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Modelling the microstructure of martensitic steels

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ABSTRACT

A method based on the kinetics of crystal growth has been developed and applied to the computation of three-dimensional microstructure in austenite–martensite steels. The detailed crystallography of the transformation is used to model a realistic martensitic microstructure during the transformation without an external system of stresses. The interaction energy based on the plastic work model is taken into account to compute the variant selection in an austenitic stainless steel and formation of martensite under externally applied stress.

1. Introduction

Martensitic transformation in steels normally occurs in an athermal manner, during cooling in a temperature range that can be accurately determined for different steels. When the martensitic transformation occurs, the austenite transforms to martensite through a shape change which is an invariant plane-strain (IPS) [1]. The rate of transformation can reach the speed of sound in metals. Martensite forms in 24 crystallographic variants in each austenite grain. The chemical driving force ΔG which depends on the composition and transformation temperature applies to all the variants equally. Generally, each variant has an equal chance of existence. However, since martensitic transformation is a deformation, an externally applied stress will favour those variants that comply with the stress and as a result variant selection occurs [2].

Consider an austenite grain with sample axes which are defined by an orthonormal set of basis vectors $[\gamma, a_1]$, $[\gamma, a_2]$, and $[\gamma, a_3]$. The matrix notation used here is due to Bowles and MacKenzie [27]. The real basis is referred to as 'γ' and its corresponding reciprocal basis is defined using the basis symbol 'γ^*'. The IPS can be represented by a 3×3 matrix $(\gamma\ \mathrm{P}\ \gamma)$ such that [1,3,4]:

$$(\gamma\ \mathrm{P}\ \gamma) = \begin{pmatrix} 1 + md_1p_1 & md_1p_2 & md_1p_3 \\ md_2p_1 & 1 + md_2p_2 & md_2p_3 \\ md_3p_1 & md_3p_2 & 1 + md_3p_3 \end{pmatrix} \quad (1)$$

where $[\gamma; \mathbf{d}] = [d_1, d_2, d_3]$ are the components of $\mathbf{d}$ in the γ basis, a unit vector which points toward the direction of the displacement. $[\mathbf{p}, \gamma^*]$ are the component of the unit invariant-plane normal in the γ^* basis (normal to the habit plane). m is the magnitude of the shape deformation.

The variant selection occurs if the transformation develops under the externally applied system of stresses. The interactions between martensite and these stresses affects the mechanical free energy of the individual variants depending on their crystallographic orientation and will produce an energy which adds to the chemical driving force. Variant selection occurs when the interaction energy is large enough compared to the chemical free energy ΔG [5,6].

Different approaches have been used to calculate the interaction energy U between applied stress and the transformation strain. Humbert et al. [6] used a method based on the elasticity theory rather than the plastic model of Patel and Cohen [2]. However, since the transformation strain is plastic, the plastic work explained in Ref. [2] gives the correct value of interaction energy [5]. According to Patel and Cohen, the interaction energy between the applied stress and martensitic transformation can be simply described as

$$U = \sigma_N \times \delta + \tau \times s \quad (2)$$

where σ_N and τ are the normal component of stress and corresponding resolved shear stress on the habit plane in the shear direction, δ and s are the dilatational and shear strains due to martensitic transformation, respectively. When the normal stress is tensile, σ is positive, while the compressive stress makes its numerical value negative. The shear component of the stress is always positive during uniaxial loading [2]. This implies that shear stresses will always

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aid the transformation while the normal stress may stimulate the martensitic transformation if it is tensile, or oppose it in the case that this component of stress is compressive. Kundu et al. [5,7,8] used the combination of crystallographic theory and interaction energy in their calculation and reliably predicted the overall texture due to martensitic transformation.

In the last few decades, the phase field modelling has been used as a powerful computational method for predicting morphological and microstructural evolution in martensitic phase transformation. Different models have been put forward by various groups of scientists, for instance, Falk [9] proposed a one dimensional model for martensitic phase transformation and exploited the shear strain as the order parameter, Barsch and Krumhansl [10,11] derived governing equation for proper martensitic phase transformation through Ginzburg–Landau theory, Saxena et al. [12] and Rasmussen et al. [13] worked with dimensionless and scaled local deviatoric strains as order parameter, Ahluwalia et al. [14,15] introduced a polycrystal model based on the continuum elasticity, Cui et al. [16] proposed a two dimensional model for generic hexagonal to orthorhombic phase transformation, Shchyglo et al. [17] suggested a systematic way to construct the Landau free energy function in NiTi and NiTiCu shape memory alloys, Wang and Khachaturyan [18] proposed a realistic three-dimensional phase field simulation for the generic improper cubic to tetragonal transformation in a single constrained crystal, Li and Chen [19] presented a model to predict the precipitation of rhombohedral in a cubic matrix in $Ti_{11}Ni_{14}$, Artemev et al. [21] studied the effect of external stress on martensitic phase transformation and shown that external stresses increase the production of those variants which are favoured by applied stresses, Artemev et al. [20] also suggested a model for proper martensitic transformation and simulated two different types of cubic to tetragonal transformation, Jin et al. [22] presented a phase field model for the cubic to trigonal transformation in AuCd alloy, Yamanaka et al. [23] suggested an elastoplastic model to simulate cubic to tetragonal transformation for an elastic perfectly plastic material. In the last years, Levitas and Preston developed the Ginzburg–Landau theory for proper martensitic phase transformation in various aspects. They proposed their model in three papers: in the first paper [24], 2–3–4 polynomial for thermal part of Gibbs energy was used and the transformation strain was coupled with the order parameter through 2–3–4 polynomial or quadratic; in the second paper [25], the austenite–martensite Landau model was developed to cover martensite–martensite transformation; and in the third paper [26], it is shown that the 2–3–4–5 polynomial is not the only Landau potential that could be used and alternative Landau potentials were introduced, 2–4–6 polynomial in the Cartesian coordinate system, and two potentials in the hyperspherical coordinate system. All these researches among others have revealed the huge capabilities of phase field modelling in predicting the microstructure evolutions at mesoscale. However, this method could be sometimes mathematically cumbersome. Therefore, the need for fast computational methods for the simulation of the microstructure evolution is becoming important.

