

Elastoplastic Phase-Field Model of Martensitic Transformation

Akinori Yamanaka^{1*}, Tomohiro Takaki², Yoshihiro Tomita³

¹ Graduate School of Science and Technology, Kobe University, 1-1, Rokkodai-chou, Nada-ku, Kobe, Hyogo, 657-8501, Japan

² Graduate School of Science and Technology, Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto, 606-8585, Japan

³ Graduate School of Engineering, Kobe University, 1-1, Rokkodai-chou, Nada-ku, Kobe, Hyogo, 657-8501, Japan

e-mail: yamanaka@solid.mech.kobe-u.ac.jp, takaki@mech.kit.ac.jp, tomita@mech.kobe-u.ac.jp

Abstract We develop an elastoplastic phase-field model of martensitic transformation that can describe the relaxation of elastic strain energy induced by both elastic and plastic deformations. In this model, to consider the plastic deformation during the martensitic transformation, the evolution of plastic strain is described by the time-dependent Ginzburg-Landau equation, which is derived from shear strain energy. The effects of the plastic accommodation of transformation strain on the transformation kinetics and morphology of a martensitic microstructure are investigated using the developed model. Results show that the martensite phase grows along a high-stress region and forms a twinned martensitic structure, eliminating a transformation-induced stress field. Furthermore, it is clarified that an increase in elastic strain energy during the martensitic transformation is largely inhibited by the plastic accommodation. The prominent release of elastic strain energy arrests the rearrangement of the orientation variants of the martensite phase. Therefore, elastoplastic-martensitic transformation does not produce a single twinned martensite, which is observed in elastic-martensitic transformation.

Key words: Elastoplastic phase-field model, Martensitic transformation, Plastic deformation, Elastic strain energy

INTRODUCTION

The microstructure of steel is produced during diffusional or displacive phase transformation [1]. It is well known that the martensite phase is formed from the austenite phase by displacive or structural phase transformation without long-range atomic diffusion, which is called martensitic transformation. Because the martensite phase exhibits desirable mechanical properties and is used as an important constituent phase of high-strength steel, the metallurgical, crystallographical and mechanical properties of steel containing a martensitic microstructure have been intensively studied experimentally and theoretically [2-5].

The martensite phase is produced by the shear deformation of the crystal lattice of the parent phase. In particular, the fcc-bcc martensitic transformation in a ferrous alloy is described using the Bain distortion [6]. Due to this distortion, elastic strain is generated in the material during the martensitic transformation. Therefore, the morphology of the martensitic microstructure is characterized by the minimization path of elastic strain energy. In references [7-10], it is suggested that elastic strain energy is reduced by the formation of a heterogeneous array of different orientation variants of the martensite phase (self-accommodation) and by plastic deformation (plastic accommodation). For example, in the case of the martensitic transformation in high-carbon steel, elastic strain energy is reduced mainly by self-accommodation, and consequently, a twinned martensite is formed. On the other hand, for low-carbon steel, elastic strain energy is generally minimized by plastic accommodation. In this case, a lath martensite is formed and dense crystal defects are introduced into the microstructure [11]. Since the morphology of these martensitic microstructures is strongly related to the mechanical properties of steel, it is quite

essential for developing a novel steel to predict the formation of martensitic microstructure precisely.

The first theoretical models describing the martensitic transformation and reproducing the formation of a martensitic microstructure were Ginzburg-Landau (GL) models for a twinned martensitic structure [7-9]. These GL models were extended to time-dependent Ginzburg-Landau (TDGL) models for the self-accommodating twinned martensitic microstructure in shape memory alloys [12,13]. In these TDGL models, the deviatoric (shear) and dilatation strains are considered as order parameters in Landau theory. Recently, a phase-field (PF) model has been extensively studied as a powerful tool for predicting microstructural evolution and has been applied to the martensitic transformation [14-17]. In particular, Khachatryan and co-workers have proposed pioneer PF models of the martensitic transformations in various alloys based on the phase-field microelasticity theory [18-21]. Their PF models consider the probability of the orientation variants of the martensite phase as an order parameter and are used to evaluate the elastic strain energy of an arbitrary mixture of austenite and martensite phases. However, to the best of our knowledge, there are no TDGL or PF models of the martensitic transformation that take into account both self-accommodation and plastic accommodation.

