Contents lists available at ScienceDirect

Computational Materials Science

Phase-field simulation of austenite growth behavior: Insights into the austenite memory phenomenon

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ABSTRACT

Austenite memory phenomenon impedes the application of reverse austenitic transformation to refine grains in steels. In this work, a phase-field model is employed to understand the austenite memory mechanism in terms of austenite growth behaviors under different mechanical boundary conditions, using the Fe–23Ni (wt.%) alloy as an example. The effect of defects formed during martensitic transformation on reverse austenitic transformation is considered by introducing a "stored energy" term. Kurdjumov–Sachs (K–S) variants of each phase are divided into three groups based on the crystallography analysis. Results show that different combinations of mechanical boundary conditions during the austenite → martensite → austenite transformation cycle have different effects on the austenite memory phenomenon, which can be attributed to the minimization of strain energy induced by phase transformations, as well as the inhomogeneous distribution of stored energy (energy of defects).

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1. Introduction

Owing to their excellent mechanical properties and low cost, martensitic stainless steels have wide applications in industry [1]. The increasing demand for high-quality steels continuously drives investigations on stainless steels with better mechanical properties. There are several methods to enhance the mechanical properties of steels, among which grain refinement is one of the most effective ways to improve both strength and toughness [2,3]. Grain refinement is usually realized by phase transformations and plastic deformations [4,5]. With severe plastic deformation, it is even possible to obtain ultrafine grain structures [6].

However, for some applications, like the steam turbine rotors used in power plants, plastic deformation is unavailable owing to the large component size and complicated shape [7]. In which case, reverse austenitic transformation could be an effective grain refinement technique [8,9]. Reverse austenitic transformations usually follow certain orientation relationships, *e.g.*, the

Kurdjumov–Sachs (K–S) relation [16,41]. In the case of high alloy martensitic stainless steels, austenite nucleates with an identical crystallographic orientation in one grain and grows into a coarse austenite grain that is crystallographically similar to original austenite grain. This is known as "austenite memory" phenomenon which is detrimental to the grain refinement [10–15]. In order to achieve refined grains in high alloy steels during reverse transformations, it is crucial to understand the underlying mechanisms of the "austenite memory" phenomenon.

Numerous efforts have been made to explain the mechanism behind the "austenite memory" phenomenon [10–20]. For example, it was proposed that coherent acicular-shaped reverse austenite particles form at the martensite lath boundaries with the K–S orientation relationship, leading to the reappearance of prior austenite [19,20]. However, since the reverse transformation occurs at high temperature, the experimental techniques (like TEM, EBSD, XRD, *etc.*) offer limited insight into the mechanism of the transformation, it has to be observed indirectly by analyzing the quenched microstructures. Undoubtedly, the quenching process affects the uncovering of "austenite memory".

On the other hand, by formulating the thermodynamic functions and transformation kinetic equations of both austenites and martensites at high temperatures, the high-temperature phase transformation and microstructure evolution processes can be predicted using theoretical methods. Among the existing theoretical

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studies [21–33], the phase-field approach stands out as a powerful computational method for modeling phase transformation and microstructure evolution at the meso-scale [25–33]. Moreover, it has been widely used to study martensitic transformations [26,28–35]. With the Bain transformation mechanism and group-subgroup symmetry relationship between the cubic austenite and the tetragonal martensite, three order parameters are usually used to express the crystallographically equivalent Bain variants; morphology and kinetics of martensitic transformations, for instance, habit planes of martensites [30], effect of applied stress or strain on martensitic transformations [31], *etc.*, have been systematically studied.

However, there has been much less focus on the reverse transformation [34]. Reverse austenitic transformations can take place diffusionally due to the high temperature whereas under certain conditions (fast heating rate, high content of austenite stabilizer alloy element such as Ni and low C content), it would appear in a displacive manner [10,13,14]. Therefore, to understand the reverse transformation mechanism, we first investigated the crystallography of both martensitic and austenitic transformations. We then performed phase-field simulations of $\gamma \rightarrow \alpha \rightarrow \gamma$ phase transformation cycle to understand the influence of initial states and mechanical boundary conditions of martensite on reverse transformation and to figure out the austenite growth behaviors that are related to the "austenite memory" phenomenon. Especially, the roles of phase-transformation-induced strain energy for both transformations and the energy of defects are carefully studied, owing to their influence on nucleation site and growth behavior of reverse austenitic transformation [53]. The distribution and amount of these energy contributions under different mechanical boundary conditions are also investigated and related to the "austenite memory" phenomenon through their effects on the nucleation and growth behavior of reverse austenite. The phase transformation cycle in Fe–23Ni alloy is taken as an example, in which the reverse austenitic transformation takes place displacively [37].

