The Bain Strain Energy in Anisotropic Fe₃Pt Crystals

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SUMMARY

The effect of the elastic anisotropy on the Bain strain energy is calculated by means of the reciprocal lattice method. With the assumption that the temperature hysteresis in the martensitic transformation is proportional to the Bain strain energy, the characteristics of the martensitic transformation in Fe₃Pt associated with ordering can be interpreted well by the fact that the elastic anisotropy exerts a large effect on the Bain strain energy.

1. INTRODUCTION

Zener [1] first proposed a close relation between the elastic anisotropy and the martensitic transformation from b.c.c. structure to f.c.c. structure. In the interpretation of their data on the Au–Cu–Zn alloy system, Nakanishi et al. [2] suggested that an important factor for the occurrence of the martensitic transformation was the temperature dependence of \( C' = (C_{11} - C_{12})/2 \). They believed that the condition for the martensitic transformation became favorable if the anisotropy factor of elastic constants increased as the temperature decreased because of a positive temperature dependence of \( C' \). Otsuka and Wayman [3] claimed that the important factor was the magnitude of anisotropy factor itself rather than the temperature dependence of the anisotropy factor. Although the above claims are different from each other, they are in agreement in that the magnitude of anisotropy factor is important for the occurrence of martensitic transformation.

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Fig. 1. The relation between the normalized Bain strain energy $E_0^{BB}$ and the anisotropy factor of the elastic constants. We assume that the Bain strain tensor is that of disordered Fe$_{76}$Pt$_{24}$ and that $C_{11} = 2.0$, $C_{12} = \alpha$ and $C_{44} = 1.0$.

decreases as the anisotropy factor increases. In the following we interpret the characteristics of martensitic transformation of Fe$_3$Pt in terms of the large effect that the elastic anisotropy has on the first-order transformation.

Fe–Pt alloys with a composition of approximately Fe$_3$Pt show a fairly marked temperature dependence of the anisotropy factor. Hausch [5] measured the temperature dependence of the elastic constants of disordered Fe$_{72}$Pt$_{28}$ and showed that below the magnetic transformation temperature the anisotropy factor increases as the temperature decreases, the value being 5.7 at 0 °C and 11 at −110 °C.

The $M_s$ temperature of Fe$_3$Pt decreases as the long-range order parameter increases [6–10], so the anisotropy factor at the $M_s$ point will be larger for a larger long-range order parameter $S$. Experimentally the character of martensitic transformation changes depending on $S$; it is non-thermoelastic when $S$ is small and is thermoelastic when $S$ is large. The morphology and internal structure of martensite do not change with $S$; twins are introduced in the martensite in order to reduce the overall transformation strain. Therefore we may be able to explain the change in character of the martensitic transformation in Fe$_3$Pt as due to the ordering because the Bain strain energy changes because of the ordering.

2. CALCULATIONS

We use the reciprocal lattice method for the calculation of the Bain strain energy. The details of the method of calculation have been described elsewhere [11]. We calculate the Bain strain energy as a function of the orientation of a short axis of an oblate spheroidal martensite. Figure 2 shows the geometry schematically. We determine the orientation so that it gives the smallest Bain strain energy for each axial ratio and the volume fraction of variants. The figures in Section 3 show the minimum Bain strain energy for each axial ratio $t$ and volume fraction $f$.

There are no data on the elastic constants of Fe$_3$Pt available as a function of $S$. Therefore we use the data of disordered Fe$_{72}$Pt$_{28}$ neglecting the effects of the composition difference and of the ordering on the elastic constants. In other words, the effect of the ordering on the elastic constants is taken into account only through the change in $M_s$ due to ordering.

The Bain strain tensor (which is equal to the ordinal Bain strain tensor minus the unit tensor) is determined from the lattice constant data for an Fe$_{76}$Pt$_{24}$ alloy [12].