The purpose of this study is to develop an elastoplastic PF model of the fcc-bcc martensitic transformation that takes into account strain energy relaxation due to both self-accommodation and plastic accommodation. Then, the two-dimensional evolution of a martensitic microstructure accompanied by elastic and plastic deformations is simulated using the developed PF model. In this paper, we discuss the effects of plastic deformation during the martensitic transformation on the minimization path of elastic strain energy and the morphology of the formed martensitic microstructure.

ELASTOPLASTIC PHASE-FIELD MODEL OF MARTENSITIC TRANSFORMATION

The elastoplastic PF model of the fcc-bcc martensitic transformation is constructed by employing the phase-field microelasticity theory for the evaluation of elastic strain energy [19] and the elastoplastic PF model suggested by Guo et al. [22].

In this model, the total free energy of the system is defined as the Ginzburg-Landau-type Gibbs free energy functional, which is the sum of chemical free energy, g_{chem} , elastic strain energy, g_{elast} , and gradient energy, g_{grad} .

$$G = \int_V (g_{chem} + g_{elast} + g_{grad}) dV \quad (1)$$

By considering that the chemical free energy is invariant with respect to any rotations and symmetries of the crystal lattice of the fcc parent phase, it can be formulated using the Landau polynomial expansion as [21]

$$g_{chem} = \Delta f \left\{ \frac{a}{2} (\phi_1^2 + \phi_2^2 + \phi_3^2) - \frac{b}{3} (\phi_1^3 + \phi_2^3 + \phi_3^3) + \frac{c}{4} (\phi_1^2 + \phi_2^2 + \phi_3^2)^2 \right\}, \quad (2)$$

where ϕ_p is the order parameter that describes the probability of the p th orientation variant of the martensite phase and $p = 1, 2, 3$ indicate three martensitic orientation variants whose tetragonality axes are along the three $\langle 100 \rangle$ directions in the martensite phase. ϕ_p changes from $\phi_p = 1$ in the p th martensite variant to $\phi_p = 0$ in the other variants and parent phases. Δf is the magnitude of driving force for the transformation, which is equal to the free energy difference between the martensite and parent phases. a , b and c are the expansion coefficients of the Landau polynomial expansion. In this study, we chose the coefficients $a = 0.15$, $b = 3a + 12$ and $c = 2a + 12$ [21, 23]. The gradient energy, which is defined as the sum of gradient energies due to the inhomogeneity of order parameters, is given as

$$g_{grad} = \frac{\kappa}{2} \sum_{p=1}^3 |\nabla \phi_p|^2, \quad (3)$$

where κ is the gradient energy coefficient.

The elastic strain energy of the system including an arbitrary mixture of martensite and parent phases is derived on the basis of the phase-field microelasticity theory as [18]

$$\mathcal{G}_{elast} = \frac{1}{2} C_{ijkl} (\varepsilon_{ij}^c - \varepsilon_{ij}^0) (\varepsilon_{kl}^c - \varepsilon_{kl}^0), \quad (4)$$

where C_{ijkl} is the elastic coefficient matrix. To describe the elastoplastic deformation during the martensitic transformation, the total stress-free strain ε_{ij}^0 is defined as the sum of the transformation stress-free strain $\varepsilon_{ij}^{00}(l)$ and plastic strain ε_{ij}^p as [23]

$$\varepsilon_{ij}^0 = \sum_{l=1}^3 \varepsilon_{ij}^{00}(l) \phi_l + \varepsilon_{ij}^p = \varepsilon_{ij}^{00}(1) \phi_1 + \varepsilon_{ij}^{00}(2) \phi_2 + \varepsilon_{ij}^{00}(3) \phi_3 + \varepsilon_{ij}^p. \quad (5)$$

As mentioned above, the three orientation variants can be produced during the fcc-bcc martensitic transformation. Thus, the transformation stress-free strains of the variants are given by the following three matrices:

$$\varepsilon_{ij}^{00}(1) = \begin{pmatrix} \varepsilon_3 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_1 \end{pmatrix}, \quad \varepsilon_{ij}^{00}(2) = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_3 & 0 \\ 0 & 0 & \varepsilon_1 \end{pmatrix}, \quad \varepsilon_{ij}^{00}(3) = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_3 \end{pmatrix}. \quad (6)$$

