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Grain size dependence of the martensite morphology – A phase-field study

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ABSTRACT

The two-dimensional elastic phase-field simulation is applied to study the grain size effect on martensite morphology with Fe–31at.%Ni alloy as the prototype material. Martensitic transformations containing one or two variants are simulated in the single-crystal and poly-crystal models, and the morphologies related to different models and their grain size dependences are displayed. The simulated results show that the accommodation ability to the martensitic shape changes plays an important role in the grain size effect of martensite morphology. Although the transformation strains in a grain can be relaxed to surrounding grains, effective self-accommodations of different variants can only proceed in the individual grain. The size of martensitic domains proportionally decreases with grain size reduction, due to harder relaxation ability induced by the grain boundaries. The decreasing of the width for multi-variant domains can be realized by decreasing the number of sub-domain variant plates without decreasing the width of the plates.

1. Introduction

Martensitic transformation (MT) still shows great importance in scientific research nowadays, because it refers to the mechanical properties and physical effects of new structural and functional materials, such as TRIP [1] and TWIP [2] effects of advanced automobile steels, magnetic-field-induced shape memory effect of shape memory alloys (SMAs) [3], high damping properties of Mn-based alloys [4] and huge superelasticity of ferrous alloys [5]. MT is a shear-dominant, lattice-distortive and diffusionless transformation occurring by nucleation and growth [6]. Internal stresses are produced because of the crystal lattice misfit between austenite and martensite. As the transformation-induced strain energy is comparable with or even larger than the chemical energy reduction of MT [7], the strain energy dominates the kinetics of MT and the martensite morphology [6]. MT usually produces several crystallographically equivalent variants with different orientations within an individual parent grain and the formation of self-accommodated multi-variant microstructure is driven by elastic energy reduction. The morphologies of martensite are different from different materials [8], such as lath shape [9], lenticular shape [10] and thin plate [11] in ferrous alloys. Complex microstructures also exist, such as lath-block-packet hierarchical structure in steels [12] and V-shaped morphology in NiTi alloy [13]. The evolution of martensitic microstructure can be observed using in situ confocal laser microscopy [14] and in situ scanning electron microscopy [15].

Reducing the grain size (GS) can improve the mechanical properties of materials [16] and will influence the characteristics of MT (*e.g.* MT start temperature [17]). In the meantime, the morphology features of MT also change with GS reduction. The grain size effects (GSEs) in lath martensitic steels have been deeply investigated [16–19] by EBSD and the microstructure and strength model has been established [12]. The experimental results show that with the decreasing of GS, the sizes of the packet (laths with the same habit plane) and block (laths of two specific variants group) decrease, but the lath width changes only slightly. The lath size is thought to be controlled by the Cottrell atmospheres and carbon segregation [12]. The three-dimensional (3D) morphology of the packets and blocks with different GSs can also be obtained by local crystallographical analyses [20]. Ultra-grain refinement of austenite makes the occurrence of multi-variant transformation difficult and leads to the suppression of MT in metastable austenite [17]. The spatial restriction effect [16] was proposed, which explains that several variants cannot be simultaneously formed due to space shortage, and he mechanical stability of austenite is independent of GS. Shibata et al. [21] found that the martensite plate size decreases with decreasing the GS in lenticular martensitic steel. Roca et al. [22] found a linear relationship between the aver-

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age plate width and GS in CuNiAl alloy, the interface energy density (act as transformation energy barrier) as a function of GS has been assessed. Martensitic microstructure would influence the mechanical properties, such as that the phase boundaries (lath and block boundaries) are effective barriers for dislocation motion, thus block boundary strengthening exists [12], and the transformation twin density has an effect on Hall–Petch relationship [23]. The GSE in nanocrystalline SMAs was simulated using the Ginzburg–Landau theory, which proposed that the inhibition effect of MT in grain boundary regions also has a strong influence on MT inside grains [24].

