Variant Selection in Phase Transformation and its Influence on Texture and Martensite Starting Temperature in Steel

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Abstract. A mechanism is proposed that can predict the textures as well as the influence of austenite grain size on martensite starting temperature in steels. The anisotropic elastic energy by shape change of martensite changes depending upon variants in neighbour austenite grains, whereas it does not in immediate parent grains in which martensite grows. A mechanism based on this behaviour of elastic energy can explain not only the texture formation of martensite but also the well-known austenite grain size dependence of Ms, particularly the abrupt drop of about 30K in the grain size range below 20 µm.

1. Introduction
Variant selection during phase transformation, in which some of the permitted child orientations by the orientation relationship between parent and child phases are preferred than others, affects microstructures and crystallographic textures of materials, thus influencing various properties. In the martensite (austenite (γ) to bcc or bct) in steels, it has been reported that anisotropic elastic energy stored in “neighbouring” γ is the most influential factor to determine the preferred variants [1, 2], while for diffusive transformation holding the orientation relation to two or more neighbouring γ grains at the same time is the most influential [2, 3]. The purpose of this article is to show that the mechanism due to the anisotropic elastic energy affects not only the microstructure and texture of martensite but also the starting temperature of martensite transformation (Ms) in steels.

Ms is well known to shift when changing austenization temperature [4] or the grain size of γ before quenching [5, 6, 7], whereas the former is now known as caused through the latter. Ms gradually decreases as the γ grain size decreases from over a few hundred µm to about 10 µm. Then, Ms abruptly drops by about 30 K in the range below 20 µm [6, 7]. This grain size dependency of Ms is still left unclarified in its mechanism.

One of the most researched mechanisms for this phenomenon is perhaps a Hall-Petch-type mechanism related to the grain refinement strengthening of γ, in which the martensite transformation is retarded due to the hardening of γ, since the nucleation and growth of martensite would cost more energy in such a hardened matrix [5, 7]. However, there is a controversy that the Hall-Petch mechanism that requires migration of dislocations over grains cannot influence Ms [6]. Although there are several other mechanisms proposed for the grain size dependence of Ms, no commonly agreed mechanism for this
phenomenon exists. In this contribution, a mechanism is proposed that is related to the anisotropic elastic energy in neighbour γ grains and explains the dependence of Ms on the γ grain size well, particularly the abrupt drop below 20 μm.

2. Theory by elastic anisotropy

In the martensite transformation in steels, the orientation relationship between γ and martensite is only a few degrees away from the Kurdjumov-Sachs (K-S) relation \([8], \{111\},/\{110\}\) and \(<110>\gamma//<111>\alpha\), and there are 24 variants due to the cubic symmetry of crystals. Preferential selection of the variants during the martensite transformation is obvious, since for instance packets and subblocks are formed, in which the variants having similar habit planes gather side by side and each variant is paired with a specific variant respectively [9]. The texture of the martensite is also known to be stronger than expected with no variant selection [1]. Proposed mechanisms for the variant selection span from several versions of habit-plane-orientation-related models to stress- or strain-related models [1]. In most of them variants are determined due to phenomena in the inside or the boundary of immediate parent grains where the variants grow in, such as stresses and dislocations within the grains and grain shape. Instead, the authors have proposed that variants may be chosen being related to “neighbour” grains, that is, the elastic energy stored in “neighbour γ grains” by displacive transformation is responsible for the variant selection [1]. Although the elastic energy is one of the major sources that require a large excess energy for the martensite transformation to occur, it does not depend on variants in the immediate parent grains, since all the variants are crystallographically equivalent. Nevertheless, outside of the parent grains, the elastic energy is dependent on the variants as well as orientations of neighbours, since the variants are not equivalent in the neighbour γ crystals anymore and γ is elastically anisotropic, thus strongly influencing the variant selection as shown in Figure 1 [1].

![Figure 1](image)

Figure 1 Comparison between textures of martensite by an experiment and prediction based on elastic energy in neighbour γ. (a) the RD fiber at 0° in Φ and 45° in \(\phi_2\) and (b) TD fiber at 90° in Φ and 45° in \(\phi_2\).

Given the elastic stiffness of the averaged matrix \(c_{ijkl}\) and the shape change of martensite \(\varepsilon_{ij}\), the stored elastic energy \(E\) due to the shape change of martensite is given by

\[
E = \frac{\varepsilon_c}{2} \sum c_{ijkl} \varepsilon_{ij} \varepsilon_{kl}. \quad (1)
\]
\( E_c \) is a coefficient introduced to roughly express the effect for which a lath-shaped martensite is embedded in a matrix; better approximation can be given by a micromechanics theory \([10]\), however it is out of the scope of this contribution. This energy is distributed in a range including not only the parent \( \gamma \) grain but also neighbour grains, especially since martensite mostly nucleates on \( \gamma \) grain boundaries. Thus, this energy in the neighbour \( \gamma \) has been thought to be a cause of variant selection and influence the texture in martensite \([1, 2]\). In the following it will be explored and discussed that this elastic energy in neighbour \( \gamma \) should be also the main mechanism of the grain size dependency of Ms.