2. Crystallography of $\gamma \rightarrow \alpha \rightarrow \gamma$ transformations

Both of the martensitic and reverse austenitic transformations proceed diffusionlessly under specific heat treatment conditions in Fe–23Ni [37,38]. The austenite, or γ phase, has a face-centered cubic (*fcc*) structure while the martensite, or α phase, is considered to be with a body-centered cubic (*bcc*) structure. The K–S or, less commonly, other orientation relationships show the crystallographic characteristics of coherent transformation [39,40]. The K–S orientation relationship is expressed as $\{111\}_\gamma // \{110\}_\alpha$ and $\langle 110 \rangle_\gamma // \langle 111 \rangle_\alpha$. The crystallographic correspondences for both transformations are shown in Fig. 1. As illustrated in the figure, for the martensitic transformation, each $\{111\}_\gamma$ plane defines six crystallographically equivalent variants, resulting in 24 distinguishable K–S variants of the martensite. In addition, the transfer of stacking model from …ABCABC… of *fcc* to …ABAB… of *bcc* is shown in Fig. 2. For the reverse austenitic transformation, four variants with different orientations are possible when the plane is fixed as $(011)_\alpha$. Because the martensite phase has six crystallographically equivalent $\{110\}_\alpha$ planes, there are also 24 variants of the austenite available during reverse austenitic transformation [16]. The transfer of stacking model from …ABAB… of *bcc* to …ABCABC… of *fcc* is shown in Fig. 3.

For simplicity, the variants for each transformation can be divided into three groups based on the analysis about the deformation tensors of both transformations. These groups are associated with a particular variant of the "Bain strain" that provides the simplest connection between the austenitic and martensitic structures [16,41,42]. Details are provided in Supplementary materials. In an existing simulation [34] on reverse austenitic transformation, the crystal structure of martensite was considered to be tetragonal; therefore, Bain strain was only applied to martensitic transformation, while the formation of reverse austenite was equivalent to the disappearance of the martensite. In addition, the effects of transformation-induced strain energy and defect energy on reverse transformations were not considered. However, for *bcc* martensites, due to the more complicated orientation relationship and the significant effects of strain energy and defect energy, the model in [34] could not reflect the crystallographic and microstructural features. Therefore, in the present work, to determine the effect of reverse austenitic transformation induced strain energy, Bain strain is also considered for modeling the reverse austenitic transformation.

Eqs. (S8) and (S13), and those listed in St1 and St2 (see Supplementary materials) show that the deformation matrices for austenite to martensite transformation contain a major part of Bain deformation, accompanied with a small rotation. The Bain deformation for austenite to martensite transformation is characterized by the compressive axis [41], lying along one of the three cubic axes of austenite, and by which we group those K–S variants of martensite into three kinds. Similarly, the Bain deformation of martensite to austenite transformation is characterized by the tensile axis. It lies along one of the three cubic axes of martensite. We label the K–S variants of both martensite and reverse austenite by their deformation axes $\{xyz\}$, as shown in Tables 1 and 2. With the strain of each variant calculated in Section 3.2, each group of variants can be represented by the same Bain strain tensor. Thus, we use three order parameters in the phase-field model to represent three groups of variants: $\{\eta_1, \eta_2, \eta_3\}$ for the martensite variant groups of martensitic transformation; $\{\phi_1, \phi_2, \phi_3\}$ for the austenite variant groups of reverse austenitic transformation.

3. Phase-field model

The $\gamma \rightarrow \alpha \rightarrow \gamma$ transformation cycle of Fe–23Ni alloy includes quenching and the subsequent reheating process. The microstructure evolution during cycling is governed by the total free energy minimization within the system. The total free energy includes the Gibbs free energy of the two phases, the interfacial energy at phase boundaries and variants boundaries, as well as the elastic strain energy due to the structural change. The sets of order parameters, $\{\eta_1, \eta_2, \eta_3\}$ and $\{\phi_1, \phi_2, \phi_3\}$, represent different variants of α and γ phases, respectively. For the martensitic transformation, $\eta_i = 0$ represents the austenite phase and $\eta_i = 1$ represents the martensite phase. For the reverse austenitic transformation, $\phi_i = 0$ represents the martensite phase and $\phi_i = 1$ represents the austenite phase. Then the total free energy of the system is given as [27,43,44]:

$$G_{total} = \int \left[G_V^{local}(\{\eta_i\}, \{\phi_j\}, T) + G_V^{grad}(\{\nabla \eta_i\}, \{\nabla \phi_j\}) + G_V^{el} \right] dV \quad (1)$$

where $G_V^{local}(\{\eta_i\}, \{\phi_j\}, T)$ is the temperature dependent local free energy density, $G_V^{grad}(\{\nabla \eta_i\}, \{\nabla \phi_j\})$ is the gradient energy density due to the inhomogeneity of order parameters at boundaries. G_V^{el} stands for the density of phase-transformation-induced strain energy.

3.1. Local free energy

The driving force for the displacive transformation cycle is the bulk energy difference between the parent phase and the new phase. We employ the Landau-type free energy to describe thermodynamics of the transformation, with its coefficients determined by the relevant physical variables of the specific system,