The phase-field microelasticity theory [25], which is based on the Time-dependent Ginzburg–Landau (TDGL) phase transition theory integrated with the Khachaturyan–Shatalov (KS) theory of elastic energy, can be used to simulate the MT process and predict the martensite morphology. The problem of transformation-induced stress can be easily solved by the KS theory, according to which the strain energy of an arbitrary coherent multiphase system can be represented in a closed form for the homogeneous modulus case [26]. Several phase-field models of MT have been developed, such as the 3D single-crystal model [25], poly-crystal model [27], external loading model [28], heterogeneous nucleation model [7] and elastoplastic model [29].

In this paper, two-dimensional (2D) elastic phase-field models are employed to study the GSEs on martensite morphology by changing the GS of the simulated system. Although little effective phase-filed model currently exists to simulate the lath martensite in steels, the present 2D model can simulate the self-accommodations of variants, and the stress relaxation changing with GS is well considered. To systematically study the GSE in different materials, the single-variant (1V) and two-variant (2V) transformations are simulated. The single-crystal (SC) and poly-crystal (PC) models are used to investigate the effect of grain boundary on MT and the stress relaxation feature in polycrystals.

2. Polycrystalline phase-field model of martensitic transformation

The phase-field model used in this paper is based on the models proposed by Wang et al. [25] and Artemev et al. [30]. As a popular approach, similar models can be found in the literature [29,31,32]. An overview of this model is presented in this section.

For the phase-field model of MT, the structural order parameters are required to simulate the structural change of a material system. In the polycrystalline phase-field model, the number of order parameters (η) is $n \times m$ where n is the number of variants in an austenite grain and m the number of grains [29]. To simplify the phase-field calculation, n equals 2 for the fcc-to-bcc MT in 2D model. The total free energy of the system G, which is the function of order parameters, is the sum of the chemical free energy, G_{ch}, the gradient energy G_{gr} and the elastic strain energy G_{el}, and is given by

$$G = G_{ch} + G_{gr} + G_{el} \tag{1}$$

The chemical energy is expressed as a Landau polynomial:

$$G_{ch} = \int_V \sum_{\alpha=1}^{m} \left[\frac{A}{2}(\eta_1(\alpha)^2 + \eta_2(\alpha)^2) - \frac{B}{3}(\eta_1(\alpha)^3 + \eta_2(\alpha)^3) + \frac{C}{4}(\eta_1(\alpha)^2 + \eta_2(\alpha)^2)^2\right] dV \tag{2}$$

where the coefficients are $A = 32\Delta G^*$, $B = 3A - 12\Delta G_m$ and $C = 2A - 12\Delta G_m$ [33]. ΔG^* is the Gibbs energy barrier and ΔG_m is the free energy difference between the parent and martensite phases, which is related with the undercooling:

$$\Delta G_m = Q(T - T_0)/T_0 \tag{3}$$

where Q is the latent heat for MT and T_0 is the thermodynamic equilibrium temperature.

The gradient energy relates to the interfacial energy and can be expressed as:

$$G_{gr} = \int_V \frac{\beta}{2} \sum_{\alpha=1}^{m} [(\nabla\eta_1(\alpha))^2 + (\nabla\eta_2(\alpha))^2] dV \tag{4}$$

where β is the gradient energy coefficient.

The elastic energy is calculated by the micromechanical approach as:

$$G_{el} = \int_V \frac{1}{2} C_{ijkl} \varepsilon_{ij}^{el} \varepsilon_{kl}^{el} dV \tag{5}$$

where C_{ijkl} is the elastic coefficient tensor and ε_{ij}^{el} the elastic strain tensor. The transformation strain produced by MT is relaxed and the distribution of the relaxed strain is given by solving the mechanical equilibrium condition. According to the theory of microelasticity, the elastic strain is defined as the difference between the total strain, ε_{ij}^{t}, and the total eigenstrain, ε_{ij}^{0}, and is expressed as:

$$\varepsilon_{ij}^{el} = \varepsilon_{ij}^{t} - \varepsilon_{ij}^{0} = \bar{\varepsilon}_{ij}^{t} + \delta\varepsilon_{ij}^{t} - \varepsilon_{ij}^{0} \tag{6}$$