Here, the components of these matrices are derived on the basis of the Bain lattice correspondence as [6]

$$\varepsilon_1 = \frac{\sqrt{2} a_{bcc} - a_{fcc}}{a_{fcc}}, \quad \varepsilon_3 = \frac{a_{bcc} - a_{fcc}}{a_{fcc}}, \quad (7)$$

where a_{bcc} and a_{fcc} are the crystal lattice parameters of the martensite and parent phases, respectively. ε_{ij}^c is the total strain, defined as the sum of the homogeneous strain $\bar{\varepsilon}_{ij}^c$ and heterogeneous strain $\delta\varepsilon_{ij}^c$ as

$$\varepsilon_{ij}^c = \bar{\varepsilon}_{ij}^c + \delta\varepsilon_{ij}^c. \quad (8)$$

The homogeneous strain, which is a uniform macroscopic strain and describes the macroscopic shape deformation of the system, is derived as the spatial average of the total stress-free strain $\bar{\varepsilon}_{ij}^0$ as

$$\bar{\varepsilon}_{ij}^c = \bar{\varepsilon}_{ij}^0 = \int_V \varepsilon_{ij}^0 dV. \quad (9)$$

On the other hand, the heterogeneous strain, which is given by the elastic theory [23, 24], is given as

$$\delta\varepsilon_{ij}^c = \frac{1}{(2\pi)^3} \int_{\vec{k}} \left\{ \Omega_{ik}(\vec{n}) n_j n_l \hat{\sigma}_{kl}^0(\vec{k}) \right\} \exp(i\vec{k} \cdot \vec{r}) d\vec{k}. \quad (10)$$

Here, $\Omega_{ij}(\vec{n})$ is the Green function tensor, which is an inverse tensor, $\Omega_{ij}^{-1}(\vec{n}) \equiv C_{ijkl} n_j n_l$. \vec{k} indicates the reciprocal space vector and $\vec{n} \equiv \vec{k}/|\vec{k}|$ is the unit vector along the \vec{k} direction. $\hat{\sigma}_{ij}^0(\vec{k}) = C_{ijkl} \hat{\varepsilon}_{ij}^0$ is the Fourier transformation of $C_{ijkl} \varepsilon_{ij}^0$. Here, $\hat{\varepsilon}_{ij}^0$ is the Fourier transformation of the total stress-free strain.

The evolution of the martensite phase is described by the following TDGL equation of the order parameter ϕ_p ,

$$\frac{\partial \phi_p}{\partial t} = -L' \frac{\delta G}{\delta \phi_p} = -L' \left(\frac{\partial \mathcal{G}_{chem}}{\partial \phi_p} + \frac{\partial \mathcal{G}_{elast}}{\partial \phi_p} - \kappa^2 \nabla^2 \phi_p \right), \quad (11)$$

where L' is the kinetic parameter.

To consider the effects of the plastic deformation on the martensitic transformation, the evolution and distribution of plastic strain should be determined. According to the elastoplasticity theory, the plastic deformation is related to the shear strain energy described by deviatoric strain [25]. Thus, we assume that the evolution of plastic strain can be expressed by the TDGL equation derived from the following shear strain energy [25]:

$$\mathbf{g}_{el}^{shear} = \frac{1}{2} \int \sigma'_{ij} (\varepsilon'_{ij}{}^c - \varepsilon'_{ij}{}^0) dV = \frac{1}{2} \int 2G (\varepsilon'_{ij}{}^c - \varepsilon'_{ij}{}^0) (\varepsilon'_{ij}{}^c - \varepsilon'_{ij}{}^0) dV. \quad (12)$$

Here, σ'_{ij} , $\varepsilon'_{ij}{}^c$ and $\varepsilon'_{ij}{}^0$ are the deviatoric components of the Cauchy stress and the total strain and total stress-free strain tensors, respectively. On the basis of shear strain energy, the evolution of plastic strain is described by the following TDGL equation:

$$\frac{\partial \varepsilon_{ij}^p}{\partial t} = -K_{ijkl} \frac{\delta \mathbf{g}_{el}^{shear}}{\delta \varepsilon_{kl}^p}, \quad (13)$$

where K_{ijkl} is the fourth-order kinetic coefficient tensor. In this study, K_{ijkl} is chosen as $K_{ijkl} = (KC_{ijkl})^{-1}$ for simplicity [22, 24]. Note that Eqn. (16) is valid only in the plastic region where the Von-Mises equivalent stress $\bar{\sigma}$ satisfies the following yield criteria [22, 25]:

$$F_Y \equiv \bar{\sigma}^2 - \sigma_y^2 = \frac{1}{2} \left\{ (\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 \right\} + 3(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2) - \sigma_y^2 \geq 0. \quad (14)$$

Here, σ_y is the yield stress of the system.