In order to determine the effect of the variants, we introduce a factor $f$. $f$ is the volume fraction of X-type Bain strain defects (see eqn. (1): we regard the transformed region as composed of Bain strain defects) and $1 - f$ is the volume fraction of Z-type Bain strain defects. X-type and Z-type Bain strain defects are twin related to each other. We assume a continuous distribution of twins instead of discrete twins [12]. Therefore the mean Bain strain tensor is given by

$$
\begin{pmatrix}
\epsilon_1 & 0 & 0 \\
0 & \epsilon_2 & 0 \\
0 & 0 & \epsilon_2
\end{pmatrix} f +
\begin{pmatrix}
\epsilon_2 & 0 & 0 \\
0 & \epsilon_2 & 0 \\
0 & 0 & \epsilon_2
\end{pmatrix} (1 - f)
$$

(1)

X type Z type
Tadaki and Shimizu [13] claimed that the change in character of the martensitic transformation due to ordering was controlled by the change in volume of the martensitic transformation due to ordering (it should be noted that, the smaller the volume change is at martensitic transformation, the larger is the value of $S$). In order to clarify the effect of volume change, we calculate the contribution of each energy term separately: the dilatational strain energy, the shear strain energy and the interaction energy between dilatational and shear components of the Bain strain tensor. In this calculation we rewrite eqn. (1) as follows:

\[
\begin{pmatrix}
\delta_1 & 0 & 0 \\
0 & \delta_1 & 0 \\
0 & 0 & \delta_1
\end{pmatrix} + \begin{pmatrix}
\frac{1}{3} - f & 0 & 0 \\
0 & \frac{1}{3} - f & 0 \\
0 & 0 & -\frac{2}{3} + f
\end{pmatrix} (\epsilon_2 - \epsilon_1) 
\]

dilatational component

The energy density in the reciprocal lattice is given by

\[
E(k) = \alpha \delta_1^2 - \phi_j^d(-k) \cdot \tilde{\phi}_U(k) \cdot \phi_j^d(k) - 2\phi_j^s(-k) \cdot \tilde{\phi}_U(k) \cdot \phi_j^s(k) + 2(\frac{1}{3} - f + f^2)(C_{11} - C_{12})(\epsilon_1 - \epsilon_2)^2 - \phi_j^s(-k) \cdot \tilde{\phi}_U(k) \cdot \phi_j^s(k)
\]

\[
k = (k_1, k_2, k_3)
\]

The first line of eqn. (3) is the dilatational energy density, the second line the interaction energy density between the dilatational and the shear parts and the third and fourth lines the shear energy density.

3. RESULTS

As shown previously [11], the Bain strain energy is given by

\[
E^{BB} = E_0^{BB} n^\beta
\]

where $\beta \approx 1.0$ and $n$ is the number of Bain strain defects which are included in an oblate spheroidal martensite.

Figure 3 shows that the Bain strain energy for $S = 0$ is dependent on the axial ratio and the volume fraction. The fraction indicated by the arrow is that expected from the phenomenological theory of martensite. Therefore Fig. 3 shows that the value of $f$ giving the minimum Bain strain energy changes from 0.5 for small axial ratios to the value expected from phenomenological theory for large axial ratios. This is an interesting result but we shall not discuss this point further.

Figure 4 shows the effect of the long-range order parameter $S$ on the minimum Bain strain energy. By the minimum Bain strain energy we mean the minimum value of the Bain strain energy for fixed values of $S$ and the axial ratio $t$; thus each point on the curves corresponds to a different value of $f$. Figure 4 shows that the Bain strain energy decreases as the degree of order increases.

Figure 5 shows the behavior of each energy term (the dilatational energy, the shear energy...
Fig. 4. The Bain strain energy as a function of the long-range order parameter.

Fig. 5. The behavior of the components of the Bain strain energy of X-type Bain strain defects (\(f = 1; t = 5; \theta = 90^\circ\)).

and the interaction energy between shear and dilatation) for X-type Bain strain defects (i.e. \(f = 1.0\) in eqn. (3)). The Bain strain energy was found to be minimum at about \(\phi = 50^\circ\). Figure 5 shows a very large change in the shear energy term due to the change in \(S\) compared with the dilatational and the interaction energy terms. Therefore, apparently Fig. 5 seems to contradict the claim of Tadaki and Shimizu [13]. However, it should be noted that the shear energy term will be greatly reduced by the introduction of a variant; this is not the case for the dilatational energy. Therefore we also calculate each energy term for \(f < 1\).

