



Phase-field modeling of austenite grain size effect on martensitic transformation in stainless steels

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ABSTRACT

A 2D elastoplastic phase-field model is developed to study the effect of prior austenite grain size on martensitic microstructure evolution in stainless steel. The effects of strain hardening and strengthening by grain size reduction (Hall-Petch effect) have been included in the model. The results show that martensite units form in different packets oriented in different crystallographic directions in simulated coarse grains, whereas uni-directional martensitic growth is observed in simulated fine grains. The number of packets and martensite block width increase with increasing grain size. With a decreasing grain size the martensitic transformation start temperature decreases, indicating strengthening of austenite. Once the transformation is initiated, at a given time, simulated fine grains give rise to higher volume fraction of martensite compared to simulated coarse grains. The von Mises equivalent stress and plastic strain are large in simulated fine grains compared to those in simulated coarse grains. The simulation results are in good agreement with experimental results.

1. Introduction

Steels are widely used as structural materials in a wide variety of industries, such as construction, automobile and aerospace. Due to the strong demand to reduce the weight of the structures with improved mechanical properties, such as strength and ductility, novel steels and steel processing methods are being developed. The new phases and the subsequent microstructure that form due to the phase transformations during the materials processing stages govern the mechanical properties. Hence the phase transformations need to be thoroughly understood in order to tailor the microstructure and mechanical properties. It is also essential to study the relationship between phase transformations and the different strengthening mechanisms, e.g. grain refinement, precipitation hardening.

Martensitic transformation (MT) is an important phase transformation that can occur in steels and many other engineering materials, such as Zr, Ti, shape memory alloys. MT in steels is a diffusionless solid state phase transformation of ductile austenite (FCC) into a high strength phase, known as martensite (BCC or BCT). Martensite can form athermally, i.e. during rapid quenching; isothermally by holding the steel close to the transformation temperature (M_s); stress-assisted, i.e. by application of stress; strain-induced, i.e. by large deformation. MT can induce internal stresses and strains in the material and when these stresses exceed the yield limit, the material undergoes plastic deformation. Therefore, MT can induce dislocations in the material and

can cause transformation induced plasticity (TRIP) effect, which can be utilized in enhancing the mechanical properties of the materials.

Martensite can form in the shape of laths or plates [1–3]. The two solid phases, austenite and martensite, are coherent and are governed by orientation relationships (OR). Based on the crystallography of the FCC–BCC phase transformation, Bain OR predicts the formation of 3 different martensite variants, Nishiyama-Wasserman OR predicts 12 variants and Kurdjumov-Sachs OR predicts 24 variants [1,4,5]. In case of lath martensite, different variants can form in groups and a hierarchical structure is observed in the experiments [1]. Martensite laths formed in an austenite grain can be grouped into several packets and within each packet there can be several blocks and sub-blocks. A group of laths that form along the same habit plane belong to the same packet. In a packet, two groups of laths with a small misorientation (10°) are collectively considered as a block, whereas each group of laths is considered as a sub-block [1,6]. Morito et al. have observed in their experiments on carbon steels that lath martensite forms in four packets, which contain 3 blocks each and within each block there are two sub-blocks. Since the packet and block boundaries are high angle boundaries, they can act as effective barriers for dislocation motion and hence can affect the strength and toughness of steels [6]. The yield strength increases with decreasing packet size in carbon steels [7].

On annealing, martensite can revert to austenite either in a martensitic (diffusionless) manner or through a diffusion-controlled mechanism. Reversed austenite formed in martensitic manner inherits

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dislocations from martensite and is beneficial in enhancing the mechanical properties [8]. Moreover, reversed austenite inherits the lath-like structure from martensite, which leads to reduction in austenite grain size [9].