Here we assume that the energy \( E \) spreads homogeneously in a spherical region of a radius \( R_c \). In a neighbour \( \gamma \) grain in this region, having the orientation of \( g_r \) and the grain volume of \( V_\gamma \), the stored energy \( E_\gamma \) may be expressed as follows,

\[
E_\gamma = \frac{3V_\gamma E_c}{8\pi R_c^3} \sum C_{ijkl} \cdot (g_\gamma^{-1} \cdot \varepsilon \cdot g_\gamma)_{ijkl} \cdot \varepsilon_{ij} \cdot (g_\gamma^{-1} \cdot \varepsilon \cdot g_\gamma)_{ij}. \tag{2}
\]

The coordinates used are fixed to the \( \gamma \) grain in which martensite grows except for the stiffness tensor of the neighbour \( \gamma \) grain \( C_{ijkl} \) that uses the coordinates fixed to this particular neighbour grain for simpler expression. The shape strain \( \varepsilon \) changes as variants change as

\[
\varepsilon_n = g_{c_n}^{-1} \cdot \varepsilon_1 \cdot g_{c_n}^c, \tag{3}
\]

where \( \varepsilon_n \) and \( g_{c_n}^c \) are the shape strain of the \( n \)-th variant and the corresponding rotation matrix of the cubic symmetry group. Then the energy \( E \) is the sum of \( E_\gamma \) for the \( \gamma \) grains in the region of the radius \( R_c \).

Thus, the energy \( E \) depends on variants as well as the circumstance in which martensite nucleates and grows, such as the orientations of neighbour grains, i.e. textures, and the number of \( \gamma \) grains within \( R_c \), i.e. “the grain size of \( \gamma \)”. It also fluctuates from a site to a site to nucleate in a material. It is obvious that the larger the fluctuation around the average of \( E \), the lower the smallest limit of the energy \( E \). Therefore, Ms that should be determined by the lower limit of \( E \) should be increased as the fluctuation increases, which depends on the texture and the grain size of \( \gamma \).

3. Influence on Ms and discussion

When the \( \gamma \) grain size is very large as compared to the radius \( R_c \), the number of neighbour \( \gamma \) grains are only one at plain grain boundaries of \( \gamma \) or two at triple junctions as shown in Figure 2a. The calculated distributions of the energy \( E/E_c \) in those cases are shown in Figures 3a and b. The energy was assumed to be equally distributed to the parent grain and one (or two) neighbour grain(s) in the former (or latter) case. The elastic moduli used is that for Fe-15%Ni-15%Cr \([11]\), and the shape strain is the one calculated by the phenomenological theory of martensite by Kelly using lattice invariant shears of \( (100)(01\overline{1})_p \) and \( (1\overline{3}1)(10\overline{1})_p \) \([1, 12]\). \( E_c \) was assumed to be constant for simplicity. Ten thousand of neighbour austenite orientations (or orientation pairs) were chosen randomly without considering textures; variants are not necessary to be considered in the texture-less case. It is observed that the elastic energy scatters in a wide range from about 65% to 135% of the averaged value in both cases. The calculated lowest and highest \( E/E_c \) in these cases are \( 0.74 \times 10^{10} \) and \( 1.52 \times 10^{10} \) Jm\(^{-3}\) respectively. Note that these energies should be one to three orders of magnitude larger than the reality, because of a small value of \( E_c \) as will be discussed later.

As the number of \( \gamma \) grains in the strained region increases as shown in Figure 2b, the energy distribution changes as shown in Figures 3c and d. Due to averaging effect by many grains, the distribution sharpens and the fluctuation decreases markedly. If the start of martensite transformation is detected by experiment when nucleation and growth occur for the lower, say, 1% of the energy distribution, the elastic energy at Ms increases with increasing the number of \( \gamma \) grains within \( R_c \) as
The elastic energy just above the lower 1% tile increases by about 30% as the number of \( \gamma \) grains increases. The number of austenite grains \( N_g \) in the radius \( R_c \) is a function of the average \( \gamma \) grain diameter \( D \) as \( R_c \) is constant. Since the first two cases with two and three grains shown in Figure 2a and Figures 3a and b correspond to an infinite grain size, the following function may be appropriate,

\[
N_g = 8 \left( \frac{R_c}{D} \right)^3 + 3. \quad (4)
\]

The elastic energy \( E \) is a part of the excess energy required for martensite transformation, and for this Ms is much lower than \( T_0 \) temperature where Gibbs energy for \( \gamma \) and ferrite are equal. The excess energy \( \Delta G \) that is dissipated as elastic, plastic and interfacial energies is known to be a function

![Schematic representation of stressed regions in \( \gamma \) by martensite](image)

Figure 2 Schematic representation of stressed regions in \( \gamma \) by martensite (a) near plane boundaries and triple junctions in large \( \gamma \) grains and (b) in the case of small \( \gamma \) grains.