Figure 6 shows the results for \(S = 0\). The Bain strain energy shows the minimum at about \(\phi = 55^\circ\). The interaction energy is negative, so the interaction between the shear and the dilatation is attractive. The dilata-

Fig. 6. The behaviors of the components of the Bain strain energy for \(f < 1\) and \(S = 0\) (\(t = 5; \theta = 90^\circ\)).

Fig. 7. The behaviors of the components of the Bain strain energy for \(f = 0.5\) and various \(S\) values (\(t = 5; \theta = 90^\circ\)).

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tional energy has a fairly weak dependence on \(\phi\) compared with the dependences of the shear and interaction energies.

Figure 7 shows the behaviors of each energy term for various values of \(S\). Again the change in the shear energy term due to the change in \(S\) is seen to be the largest.

4. DISCUSSION

The long-range order parameter will affect the free energy of the high temperature phase
and that of the martensitic phase. Therefore it is difficult to discuss fully the dependence of $M_s$ on the long-range order parameter. We shall discuss the relation between supercooling, which is a measure of the contribution of the non-chemical free energy, and the Bain strain energy under a simple assumption that the relative temperature dependence of the free energy of the ordered phase is the same as that of the disordered phase. Moreover, we neglect the contribution of twin boundary energy for $f < 1$, because we do not know the twin boundary energy as a function of the order parameter. If we introduce the twin boundary energy, we can determine not only the volume fraction $f$ but also the magnitude of the thickness of each variant [14, 15].

Even so, we cannot show the relation between supercooling and the Bain strain energy without details of the nucleation and growth mechanism. We discuss the above relation with the following assumptions.

1. The axial ratio of an oblate spheroidal martensite at the beginning of growth is constant, irrespective of the value of the long-range order parameter.

2. Growth starts when the gain in chemical free energy exceeds the Bain strain energy for the above axial ratio.

3. The width of the temperature hysteresis is twice that of the degree of supercooling.

The assumptions (1) and (2) may be rationalized if we assume that the nucleation and growth of martensite takes place near a dislocation or a group of dislocations.

In Fig. 8 Umemoto and Wayman's [16] experimental results and the results of the present calculation are compared. The temperature hysteresis $\Delta T$ is assumed to be proportional to the strain energy; both are normalized with respect to the values of the disordered phase. The general tendency shows fairly good agreement between calculation and experiment. If the elastic constants of the ordered phase are smaller than those of the disordered phase and/or the anisotropy factor of the ordered phase is larger than that of the disordered phase, which is the situation as judged from ref. 17, Fig. 2, the agreement will be better.

Figures 5 and 7 show that the largest reduction in strain energy occurs in the shear energy term when the order parameter becomes large. This is also true when we introduce the Z-type variant. Even so, the largest term is the shear energy term even for large order parameters. Therefore we know that the largest contribution comes from the shear energy term and that it will determine the character of the martensitic transformation. This is consistent with, although indirectly, the fact that the habit plane of $\text{Fe}_3\text{Pt}$ does not change with ordering.

Therefore we can understand roughly the change in hysteresis due to ordering in terms of the change in the Bain strain energy, and especially the change in the shear energy component due to ordering. If we define the thermoelastic martensitic transformation as a martensitic transformation with a small hysteresis, we can understand approximately the change in character of the martensitic transformation in $\text{Fe}_3\text{Pt}$ due to ordering from the above discussion. However, the actual situation seems to be more complex. We must take into account the reversibility of the transformation and therefore the characters of the defects which are introduced during the martensitic transformation and also of the plastic zone around a martensite particle (this idea was introduced by Olson and Owen [18]). These considerations will be published in a future paper.

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