

Full length article

Non-conservative dynamics of lattice sites near a migrating interface in a diffusional phase transformation



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ABSTRACT

Migration of phase boundaries in crystalline solids eliminates one set of lattice sites and establishes another. Using a combination of phase field crystal modeling and crystallographic analysis, we present here a complete atomistic description of the migration mechanism of a high-index planar interface during a diffusional hexagon to square phase transformation. In particular we show that a terrace-step interface advances macroscopically in the form of growth ledges, while microscopically its migration occurs by opposite shearing on the terraces and a *one-to-two splitting* of lattice sites, giving a new class of lattice site correspondence and superabundant vacancies. In addition, a new approach capable of finding a critical nucleus with atomic resolution is developed by combining the phase field crystal energetics with the free-end nudged elastic band algorithm.

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1. Introduction

When people invoke “atoms” to describe plasticity or phase transformation of crystalline materials, they very often really mean “atomic sites” (lattice site or site in this paper). The distinction between “site” and “atom” is parallel to the distinction between the governmental structure of a country and who is occupying which office at the moment. “Site” can be enduring, for instance a particular lattice site in bronze may be occupied by Cu atom, Sn atom or vacancy at different times. However, in plasticity and in phase transformations, the site lattice may necessarily change. Unlike atoms which cannot be created/annihilated and therefore must satisfy local conservation, there is no conservation rule of lattice sites, so concepts like “lattice correspondence”, “ledge motion” and “transformation strain” need to be carefully considered in light of this [1]. Here we examine the creation/annihilation/motion dynamics of lattice sites in a model hexagon-to-square lattice phase

transformation, and try to address the fundamental question of “where, when and how does lattice site arise?”

Interfaces play essential roles in microstructural evolution [2,3]. Compared to crystallographic theories of interface structures [4–13], how these interfaces migrate in plasticity and phase transformation is less clear. The structure of a phase boundary dictated by the invariant plane strain (IPS) condition consists of terraces and steps, referred to as structural ledges (SLs) or disconnections. It is often assumed that a *collective* motion of SLs within the terrace plane accounts for the advance of the macroscopic interface [3,10,13]. Chiao and Chen [10] reported that the steps/ledges of the orthorhombic/monoclinic interface move synchronously as an entity. This view has been followed by Pond and Hirth [13] and is also accepted in the Book by Sutton and Balluffi [3]. But the Moiré ledge (ML) approach suggests that, an extrinsic ledge, defined as the ML between two adjacent Moiré planes, could be responsible for the migration of a terrace-step interface [14–16].

Moreover, the practice of one-to-one lattice site correspondence, which is implicitly assumed in all ledge-wise migration mechanisms [17,18], may not be satisfied. This is where the confusion between “site” and “atom” tends to cause trouble. While an atom can only be at one place at a time, a “site” can move, split

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into two, or be eliminated when a phase boundary sweeps across. This is because a site is just the location where there is significant probability of finding an atom, so an atom occupying an old site, when that old site is eliminated, can find itself presented with two new sites nearby (in the one-to-two splitting case) with certain probability to migrate to, like in quantum mechanics. For example, if there is a significant molar volume difference between the product and matrix phases, the number of lattice sites before and after the transformation might be different. In order to accommodate the molar volume change, creation or annihilation of lattice sites becomes necessary, such as the formation of a large amount of excess vacancies observed in the ordering processes of Ni₃Fe and Cu₃Au [19]. “Superabundant vacancies” is therefore one way to reconcile the conservation of mass with the non-conservation of sites when the phase boundary sweeps across. Crystal displacements $\mathbf{u}(\mathbf{r})$ like in the Kirkendall effect [20] or elastic strain $\epsilon(\mathbf{r})$ (and stress $\sigma(\mathbf{r})$) are other ways of accommodating the large molar volume change.

In this paper, combining the phase field crystal (PFC) method [21–24], theory of crystallography [6,8,11,14] and nudged elastic band method (NEB) [25,26], we investigate the atomistic mechanisms of interface migration during a model diffusional phase transformation from hexagon lattice to square lattice with large molar volume differences. Relying on a properly time-averaged atomic density field [27], PFC can capture lattice site movements at diffusional time scale [28–30]. Theories of O-line, SL and coincidence site lattice (CSL) are used to analyze the structure of interfaces. In order to obtain a complete picture of the phase transformation including nucleation and growth, a new approach capable of capturing the critical nucleus configuration with atomic resolution is developed by combining the free-end NEB algorithm [25,26] with PFC energetics.