![Distribution of elastic energy in \( \gamma \) where there are (a) 2, (b) 3, (c) 10, (d) 50 grains in the stressed region.](image)

Figure 3 Distribution of elastic energy in \( \gamma \) where there are (a) 2, (b) 3, (c) 10, (d) 50 grains in the stressed region.
approximately linear to transformation temperature \[ T_0 \] and becomes zero at \( T_0 \). It is also known that \( \Delta G \) and \( M_s \) for a large grain size (\( \Delta G_\infty \) and \( M_s_\infty \)) are about 1200 J·mol\(^{-1}\) (or \( 1.7 \times 10^8 \) J·m\(^{-3}\)) and about 300 K lower than \( T_0 \), respectively [7]. Therefore, assuming \( E = \Delta G/3 \), \( E \) in J·m\(^{-3}\) can be expressed as a function of \( M_s \) in K as

\[
E = \frac{1}{3} \left[ \frac{1.7 \times 10^8}{300} (M_\infty - M_s) + 1.7 \times 10^6 \right] (J \cdot m^{-3}). \tag{5}
\]

Then it follows that

\[
M_\infty - M_s = (5.3 \times 10^{-6} \cdot E - 300) \ (K). \tag{6}
\]

From this equation, \( E \) is about \( 5.7 \times 10^7 \) J·m\(^{-3}\) at the temperature of \( M_s_\infty \). On the other hand, \( E/E_c \) at \( M_s_\infty \), where \( N_g \) is two to three in our model, is about \( 8.2 \times 10^9 \) J·m\(^{-3}\) as observed in Figure 4. Therefore, \( E_c \) is derived as around \( 7 \times 10^3 \). This small value of the coefficient tells us something about the aspect ratio of a martensite lath, which is estimated to be of the order of \( 10^2 \) by micromechanics [10].

From equations 4 and 6, the above value of \( E_c \) and the data in Figure 4, the influence of \( \gamma \) grain size on \( M_s \) is predicted as shown in Figure 5a, where three cases of \( R_c=5, 8 \) and \( 15 \) \( \mu \)m are presented. An abrupt drop of \( M_s \) is observed below the average \( \gamma \) grain size of about \( 2R_c \), and the total decrease is about 30 K in all the cases.

![Figure 4](image)

Figure 4 Elastic energy at lower 1\% tiles of elastic energy distributions vs the number of \( \gamma \) grains in the stressed region.

The above theoretical results particularly for \( R_c \) being 8 \( \mu \)m agree well with the experimental results for Fe-5\%Ni-2.3\%Mn-C shown in Figure 5b [6] where \( M_s \) rapidly decreases by about 30K as the \( \gamma \) grain diameter decreases from 20 to a few \( \mu \)m. However, the gradual decrease of about 10 K observed in the range over 20 \( \mu \)m cannot be well explained by the present theory. Nevertheless, it is important that this elastic-energy-based prediction of \( M_s \) has only one parameter of \( R_c \) that has a clear physical meaning, “the radius of the elastically strained region”. The model is capable of predicting how \( M_s \) decreases as \( \gamma \) grain refines by knowing the internal energy variation between austenite and ferrite, elastic moduli of \( \gamma \), the shape strain and \( E_c \) for martensite and \( R_c \), all of which can be evaluated theoretically.

Justification of \( R_c \) of around 8 \( \mu \)m is a matter for discussion. Elastic displacement by inclusions is known to change being inverse proportional to the square of distance in a remote distance, and its
behaviour in a close distance is complicated [10]. A relevant question is how large the size of martensite lath that determines $R_c$ at Ms is. If it is the size of an embryo of martensite, $R_c$ would not be as large as 8 $\mu$m. The texture of $\gamma$ is an influential factor as well. When a strong texture is present in austenite, the distribution and fluctuation in the elastic energy as shown in Figure 3 would change largely. However, further work is required to answer those questions.

![Figure 5](image.png)

Figure 5 (a) Predicted and (b) observed changes of Ms by grain refinement of $\gamma$. Figure b was a replot of the data in ref. 6.

4. Conclusion
The influence of elastic energy in neighbour $\gamma$ grains on variant selection as well as Ms of martensite transformation in steels has been studied. A mechanism has been introduced that can predict the textures as well as the grain size dependence of martensite starting temperature in steels. Whereas the elastic energy by shape strain of martensite in immediate parent grains does not depend on variants, the elastic energy in neighbour austenite grains does depend on the variants and largely affects the textures of martensite and Ms. It is predicted by the proposed mechanism that Ms rapidly decreases when the average grain size of $\gamma$ decreases to below 20 $\mu$m as observed experimentally, if the elastic energy is distributed in a surrounding region of 5 to 10 $\mu$m in radius.

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