In the present work, mathematical models have been programmed to simulate the martensitic transformation. The microstructure of martensite is, firstly, computed when no external stress is applied. For this, a set of crystallography data is deduced using the theory of martensite and employed in calculations. Secondly, during the transformation under an external system of stresses, the same method as used in Ref. [5] is employed. A set of crystallographic data for an austenitic stainless steel is used to programme the growth of martensitic variants in an individual austenite grain. This theory is consistent with all the experimentally observed features of the martensitic transformation [1,3,27,28]. Through the present work, it is assumed that the materials is free from defects. However, the real materials always have defects which play a significant role in the evolution of martensitic microstructure. Also in the present computation, the stress or strain interactions between plates are not accounted for. The presented model can be used for modelling the martensitic transformation in steels as an alternative method for phase filed method. This model is mathematically simpler and is able to compute the microstructure much faster than phase field method. The proposed model benefits from using the phenomenological theory of martensite crystallography which describes the crystallography and shape of martensite plates correctly.

2. Crystallography

Eq. (1) can be simplified as:

$$(\gamma\ \mathrm{P}\ \gamma) = I + m[\gamma;\mathbf{d}](\mathbf{p};\gamma^*) \tag{3}$$

where I is the identity matrix. There exist 24 different martensite variants in any austenite grain, and hence resulting in 24 different IPSs. Fig. 1a shows an arbitrary vector u traversing an austenite grain before transformation. Δu indicates its intercept with the austenite grain which will transform to martensite. Because of the transformation, the vector u becomes a new vector v as illustrated in Fig. 1b. The components of this new vector can be determined as follows [5]:

$$v = P\Delta u + (u - \Delta u) \tag{4}$$

The change in shape caused by the formation of a particular martensite plate i in an austenite grain, $(\gamma\ \mathrm{P}_i\ \gamma) \equiv \mathrm{P}_i$ is known from the crystallographic theory developed for martensite [3,28]. Knowing this deformation, it is possible to deduce the remaining 23 matrices for a grain of austenite in the sample frame of reference using symmetry operations. Each can be formulated using a similarity transformation as follows:

$$(S\ \mathrm{P}_i\ S) = (S\ \mathrm{J}\ \gamma)(\gamma\ \mathrm{P}_i\ \gamma)(\gamma\ \mathrm{J}\ S) \tag{5}$$

where the matrix $(S\ \mathrm{J}\ \gamma)$ refer to rotation relating the grain of austenite to the sample axes, and $(\gamma\ \mathrm{J}\ S)$ indicates the inverse of this rotation matrix. In such a way, one is able to calculate the components of vector v in the reference frame of the sample.

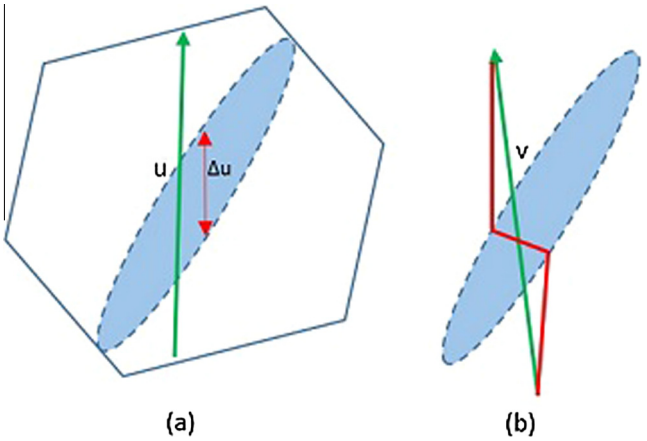

Fig. 1. The formation of an initial vector u due to the formation of martensite. (a) An austenite grain prior to transformation, with the ultimate location of a plate of martensite marked. (b) The following martensite transformation.