NUMERICAL MODEL AND INITIAL CONDITION

The evolution of a martensitic microstructure during isothermal fcc-bcc martensitic transformation is simulated in two dimensions. The system is assumed to be an elastic-perfectly plastic material. Governing equations (Eqns. (11) and (13)) are solved by the finite difference method with periodic boundary conditions. The size of the computational domain is $0.25 \times 0.25 \mu\text{m}^2$ and the domain is divided into 128×128 meshes. The mesh size is $\Delta x = 3.9 \text{ nm}$ and the plane strain condition is assumed. Because we perform a two-dimensional simulation, the governing equations for ϕ_1 and ϕ_2 are solved. In this case, we assume that the total stress-free strain is reduced to,

$$\varepsilon_{ij}^0 = \begin{pmatrix} \varepsilon_3 & 0 \\ 0 & \varepsilon_1 \end{pmatrix} \phi_1 + \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_3 \end{pmatrix} \phi_2 + \varepsilon_{ij}^p \quad (15)$$

The initial condition in the computational domain is assumed to be the austenite phase and all order parameters are set to be zero. One circular nucleus of the martensite phase with diameter $d_0 = 55 \text{ nm}$, which is given by random numbers between 0 and 0.1, is located at the center of the computational domain. The isothermal transformation temperature is set to be constant at $T = 300 \text{ K}$. The transformation stress-free strains in Eqn. (15) are given by $\varepsilon_1 = 0.1112$ and $\varepsilon_2 = -0.1756$ [18]. The elastic and shear strain energies, i.e., Eqns. (4) and (12), are calculated using the following elastic constants: $C_{11} = 242$, $C_{22} = 112$ and $C_{12} = 84 \text{ GPa}$ [6]. The other numerical values and parameters are as follows: the gradient energy coefficient is $\kappa = 1.0 \times 10^{-15} \text{ J m}^2 / \text{mol}$ and the kinetic parameters of the TDGL equation for ϕ_p and ε_{ij}^p are set to be $K = 0.001$ and $L' = 1$, respectively.

RESULTS AND DISCUSSION

To study the effects of plastic deformation during the martensitic transformation on the kinetics of transformation and the morphology of the formed martensitic microstructure, we simulate the martensitic transformation in a linear elastic material whose yield stress is assumed to be $\sigma_y = 10000 \text{ MPa}$ and in an elastoplastic material with $\sigma_y = 800 \text{ MPa}$. Hereafter, we call the former case the elastic-martensitic transformation and the latter case the elastoplastic-martensitic transformation.

Figures 1 (a) and (b) show the evolutions of the martensitic phase on the (001) plane of the parent phase during the elastic- and elastoplastic-martensitic transformations, respectively. Here, yellow, red and blue regions correspond to the first and second orientation variants of the martensite phase, which are defined as $\phi_1 \geq 0.6$ and $\phi_2 \geq 0.6$, and the austenite phase, respectively. The time unit s' in Fig. 1 denotes dimensionless time. In the early stages of the transformations at $40 s'$, both results show that thin plate-shaped martensitic phases grow from the initial seed of the martensite phase into the $\langle 110 \rangle$ directions. The evolutions of equivalent stress during these transformations are shown in Figs. 2 (a) and

(b). A transformation-induced stress field is observed in and around the newly formed martensite phase due to transformation strain. Furthermore, we observe that the morphology of the simulated martensitic microstructure is similar to that of the butterfly-type martensite observed experimentally and by finite element simulation [26, 27]. As the martensitic transformation proceeds, the martensite phase grows along a transformation-induced high-stress region. It can be seen that a twin-related variant is formed near the variant formed in the early stages by the autocatalytic effect, as indicated by a white arrow in the figure at 45 s' in Fig. 1 (a) [28]. The morphology of the growing martensite phase exhibits the twin-related pair structure of the martensitic variants so as to eliminate the shear strain caused by the transformation.