The total strain is defined as the sum of the homogeneous strain, $\bar{\varepsilon}_{ij}^{t}$, and the heterogeneous strain, $\delta\varepsilon_{ij}^{t}$. The eigenstrain is the summation of transformation strain and defect strain, and can be written as:

$$\left[\varepsilon_{ij}^{000}(1)\right] = \begin{pmatrix} \varepsilon_3 & 0 \\ 0 & \varepsilon_1 \end{pmatrix}, \quad \left[\varepsilon_{ij}^{000}(2)\right] = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_3 \end{pmatrix} \tag{7}$$

$$\varepsilon_{ij}^{00}(p,\alpha) = R_{ik}^{\alpha} R_{jl}^{\alpha} \varepsilon_{kl}^{000} \tag{8}$$

$$\varepsilon_{ij}^{0} = \left[\sum_{\alpha=1}^{m}\sum_{p=1}^{2} \varepsilon_{ij}^{00}(p,\alpha)\lambda(\eta_p(\alpha))\right] + \varepsilon_{ij}^{de} \tag{9}$$

where ε_{ij}^{000} is the transformation strain of martensitic variant, R_{ij}^{α} is the rotation tensor of the grain α from the local to global coordinate system, ε_{ij}^{de} is the defect strain. The polycrystal structure is generated by the Voronoi tessellations under a periodical boundary constraint, and the grains are randomly oriented [34]. Unlike other works [32,35], we have no special treatment of the grain boundaries. To avoid the unphysical values of the order parameter driven by strain energy reduction, $\lambda(\eta_p(\alpha))$ is given by [32]:

$$\lambda(\eta_p(\alpha)) = \begin{cases} \eta_p(\alpha) & (when\ \eta_p(\alpha) \geqslant 0) \\ \eta_p^2(\alpha) & (when\ \eta_p(\alpha) < 0) \end{cases} \tag{10}$$

$\bar{\varepsilon}_{ij}^{t}$ relates to the boundary conditions and is given as:

$$\bar{\varepsilon}_{ij}^{t} = \begin{cases} \bar{\varepsilon}_{ij} & (for\ strain - controlled\ condition) \\ S_{ijkl}\sigma_{kl}^{appl} + \bar{\varepsilon}_{ij}^{0} & (for\ stress - controlled\ condition) \end{cases} \tag{11}$$

where $\bar{\varepsilon}_{ij}$ and σ_{kl}^{appl} are the given strain and stress conditions respectively, S_{ijkl} is the compliance coefficient tensor, and $\bar{\varepsilon}_{ij}^{0}$ is the homogeneous eigenstrain. The heterogeneous strain is given by solving the mechanical equilibrium equation [29], as:

$$\delta\varepsilon_{ij}^{t} = \frac{1}{(2\pi)^2} \int_k \frac{1}{2} [e_i\Omega_{mj}(\boldsymbol{e}) + e_j\Omega_{mi}(\boldsymbol{e})] \hat{\sigma}_{mn}^{0}(\boldsymbol{k}) e_n \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) d\boldsymbol{k} \tag{12}$$

where $\boldsymbol{k}$ indicates the reciprocal space vector, and $\boldsymbol{e} = \boldsymbol{k}/|\boldsymbol{k}|$ is the unit vector along the $\boldsymbol{k}$ direction. $\Omega_{il}(\boldsymbol{e})$ is the Green function tensor inverse to the tensor $\Omega_{il}^{-1}(\boldsymbol{e}) = C_{ijkl}e_j e_k$.

The time evolution of the order parameters is described by the following TDGL equation: