Note

Variant Selection in Mechanically-induced Martensitic Transformation of Metastable Austenitic Steel

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(Received on March 7, 2005; accepted on April 27, 2005)

1. Introduction

During martensite transformation, parent austenite usually has an orientation relationship with newly transformed martensite and thereby a crystallographic texture of the austenite has a great influence on a texture development in the inherited martensite. For a given orientation relationship, there are several equivalent orientations of the inherited phase, which is called variant. **Table 1** shows the 24 variants for Kurdjumov–Sachs (K–S) orientation relationship which is usually observed in carbon steels. In idealized case, all variants can appear in an austenite grain with an equal probability during the transformation. However, it has been reported that some variants preferentially appeared during the transformation. In other words, some variants possibly have greater relative probability to be selected. This phenomenon, which is called variant selection, is known to have a significant effect on the texture development in the inherited phase.

The slip system of parent phase,^{1–3)} the grain boundary orientation⁴⁾ and the existence of stress^{5–8)} have been known to affect the variant selection during the transformation and the development of transformation texture. As for the slip activity, the criterion of variant selection was imposed in terms of slip distribution and was applied to diffusion-controlled transformation.³⁾ Ray *et al.*^{9,10)} reviewed the various

kinds of transformation texture that is normally encountered in austenite-to-ferrite transformation in steel. As for the bainitic transformation in steel, the variant selection had been investigated by an experimental observation.¹¹⁾ Recently, present authors suggested that the probability for a nucleation site to really act during displacive transformation could be derived for each variant as a function of the mechanical interaction energy between externally applied stress and lattice deformation based on the Kurdjumov–Sachs (K–S) relationship.^{6–8)}

In present study, the variant selection in mechanically induced martensitic transformation of metastable austenite is investigated with respect to the interaction between external stress and lattice deformation of the transformation. The orientations of parent austenite and newly transformed martensite are measured for tensile and compressive deformation using electron back-scattered diffraction (EBSD). For an individual austenite grain, the orientation of 24 K–S variants are evaluated and compared with measured orientation of martensite. The interaction energy between externally applied stress and lattice deformation is calculated for each 24 K–S variant and the probability of variant selection is assessed. The assessed probability is compared with the experimental results.

2. Experimental

The alloy used in present study is SUS 301 that has fully austenitic structure at room temperature. Chemical composition of the alloy is Fe–0.13C–17Cr–7Ni–2Mn–1Si in wt% and the Ms temperature is estimated to be –102°C from Nehrenberg's equation.¹¹⁾ The alloy is prepared by vacuum induction melting. The ingot is homogenized at 1200°C for 10 h and then austenitized at 1066°C for 10 min followed by water quenching.

Tensile test specimen of 12.5 mm in gauge length and 4 mm in diameter is machined from the ingot. The compression test specimen with a diameter of 8 mm and height of 12 mm is also machined. To obtain mechanically transformed martensite from metastable austenite, the tensile specimen is deformed with a uniform elongation of 10% at room temperature. The flow stress at 10% elongation is around 350 MPa. For the compressive specimen, nominal reduction ratio of 10% is adopted.

The microstructure and orientation of deformed specimen are investigated with FE-SEM equipped with EBSD system. The orientation mapping with EBSD enables us to assess the orientation of each phase as well as to evaluate their distribution.

3. Mechanical Interaction Energy under Applied Stress

It is well known that the transformed martensite usually has orientation relationship with its parent austenite called as K–S relation. Each of the 24 variants of K–S relation has one compressive axis and two tensile axes for the martensitic transformation, which is called the Bain distortion. When a compressive stress is applied, it is natural that the variant whose compressive axis is nearly parallel to the direction of the applied stress should have larger probability for the variant selection. It could be easily understood that the tensile stress state comes to the same thing.

To analyze quantitatively the probability of variant selection, the probability for a nucleation site to really act should be derived as a function of external stress state for each martensitic variant. Based on the Koistinen and

Table 1. Twenty four variants of K–S relation.

Variant No.	Plane Parallel ($\gamma // \alpha'$)	Direction Parallel [$\gamma // \alpha'$]	Variant No.	Plane Parallel ($\gamma // \alpha'$)	Direction Parallel [$\gamma // \alpha'$]
1	(111) // (011)	$[\bar{1}10] // [\bar{1}\bar{1}\bar{1}]$	13	($\bar{1}\bar{1}$) // (011)	$[110] // [\bar{1}\bar{1}\bar{1}]$
2	(111) // (011)	$[\bar{1}10] // [\bar{1}\bar{1}\bar{1}]$	14	($\bar{1}\bar{1}$) // (011)	$[110] // [\bar{1}\bar{1}\bar{1}]$
3	(111) // (011)	$[\bar{1}01] // [\bar{1}\bar{1}\bar{1}]$	15	($\bar{1}\bar{1}$) // (011)	$[011] // [\bar{1}\bar{1}\bar{1}]$
4	(111) // (011)	$[\bar{1}01] // [\bar{1}\bar{1}\bar{1}]$	16	($\bar{1}\bar{1}$) // (011)	$[011] // [\bar{1}\bar{1}\bar{1}]$
5	(111) // (011)	$[0\bar{1}1] // [\bar{1}\bar{1}\bar{1}]$	17	($\bar{1}\bar{1}$) // (011)	$[\bar{1}01] // [\bar{1}\bar{1}\bar{1}]$
6	(111) // (011)	$[0\bar{1}1] // [\bar{1}\bar{1}\bar{1}]$	18	($\bar{1}\bar{1}$) // (011)	$[\bar{1}01] // [\bar{1}\bar{1}\bar{1}]$
7	($\bar{1}\bar{1}$) // (011)	$[\bar{1}\bar{1}0] // [\bar{1}\bar{1}\bar{1}]$	19	($\bar{1}\bar{1}$) // (011)	$[1\bar{1}0] // [\bar{1}\bar{1}\bar{1}]$
8	($\bar{1}\bar{1}$) // (011)	$[\bar{1}\bar{1}0] // [\bar{1}\bar{1}\bar{1}]$	20	($\bar{1}\bar{1}$) // (011)	$[1\bar{1}0] // [\bar{1}\bar{1}\bar{1}]$
9	($\bar{1}\bar{1}$) // (011)	$[0\bar{1}\bar{1}] // [\bar{1}\bar{1}\bar{1}]$	21	($\bar{1}\bar{1}$) // (011)	$[101] // [\bar{1}\bar{1}\bar{1}]$
10	($\bar{1}\bar{1}$) // (011)	$[0\bar{1}\bar{1}] // [\bar{1}\bar{1}\bar{1}]$	22	($\bar{1}\bar{1}$) // (011)	$[101] // [\bar{1}\bar{1}\bar{1}]$
11	($\bar{1}\bar{1}$) // (011)	$[101] // [\bar{1}\bar{1}\bar{1}]$	23	($\bar{1}\bar{1}$) // (011)	$[011] // [\bar{1}\bar{1}\bar{1}]$
12	($\bar{1}\bar{1}$) // (011)	$[101] // [\bar{1}\bar{1}\bar{1}]$	24	($\bar{1}\bar{1}$) // (011)	$[011] // [\bar{1}\bar{1}\bar{1}]$

Marburger's empirical equation,¹³⁾ Han *et al.*⁸⁾ derived the probability, P^i , for the operational nucleation site of i -th martensitic variant as follows

$$P^i = -A (\Delta G + U^i) \dots\dots\dots(1)$$

where ΔG and U^i are the chemical free energy change for austenite-to-martensite transformation and the mechanical driving force given by the interaction between the applied stress field and the lattice deformation during the transformation, respectively. A is a constant at a given temperature. Notice that in the above expression, a negative value of U^i indicates a favorable interaction with the applied stress.

If the transformation strain tensor on the specimen coordinate is denoted as ϵ_{ij}^S , the interaction energy, U^i , can be defined as

$$U^i = \sigma_{ij} \cdot \epsilon_{ij}^S \dots\dots\dots(2)$$

where σ_{ij} is the externally applied stress on the specimen coordinate and the superscript i means i -th variant. To analyze more precisely the mechanical contribution in martensitic transformation, it is necessary to consider the invariant plane strain (IPS) together with the Bain distortion. According to Wechsler–Lieberman–Read (W–L–R) crystallographic theory,¹⁴⁾ the lattice deformation associated with the displacive transformation (**F**) without rigid body rotation can be expressed as follows.

$$\mathbf{F} = \mathbf{B}\mathbf{P} \dots\dots\dots(3)$$

where **B** and **P** represent the Bain deformation and the lattice-invariant shear, respectively. The Bain deformation, **bFb**, defined on the crystallographic coordinate system of parent austenite (FCC) can be expressed by the following form.

$$\mathbf{bFb} = \begin{bmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_3 \end{bmatrix} \dots\dots\dots(4)$$

where η_1 and η_3 are the expansion ratio and the contraction ratio accompanying with the Bain deformation. η_1 and η_3 can be calculated from the density ratio of FCC and BCT.^{6,15)} Then, the lattice deformation associated with the transformation on the reference of the crystallographic coordinate of inherited martensite, **bFb**, can be calculated by W–L–R theory assuming an appropriate direction and plane for the lattice-invariant shear.^{8,16)} Once **bFb** is calculated, we can get the transformation strain of each variant on the reference coordinate of BCT as follows

$$\epsilon_{ij}^C = \frac{1}{2} [(\mathbf{bFb})^T (\mathbf{bFb}) - \mathbf{I}] \dots\dots\dots(5)$$

where **I** is identity tensor. To calculate the transformation strain on the specimen coordinate, it is necessary to convert the transformation strain on the crystal coordinate of BCT into the one on the specimen coordinate. The nucleation of the martensitic variant, whose orientation is related to the austenite by K–S relationship, involves the transformation strain of Eq. (5). This orientation relation corresponds to the 24 rotation matrices, $\Delta \mathbf{g}_{KS}^m$ ($m=1, \dots, 2, 4$), which indicate the orientations of 24 K–S variants with the reference of the crystallographic coordinate of parent austenite. Thus, if the orientation of parent austenite is characterized by **g**, each orientation of 24 K–S variants is given as $\Delta \mathbf{g}_{KS}^m \cdot \mathbf{g}$ ($m=1, \dots, 2, 4$). By tensor transformation rule, the transformation strain on the specimen coordinate can be calculated