Figure 3 shows the transformation curves for the elastic- and elastoplastic-martensitic transformations. The volume fraction of the martensite phase rapidly increases during the transformation. In both cases, elastic strain energy increases with increasing volume fraction of the martensite phase, as shown in Fig. 4. As mentioned above, elastic strain energy is reduced by the formation of self-accommodating martensite variants and by plastic deformation. In the case of the elastic-martensitic transformation, the orientation variants of the martensite phase formed in the early stages are rearranged so as to eliminate the twinned domain with a (110) habit plane, as indicated by black arrows in the figure at 60 s' in Fig. 1 (a). As a result, it can be observed that the final morphology of the martensitic microstructure produced by the elastic-martensitic transformation exhibits a single twinned martensitic structure with a (-110) habit plane. Because this self-accommodation of the martensitic variants induces the relaxation of internal stress, elastic strain energy decreases to zero.

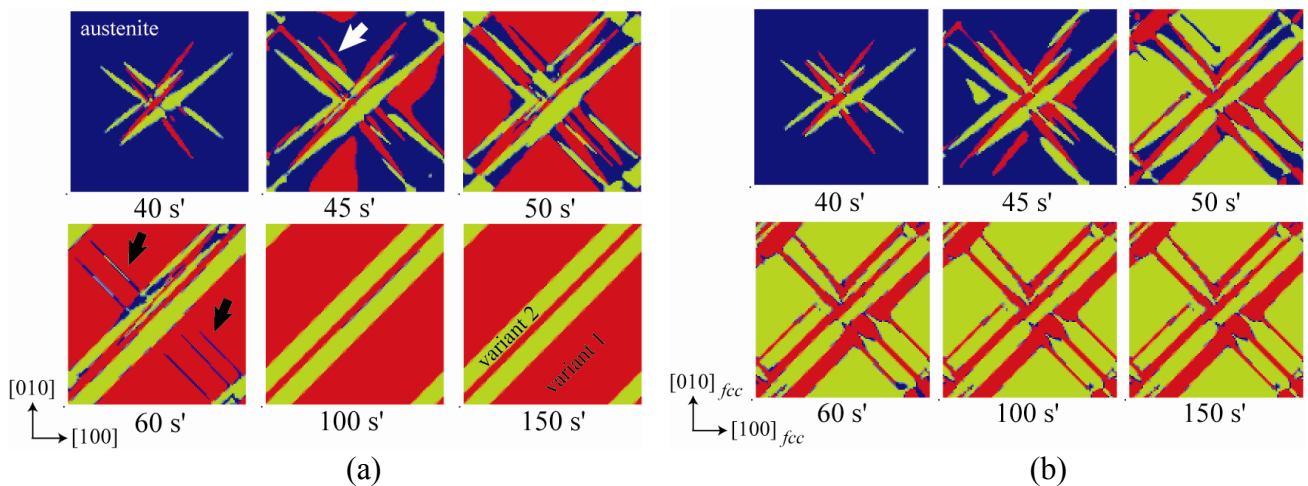


Fig. 1 Evolutions of orientation variants of martensite phase during (a) elastic- and (b) elastoplastic-martensitic transformations