Note that as a general phenomenon of pattern formation and evolution, the square to hexagon transformation has been studied extensively in the literature [31–37], but the focus of the current study is completely different, with particular emphases on (i) when the orientation relationship between the parent and product phases is formed (e.g., during nucleation or growth), (ii) detailed atomic arrangement at the interface including steps, terraces and dislocation structures, (iii) how a high-index terrace-step interface moves (e.g., via structural ledge or ML), (iv) whether the commonly assumed one-to-one lattice site correspondence holds, and (v) how the large volume change is accommodated.

2. Methods

2.1. Phase field crystal model

The PFC model uses the Helmholtz free energy to describe an inhomogeneous system in reference to a homogenous liquid state of density ρ_L and the dimensionless form of the Helmholtz free energy is given as [23],

$$F_{PFC} = \int \left\{ \left[\frac{n(\mathbf{r})^2}{2} - \eta \frac{n(\mathbf{r})^3}{6} + \nu \frac{n(\mathbf{r})^4}{12} \right] - \left[\frac{1}{2} n(\mathbf{r}) \int C_2(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}') d\mathbf{r}' \right] \right\} d\mathbf{r} \quad (1)$$

where $n(\mathbf{r}) \equiv \rho(\mathbf{r})/\rho_L - 1$ is the dimensionless number density field. Parameters η and ν are the expansion coefficients and they are assumed unity (i.e., $\eta = \nu = 1$) in the current study. The direct pair correlation function $C_2(|\mathbf{r} - \mathbf{r}'|)$ is constructed by the envelope of two Gaussian peaks in the reciprocal space as [23],

$$\widehat{C}_2(|\mathbf{k}|) = \begin{cases} e^{-\frac{\tau^2 k_1^2}{2\rho_1 \beta_1}} e^{-\frac{(|\mathbf{k} - \mathbf{k}_1|)^2}{2\alpha_1^2}}, & |\mathbf{k}| \leq k_c \\ e^{-\frac{\tau^2 k_2^2}{2\rho_2 \beta_2}} e^{-\frac{(|\mathbf{k} - \mathbf{k}_2|)^2}{2\alpha_2^2}}, & |\mathbf{k}| > k_c \end{cases} \quad (2)$$

where k_c is the intersection point of the two peaks. The wave vector $k_1 = 2\pi$, $k_2 = \sqrt{2}k_1$, and other symmetry-related parameters ρ_i and β_i ($i = 1, 2$) are determined in accordance with a square lattice [23]. Depending on temperature T , the contribution from different peaks varies, thus leading to the formation of a hexagon phase at high temperature where the first peak dominates and a square phase at low temperature where both peaks play a role.

The phase diagram is determined by common tangent construction on the free energy curves of different phases at each temperature. In particular, the free energy of the liquid phase is calculated by imposing a constant density field with $n_{liq} = \bar{n}$. For the solid phases, the density field for the square lattice is represented using a two-mode approximation,

$$n_{sq} = \bar{n} + 2A_{sq}^1 [\cos(k_{sq}x) + \cos(k_{sq}y)] + 4A_{sq}^2 \cos(k_{sq}x) \cos(k_{sq}y) \quad (3)$$

and the density field for the hexagon lattice is represented by a one-mode approximation,

$$n_{hex} = \bar{n} + 4A_{hex} \cos(k_{hex}x) \cos(k_{hex}y/\sqrt{3}) - 2A_{hex} \cos(2k_{hex}y/\sqrt{3}) \quad (4)$$

where the wave vectors $k_{sq} = k_1$ and $k_{hex} = 2/\sqrt{3}k_1$. The amplitudes A_{sq}^1 , A_{sq}^2 and A_{hex} can be obtained by free energy minimization. Analytic expressions of the free energy densities for all the phases are presented in Appendix A, and the resultant phase diagram is shown in Fig. 1.

The transformation and interface migration are characterized by the time-evolution of the atomic number density field $n(\mathbf{r})$ that is governed by the conserved equation of motion,

$$\frac{\partial n}{\partial t} = \nabla^2 \frac{\delta F_{PFC}}{\delta n} + \xi \quad (5)$$

where ξ represents a colored Gaussian noise described by

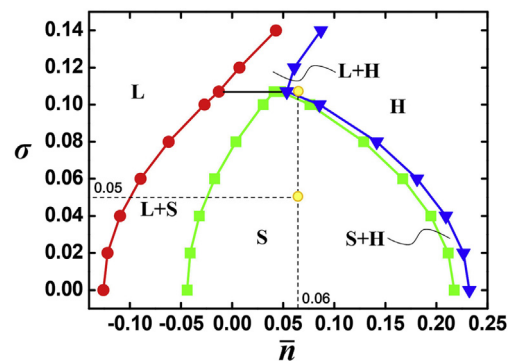


Fig. 1. Phase diagram constructed by using the free energy model presented in the text, showing phase equilibria among the liquid (L), square (S), and hexagon (H) phases. The yellow circles denote the system and temperatures considered in the simulations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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