as follows

$$\epsilon_{ij}^S = a_{ik} a_{jl} \epsilon_{kl}^C \dots\dots\dots(6)$$

where a_{ij} is the direction cosine which links the crystal coordinate to the specimen coordinate and can be calculated by $[\Delta \mathbf{g}_{KS}^m \cdot \mathbf{g}]^{-1}$. By using Eq. (6), the transformation strain tensor on the specimen coordinate for each K–S variant can be obtained and used to determine the interaction energy, U^i . From the assessment of the mechanical driving force, U^i , for each variant, then, the probability of variant selection under the applied stress state can be estimated.

4. Results and Discussion

Figures 1(a) and **1(b)** show the orientation mapping of parent austenite grains and inherited martensite after tensile deformation. The retained austenite phase allows identification of parent austenite grains in the EBSD map. The orientation of the martensite from a parent austenite grain could also be identified. Here, the external tensile stress was assumed to be applied along RD-axis.

The theoretical orientations of 24 K–S variants for austenite grains A1 and A2 in Fig. 1 could be obtained from the crystal orientation of the individual austenite grain and the K–S relationship listed on Table 1. Then, the measured martensite phase could be linked to the appropriate K–S variant by comparing the deviation angle between the theoretical orientation of the K–S variants and the measured orientation of the martensite. The variant to which the transformed martensite belongs will make smallest deviation angle with the measured orientation of martensite. From the smallest angle deviation, martensite M1 and M2 correspond to K–S variant No. 20 in Fig. 2(a) and No. 21 in Fig. 2(b), respectively. The variant number indicates the sequence listed on Table 1. The deviation angles of M1 and M2 were obtained as 3.8° and 1.94°, respectively. Figure 2 shows the calculated mechanical interaction energy, U^i , for each K–S variant number. Note that K–S variants No. 20 in Fig. 2(a) (corresponding to M1) and No. 21 in Fig. 2(b) (corresponding to M2) have very large negative value of U^i .

Figures 3(a) and **3(b)** show the EBSD orientation maps of the parent austenite grains and the inherited martensite variants observed after compressive deformation. The compressive stress was assumed to be applied along ND-axis. Two martensites, M3 and M4, could be identified from austenite grain, A3. M3 and M4 could be linked to K–S variant No. 1 and 2, and the deviation angles were obtained as 2.48° and 2.03°, respectively. From Fig. 4, it can be confirmed that the U^i of K–S variant No. 1 (corresponding to M3) is the largest negative value and the other variant (K–S variant No. 2) corresponding to M4 has also relatively large negative value of U^i . These negative values of U^i for some specific variants under the tensile and compressive stress state are related with the favorable interaction with the applied stress as shown in Eq. (1) and it means that the probability for these variants to be selected becomes increased due to the external stress.

Under the compressive stress state, the number of variants, which have a negative value of mechanical interaction energy, is smaller than the one under the tensile stress state. In addition, the absolute value of U^i in case of the compressive stress state was smaller than the one under the tensile stress state. It can be understood from the fact that each of the 24 K–S variants has one compressive axis and two tensile axes for the martensite transformation and tensile stress is more effective on increasing the driving force for the mechanically-induced transformation. It accords with the ob-

Fig. 1. EBSD orientation mapping of (b) martensitic variants transformed from (a) single parent austenite grains after 10% tensile test. Martensites M1 and M2 seem to be transformed from austenite grains A1 and A2, respectively.

(a)

(b)

Fig. 2. The mechanical interaction energies calculated for 24 K-S variants of parent austenites (a) A1 and (b) A2 under the 10% tensile condition.

Fig. 3. EBSD orientation mapping of (b) martensitic variants (M3 and M4) transformed from (a) a single parent austenite grain (A3) after 10% compression test.

Fig. 4. The mechanical interaction energies calculated for 24 K-S variants of parent austenite A3 under the 10% compressive condition.

servation that the applied tensile stress more effectively accelerates the martensite transformation than the compressive stress.^{8,17)}

5. Summary

The orientation relationship between the parent austenite and the inherited martensite which had been mechanically-induced transformed under both uniaxial tension and compression state was observed by an electron backscattered diffraction (EBSD). The probability of variant selection was assessed with the interaction energy between externally applied stress and lattice deformation for each martensitic variant. The interaction energy was calculated from the Bain deformation and the invariant shear strain on the basis of K-S orientation relationship. It could be confirmed that the calculated interaction energy for the transformed martensitic variant has the relatively very large negative value. The negative value of the interaction energy under

the tensile and compressive stress state is related with the favorable interaction with the applied stress and it means that the probability for some specific variants to be selected becomes increased due to the external stress.

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