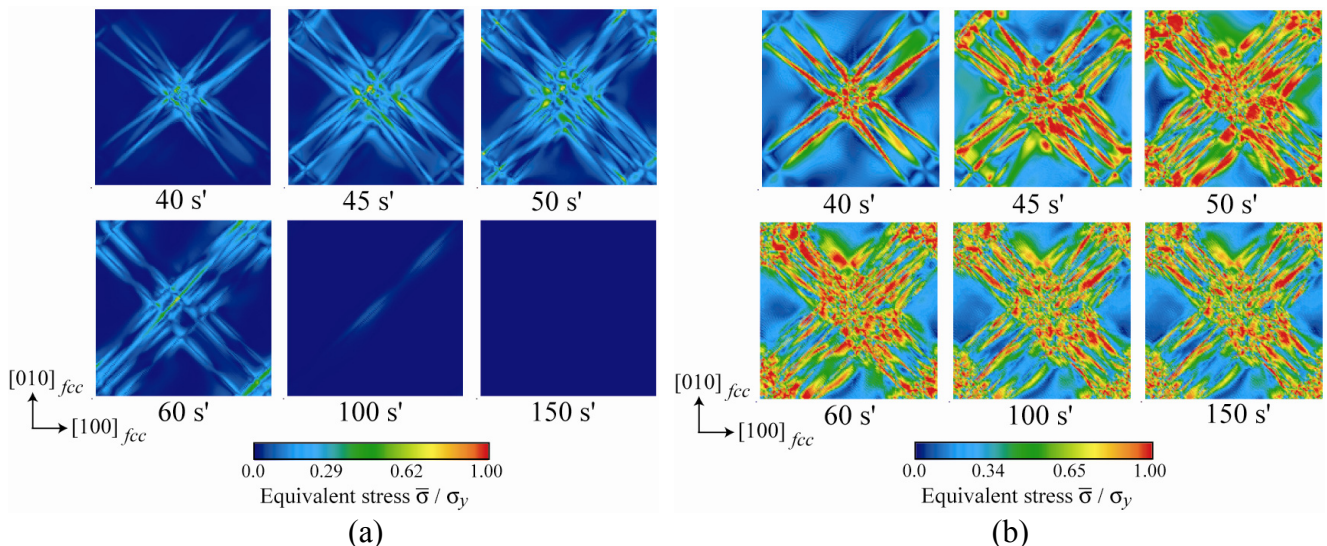


Fig. 2 Distributions of equivalent stress in (a) elastic- and (b) elastoplastic-martensitic transformations.

In the case of the elastoplastic-martensitic transformation, the growth of the martensite phase is accompanied by plastic deformation. The evolution of a plastically deformed region ($\varepsilon_{ij}^p > 0$) with the growth of the martensitic variants is shown in Fig. 5. Plastic strain is generated in both the martensite and austenite phases to compensate for the transformation strain. In this case, it is revealed that an increase in elastic strain energy in the elastoplastic-martensitic transformation is largely inhibited not only by the self-accommodation, i.e., the formation of a twinned martensitic structure, but also by the plastic accommodation. Owing to the marked release of elastic strain energy by the plastic accommodation, the rearrangement of twinned martensitic structures with a (-110) habit plane is arrested, as shown in Fig. 1 (b). Thus, the martensitic structure formed in the elastoplastic-martensitic transformation includes two different twinned martensitic structures with (110) and (-110) habit planes. Furthermore, it can be confirmed that the plastic deformation during the transformation causes residual stress in the microstructure and that the final value of elastic strain energy does not decrease to zero even long after isothermal holding.

Finally, it should be noted that our elastoplastic PF model can demonstrate the martensitic transformation accompanied by the elastic and plastic deformations in an elastic-perfectly plastic material. However, in real materials, since the evolution of the martensite phase is strongly affected by slip systems, we may need to extend our PF model to consider the slip systems and dislocation hardening in future studies.

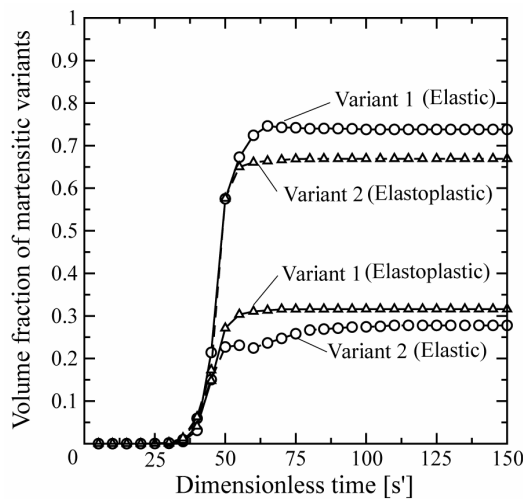


Fig.3 Variations in volume fractions of martensitic variants during (a) elastic- and (b) elastoplastic-martensitic transformations

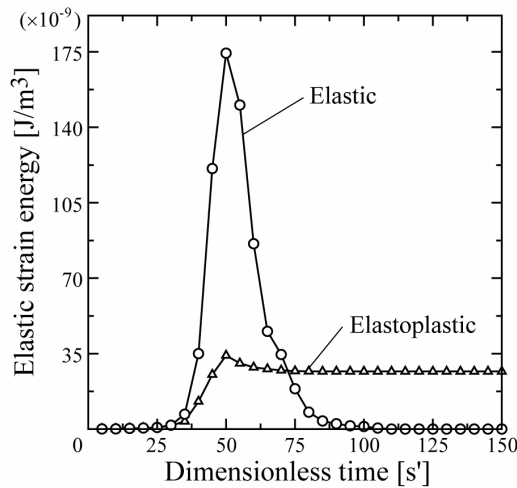


Fig.4 Variations in elastic strain energy during (a) elastic- and (b) elastoplastic-martensitic transformations