Grain refinement [8–12] and grain boundary strengthening [13] are reported to be effective strengthening mechanisms. Several studies have shown that martensitic transformation and reverse phase transformation of martensite to austenite can be utilized to design fine grain and ultra-fine grained steels [9,10,12]. Reduction of grain size has a considerable effect on martensite formation. Grain refinement can lead to reduction of M_s temperature [14], increased retained austenite [15,16] and dislocation density [17]. Grain refinement can lead to decrease in block width and packet size, although the change in lath width is small [6]. As the grain refinement leads to a decreased tendency to form martensite and can sometimes inhibit the transformation completely, it is difficult to study by experiments the effect of austenite grain size on M_s temperature, morphology and mechanical properties [18]. Under extreme thermo-mechanical service conditions, martensitic transformation could occur in the stable fine and ultra-fine grained austenitic steels and hence this aspect needs to be accounted for during material design. Therefore, it is essential to understand the behavior of fine and ultra fine grains during martensitic transformation using theoretical approaches.

Due to its technical and scientific importance, MT has been thoroughly studied using mathematical models and experiments. The interaction between phase transformation, twinning and plasticity has been studied using phenomenological models [19,20] and constitutive models based on continuum mechanics approaches [21–29]. The evolution of plastic strains due to martensitic transformation was also modeled [23,25,26,28]. The phase-field approach [30–32] has been successfully applied to study martensitic transformation [33–46] as well as the reversion of martensite to austenite by shear mechanism [47]. The evolution of martensitic microstructure and dislocations using the phase-field approach has been studied [48,49]. The phase-field approach was also applied to study the effect of austenite grain size on martensite formation in Fe-Ni alloy [40] and shape memory alloy [42]. However, the effect of grain size on martensitic transformation coupled with plasticity has not been studied using the phase-field method. In the present work, 2D phase-field model coupled with continuum plasticity is used to study the effect of grain size on martensite formation (FCC to BCC) in stainless steel [33]. As the focus of the present work is to study the evolution of martensite morphology at the microscopic level, continuum plasticity is considered instead of modeling the dislocations at nanoscale level as in Refs. [48,49]. The effects of strain hardening and Hall-Petch effect (effect of grain size on yield strength) are included in the model. The results show the microstructure evolution along with the formation of different packets. The average block width as well as M_s temperature for different grain sizes are also predicted. The present work also discusses the effect of grain refinement on the chemical driving forces for initiation and progression of the transformation.

2. Phase-field model

The phase-field equation governing the microstructure evolution is given by:

$$\frac{\partial \eta_p}{\partial t} = - \sum_{q=1}^{q=v} L_{pq} \frac{\delta G}{\delta \eta_q} \quad (1a)$$

and

$$\frac{\delta G}{\delta \eta_p} = \frac{\partial G_v}{\partial \eta_p} - \nabla \cdot (\boldsymbol{\beta} \cdot \nabla \eta_p) \quad (1b)$$

where G is the Gibbs energy of the system, η_p is the phase field variable that tracks the evolution of martensite, v is the total number of

martensite variants, $\boldsymbol{\beta}$ is gradient coefficient and L_{pq} is a matrix of kinetic parameters.

Martensite variants (laths), which form in 24 different crystallographic orientations, can be grouped into three basic variants known as Bain variants [4,5]. Bain variants are obtained when the cubic crystal is compressed along one of the three orthogonal axes, i.e. X, Y and Z, and is elongated along the other two axes. This gives rise to three compression possibilities, i.e. along X, Y and Z, and hence three Bain variants can be obtained [5]. In the present two dimensional (2D) case, two phase-field variables (η_1, η_2) that correspond to the two Bain variants with compression along X- and Y-axes, respectively are considered.

The Gibbs energy of a system undergoing athermal martensitic transformation can be expressed as:

$$G = \int_V (G_v^{chem} + G_v^{grad} + G_v^{el}) dV \quad (2)$$

where G_v^{chem} corresponds to the chemical part of the Gibbs energy density, G_v^{grad} is the gradient energy term, G_v^{el} is the strain energy density.

