTEM by Moritani [7]. A classic example of disconnections facilitating a diffusional as opposed to martensitic phase transformation is the growth of the hexagonal γ (Ag_2Al) phase into Al by the lateral motion of steps on the (0 0 0 1) basal plane of γ [8–12]. However, as reviewed by Muddle et al. [13], a

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similar mechanism applies to the case of the growth of ordered phases in a disordered matrix in the AuCu and AgCd binary systems. In addition, Pond et al. [14,15] have described the disconnection structure observed at the interface between γ-TiAl and the ordered α_2-Ti_2Al phase. Purdy and Hirth [16] studied the precipitation of the θ′ phase in the Al–Cu system and identified two types of disconnections, one glissile and one sessile, at the precipitate–matrix interface. In a more recent study, Medlin and Sugar [17] demonstrated how glissile disconnections facilitate the transformation of the tradymite structure to the rocksalt structure in the $AgSbTe_2$ thermoelectric material.

In a previous publication, Song and Hoyt investigated the velocity, driving forces and mobilities of an interface between the bcc and face-centered-cubic (fcc) phase in pure Fe using classical molecular dynamics simulations [18]. The interphase boundary is given by $(1\,1\,0)_{bcc}$ // $(7\,7\,6)_{fcc}$ and $[0\,0\,1]_{bcc}$ // $[-1\,1\,0]_{fcc}$ but can best be described as a small tilt, in an axis lying within the boundary, about the Nishiyama–Wasserman orientation relationship, such that a regularly spaced array of structural disconnections is introduced. It was demonstrated that the presence of the disconnections leads to interface motion observable on the timescale of molecular dynamics (MD). Since the disconnections are sessile and no diffusive transport takes place in MD simulations, the observed mobility of the interface is surprising.

A distinct advantage of MD simulations in the study of interface migration is the fact that the motion of individual atoms can be monitored. In previous studies of grain boundaries, the important atomic mechanisms controlling the motion have been observed and in some cases quite unexpected processes have been identified [19–21]. Therefore the purpose of the present paper is to analyze in detail the atomic mechanisms taking place during the interface motion of the fcc–bcc boundary studied previously. We argue that the disconnections act as heterogeneous sites for the nucleation of a second set of glissile disconnections on the terraces. Although only one orientation is investigated here, the results may provide important insights into the atomic processes occurring in more general incoherent crystalline heterophase boundaries.

2. Theoretical background and numerical procedures

2.1. Disconnections

A disconnection is a type of interphase boundary defect that possesses both dislocation and step character. The crystallography of a disconnection can be understood from Fig. 1, which depicts the interface between a phase α (top) and γ (bottom). To form a disconnection we consider the joining of the phases where the two crystals have opposing ledge directions. The vector $\boldsymbol{n}$ is normal to the terrace surface and a step is identified as positive if the step translates the terrace in the direction of $\boldsymbol{n}$. Also shown in Fig. 1, $\boldsymbol{l_a}$ and $\boldsymbol{l_\gamma}$ are the ledge translation vectors, which can either

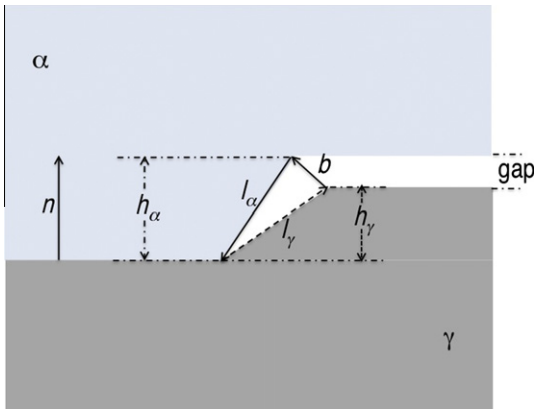

Fig. 1. A schematic of a single step disconnection structure. Two crystals α and γ with ledge vectors $\boldsymbol{l_a}$ and $\boldsymbol{l_r}$ respectively are shown and n is the plane normal. The two steps heights, h_α and h_γ, are computed from the dot product of the ledge vectors and n. Since the lattice parameters and crystal structures of the two phases are different, h_α does not equal h_γ and a gap must be closed.

be normal to or have some angle to the terrace surface. Therefore, the step height for the α phase can be determined as $h_\alpha = \boldsymbol{n} \cdot \boldsymbol{l_\alpha}$ and a similar construction is applied to determine the step height of the γ phase. Since the lattice parameter and crystal structures for the two sides are different ($\boldsymbol{l_a} \neq \boldsymbol{l_r}$), a gap, equal to the difference in step heights, is necessary at the right of the step. The gap is closed by intermolecular forces and the dislocation character of the disconnection is created. The Burgers vector of the disconnection is the sum of the individual ledge translations, i.e.

$$\vec{b} = \boldsymbol{l_\alpha} + \boldsymbol{l_\gamma} \tag{1}$$

The dislocation character of a disconnection can also be derived by a Burgers circuit construction; however, since the circuit will necessarily involve two distinct phases, care must be taken in the definition of $\boldsymbol{b}$. For two phases α and γ the Burgers vector can be written as:

$$\vec{b} = -(\boldsymbol{t_\gamma} + \boldsymbol{P}_{coh}\boldsymbol{t_\alpha}) \tag{2}$$

Here $\boldsymbol{t_\alpha}$ and $\boldsymbol{t_\gamma}$ are vectors referred to the coordinate system of each phase and $\boldsymbol{P}_{coh}$ is a rotation matrix that maps the γ phase coordinate system into that of the α phase (including coherency strain). From the point of view of interphase boundary mobility, an important geometrical consideration is the orientation of $\boldsymbol{b}$ relative to the boundary normal. In most of the experimental studies summarized in Section 1, for example the Al–Ag work by Howe et al. [22], the disconnections are characterized by a $\boldsymbol{b}$ vector lying within the boundary plane, such that the phase transformation proceeds by the lateral motion of disconnections. In our previous paper [18], however, an fcc–bcc boundary that is mobile on MD timescales and contains a parallel array of steps at the interface was identified, but the motion of the boundary is not controlled by the lateral motion of disconnections.