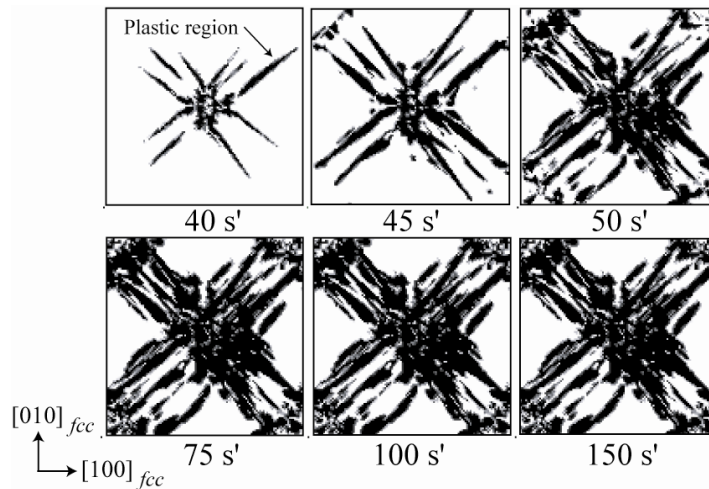


Fig. 5 Evolution of plastically deformed region during elastoplastic-martensitic transformation

CONCLUSIONS

An elastoplastic PF model for the martensitic transformation accompanied by the relaxation of elastic strain energy induced by elastic and plastic deformations was proposed. In this study, we investigated the effects of plastic deformation during the martensitic transformation on the kinetics of the transformation and the morphology of a martensitic microstructure using the proposed elastoplastic PF model. The results obtained from this study are as follows:

1. The proposed elastoplastic PF model can describe the evolution of the plastic deformation associated with the martensitic transformation by solving the TDGL equations for plastic strain. This model is utilized to predict the morphology of the martensite phase and the distribution of residual stress in the microstructure after the martensitic transformation.
2. For the elastic-martensitic transformation, the orientation variants of the martensite phase are self-accommodated to compensate for the transformation-induced stress field and to reduced elastic strain energy, which increases owing to the martensitic transformation. In this case, the final morphology of the martensite phase exhibits a single twinned martensitic structure, which results in zero elastic strain energy.
3. In the elastoplastic-martensitic transformation, the increase in elastic strain energy during the transformation is markedly suppressed by the plastic accommodation. Thus, the self-accommodation of the martensitic variants driven by elastic strain energy is inhibited, and a single variant martensitic structure is not formed.
4. Due to the plastic deformation during the elastoplastic-martensitic transformation, residual stress is arised in the microstructure. Because of this effect, elastic strain energy does not decrease to zero even long after isothermal transformation.

Acknowledgements The authors greatly acknowledge financial support though by the Japan Society for the Promotion of Science for Young Scientists.

REFERENCES

- [1] J. W. Christian, *The theory of transformation in metals and alloys*, Pergamon, Oxford, (2003).
- [2] P. M. Kelly and J. Nutting, *The martensite transformation in carbon steel*, Proc. R. Soc. Lond., Ser. A, Math. phys. Sci., 259, (1960), pp.45-58.
- [3] T. Maki and I. Tamura, *Morphology and Substructure of Lath Martensite in Steels*, Trans. ISIJ., 67, (1981), pp.852-866. (in Japanese)
- [4] Y. Tomita and T. Iwamoto, *Computational prediction of deformation behavior of of TRIP steels under cyclic loading*, Int. J. Mech. Sci., 43, (2001), pp.2017-2034.