G_v^{chem} is expressed as a Landau-type polynomial [33,34]:

$$G_v^{chem}(\eta_1, \eta_2) = \frac{1}{V_m} \left[\frac{1}{2} A (\eta_1^2 + \eta_2^2) - \frac{1}{3} B (\eta_1^3 + \eta_2^3) + \frac{1}{4} C (\eta_1^2 + \eta_2^2)^2 \right] \quad (3)$$

where V_m is the molar volume and the coefficients A, B, C are expressed in terms of Gibbs energy barrier (ΔG^*) and the driving force (ΔG_m) as: $A = 32\Delta G^*$, $B = (3A - 12\Delta G_m)$, $C = (2A - 12\Delta G_m)$ and $\Delta G^* = \frac{V_m \beta}{2\delta^2}$ [33]. δ is the physical interface thickness, V_m is molar volume and β is gradient coefficient as explained below.

G_v^{grad} is expressed as [33,34]:

$$G_v^{grad} = \frac{1}{2} \sum_{p=1}^{p=v} \beta_{ij}(p) \frac{\partial \eta_p}{\partial r_i} \frac{\partial \eta_p}{\partial r_j} \quad (4)$$

where $\mathbf{r}(x, y)$ is the position vector expressed in Cartesian coordinates. The term on the right hand side is same as the second term in Eq. (1b). β_{ij} is the gradient coefficient matrix expressed in terms of the interfacial energy (γ), molar volume and the Gibbs energy barrier. In this work isotropic interfacial properties are considered and it is also assumed that both austenite-martensite and martensite-martensite interfaces have same interfacial properties. Hence $\beta_{ij}(p) = \beta = \frac{9\gamma^2 V_m}{16\Delta G^*}$.

G_v^{el} can be expressed as [33,34,37]:

$$G_v^{el} = \int_{\epsilon_{ij}^0(\mathbf{r})}^{\epsilon_{ij}^{ej}(\mathbf{r})} \sigma_{ij}(\mathbf{r}) d\epsilon_{ij}(\mathbf{r}) = \int_{\epsilon_{ij}^0(\mathbf{r})}^{\epsilon_{ij}^{ej}(\mathbf{r})} c_{ijkl} (\epsilon_{kl}(\mathbf{r}) - \epsilon_{kl}^0(\mathbf{r}) - \epsilon_{kl}^{pl}(\mathbf{r})) d\epsilon_{ij}(\mathbf{r}) \quad (5)$$

where $\sigma_{ij}(\mathbf{r})$ is the stress, c_{ijkl} is the tensor of elastic constants, $\epsilon_{ij}(\mathbf{r})$ is the total strain, $\epsilon_{kl}^{pl}(\mathbf{r})$ is the plastic strain. Small strain theory is assumed in the present work and therefore $\epsilon_{ij}(\mathbf{r})$ can be expressed as:

$\epsilon_{ij}(\mathbf{r}) = \frac{1}{2} \left(\frac{\partial u_i(\mathbf{r})}{\partial r_j} + \frac{\partial u_j(\mathbf{r})}{\partial r_i} \right)$, where $\mathbf{u}(\mathbf{r})$ is the local displacement vector. Earlier works have considered finite strain theory [23,28,35,48,49]. $\epsilon_{ij}^0(\mathbf{r})$ is the stress-free transformation strain, given by:

$$\epsilon_{ij}^0(\mathbf{r}) = \sum_{p=1}^{p=2} \eta_p(\mathbf{r}) \epsilon_{ij}^{00}(p) \quad (6)$$

where $\epsilon_{ij}^{00}(p)$ are the Bain strain tensors that govern the two phase-field variables (η_1, η_2) and are given by:

$$\epsilon_{ij}^{00}(1) = \begin{bmatrix} \epsilon_3 & 0 \\ 0 & \epsilon_1 \end{bmatrix}, \quad \epsilon_{ij}^{00}(2) = \begin{bmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_3 \end{bmatrix} \quad (7)$$

where ϵ_3 and ϵ_1 are compressive and tensile transformation strains, respectively.

The material undergoes plastic deformation when the internal stress ($\sigma_{ij}(\mathbf{r})$) exceeds the yield limit. In this work von Mises yield criterion is

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