- [5] V. I. Levitas, A. V. Idesman and D. L. Preston, *Microscale simulation of martensitic microstructure evolution*, Phys. Rev. Lett., 93, (2004), 105701.
- [6] Z. Nishiyama, *Martensitic transformations*, Academic press inc., New York, (1978).
- [7] F. Falk, *Ginzburg-Landau theory of static domain walls in shape-memory alloys*, Z. Physik B – Condensed Matter., 51, (1983), pp.177-185.
- [8] G. R. Barsh and J. A. Krumhansl, *Twin boundaries in ferroelastic media without interface dislocations*, Phys. Rev. Lett., 53, (1983), pp.1069-1072.
- [9] A. E. Jacobs, *Landau theory of a constrained ferroelastic in two dimensions*, Phys. Rev. B., 52, (1995), pp. 6327-6331.
- [10] S. Xiaoyan and G. Nanju, *The self-accommodation and plastic accommodation effects during the formation of $\{259\}_f$ lenticular martensite*, ISIJ Int., 36, (1996), pp.592-594.
- [11] S. Morito, H. Tanaka, R. Konishi, T. Furuhashi and T. Maki, *The morphology and crystallography of lath martensite in Fe-C alloys*, Acta Mater., 51, (2003), pp.1789-1799.
- [12] S. R. Shenoy, T. Lookman, A. Saxena and A. R. Bishop, *Martensitic textures : Multiscale consequences of elastic compatibility*, Phys. Rev. B, 60, (1999), R12537.
- [13] R. Ahluwalia, T. Lookman, A. Saxena and R. C. Albers, *Landau theory for shape memory polycrystals*, Acta Mater., 52, (2004), pp.209-218.
- [14] R. Kobayashi, *Modeling and numerical simulations of dendritic crystal growth*, Phys. D, 63, (1993), pp.410-423.
- [15] A. Yamanaka, T. Takaki and Y. Tomita, *Phase-Field simulation of austenite to ferrite transformation and Widmännstätten ferrite formation in Fe-C alloy*, Mater. Trans., 47, (2006), pp.2725-2731.
- [16] T. Takaki and Y. Tomita, *Two-dimensional phase-field simulation of self-assembled quantum dot formation*, J. Crystal Growth, 287, (2006), pp.459-499.
- [17] Y. -W. Cui, T. Koyama, I. Ohnuma, K. Oikawa, R. Kainuma and K. Ishida, *Simulation of hexagonal-orthorhombic phase transformation in polycrystal*, Acta Mater., 55, (2007), pp.233-241.
- [18] A. G. Khachaturyan, *Theory of structural transformations in solids*, John Wiley & Sons Ltd., New York, (1986).
- [19] Y. Wang and A. G. Khachaturyan, *Three-dimensional field model and computer modeling of martensitic transformations*, Acta Mater., 45, (1997), pp.759-773.
- [20] A. Artemev, Y. Jin and A. G. Khachaturyan, *Three-dimensional phase field model of proper martensitic transformation*, Acta Mater., 49, (2001), pp.1165-1177.
- [21] Y. M. Jin, A. Artemev and A. G. Khachaturyan, *Three-dimensional phase field model of low-symmetry martensitic transformation in polycrystal: simulation of ζ'_2 martensite in AuCd alloys*, Acta Mater., 49, (2001), pp.2309-2320.
- [22] X. H. Guo, S-Q. Shi, X. Q. Ma, *Elastoplastic phase field model for microstructure evolution*, Appl. Phys. Lett., 87, (2005), 221910.
- [23] T. Koyama and H. Onodera, *Phase-field simulation of microstructure changes in Ni_2MnGa ferromagnetic alloy under external stress and magnetic fields*, Mater. Trans., 44, (2003), pp.2503-2508.
- [24] Y. U. Wang, Y. M. Jin and A. G. Khachaturyan, *The effects of free surfaces on martensitic microstructures: 3D phase-field microelasticity simulation study*, Acta Mater., 52, (2004), pp.1039-1050.
- [25] Y. Tomita, *Computational elastoplasticity*, (1990), YOKENDO Ltd. (in Japanese)

- [26] M. Umemoto, E. Yoshitake and I. Tamura, *The morphology of martensite in Fe-C, Fe-Ni-C and Fe-Cr-C alloys*, J. Mater. Sci., 18, (1983), pp.2893-2904.
- [27] P. Xu and J. W. Morris, Jr., *Computer simulation of martensitic transformation in constrained two-dimensional crystals under external stress*, Metall. Trans., 24A, (1993), pp.1281-1294.
- [28] Q. P. Meng, Y. H. Rong and T. Y. Hsu, *Effect of internal stress on autocatalytic nucleation of martensitic transformation*, Metel. Mater. Trans. A., 37A, (2006), pp. 1405-1411.