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Phase-field simulation of lenticular martensite and inheritance of the accommodation dislocations

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Abstract. A phase-field simulation is performed to study the substructure evolution of lenticular martensite in TRIP steels. The evolution of martensitic phase variants and dislocations is calculated by a coupled phase-field micro-elasticity model. The simulations at isothermal conditions show that during the phase transformation, the accommodation dislocations evolving in the austenite are inherited by the martensitic phase and cause the further evolution of a single martensitic variant in the direction of the dislocation slip. As a result of the interaction, a change of the growth mode from twining to slip can be observed in accordance to the substructure formation of lenticular martensite. This interaction between the dislocations and martensitic phase depends on dislocation slip systems and the orientation of the martensitic variants as well as on the energy barriers for the phase transformation and for the dislocation motion.

1 Introduction

The interaction between the martensitic transformation (MT) front and plastic deformation is one of the most important phenomenon in the theory of solid-solid transformations due to their numerous applications in material science. During MT, the accommodation dislocations evolve in the austenitic matrix and interact with the transformation front. This interaction can change thermodynamics, nucleation, growth kinetics, microstructure, hysteresis and irreversibility of the phase transformation. The plastic accommodation process in soft matrix caused by MT is often called the "Greenwood-Johnson" effect. The plastic deformation process due to the formation of preferred variants under small stresses is often denominated as "Magee" effect. Both processes belong to the transformation-induced plasticity (TRIP) phenomenon and can occur simultaneously [1, 2]. The phenomena of TRIP is utilized in many hight temperature deformation processes to obtain an optimal combination of strength and ductility of steels and ceramics.

The phase-field (PF) models have been extensively developed as a powerful tool for predicting the nucleation and microstructure evolution during MT. Khachaturyan and co-workers proposed a PF model for the simulation of MT in various alloys based on the micro-elasticity theory of Khachaturyan and Shatalov [3–6]. This approach integrates micro-elasticity into the phase-field model based on the time-dependent Ginzburg-Landau (TDGL) equations and enables the development of a reciprocal-space formulation of the strain energy as an explicit functional of arbitrary continuous distributions of structural and/or compositional non-uniformities. The method considers in a continuous way, the evolution of martensitic orientation variants as the evolution of order parameters and it can be used to evaluate the elastic strain energy of an arbitrary mixture of solid phases and their orientation variants. The method has been extended to investigate martensitic transformations in single crystals [7], polycrystalline systems [8] and to investigate the effect of applied stresses and defects on MT [9].

For the investigation of the dislocation dynamics, a phase-field model of dislocations was developed utilizing the similarity between the solid-solid phase transformations and dislocations by Wang et al. [10–12], Hu et al. [13, 14], Jin et al. [15], Shen et al. [16], Levitas et al. [17]. The main idea follows from the phase-field microelasticity theory developed for martensitic phase transformations. It is widely used along with other dislocation models reviewed in Ref. [18] for modeling plastic deformation by dislocation motion at the nanoscale.

Recently, the study of the interaction of solid-solid phase transformation and dislocation evolution by means of the phase-field model were started by Levitas et al. [19]. They developed a coupled phase-field approach as a combination of the own advanced phase-field models for MT [20] and dislocation evolution [17] with nontrivial coupling terms. The simulations were carried out by means of finite element approach in a small 2D system with one martensitic variant. The nucleation of the dislocations on the transformation front and their evolution in both phases were observed and analyzed.

A similar phase-field approach is adopted in the present work to study the effect of individual dislocations distributed in the austenite near the MT front on the substructure formation during the growth of a single plate of

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lenticular martensite as well as the effect of MT on dislocation dynamics. For this study, we have chosen the lenticular martensite as a representative complex system with two structure elements: twins and dislocations. The substructure of lenticular martensite consist of three regions: (i) the completely twinned “midrib” region which is similar to thin plate martensite, (ii) the “twinned region” which consist of the twins extending from the midrib and has not regular structure, (iii) the “untwinned” or “slip” region which consist of two areas, the first one with several sets of screw dislocations and the second one with a high density of accommodation dislocations which are inherited from the parent austenite [21]. It is expected that the change of the growth mode from twining to slip can be caused by an increase in the local temperature produced by the latent heat of the transformation.

Recently, we developed a continuous approach which combines the phase field model of MT with the evolution of the plastic strain and the dislocation density field calculated by the slip evolution law [22, 23]. This approach uses phenomenological interaction parameters which have to be estimated. Furthermore, it can be applied only on microscale because of the continuous dislocation field. In this work we use the phase-field model for the evolution of individual dislocations along with the phase transformation to study the mechanism of the interaction of the MT front with the accommodation dislocations on the nanoscale. The kinetics of MT is described as before by the elasto-plastic phase-field model for MT based on the works Wang et al. [4] and Zhang et al. [9]. The evolution of the dislocations is calculated according to the phase-field model of dislocations based on the models of Wang et al. [11] and Levitas et al. [17, 24] in 3 dimensions. We simulate the evolution of a martensitic plate with and without dislocations and show the transition from the twinned to untwinned region in the presence of the dislocations of a specific slip system.

2 Evolution of phase field order parameters of MT

In order to model the microstructure evolution of a lenticular martensitic plate, we choose the phase-field model variant suggested in Ref. [4] and extend it by the improvements from the model variant in Ref. [9] concerning the incorporation of the dislocation field and the new form of the Fourier transform. Here, the evolution of the order parameters of martensitic variants η_p will be combined with the evolution of the order parameters of dislocations ψ_β. The elasto-plastic phase-field kinetic equation for a martensitic variant p in dimensionless form is

$$\frac{\partial \eta_p(\mathbf{r})}{\partial t} = \phi \nabla^2 \eta_p(\mathbf{r}) - f'_{\eta_p} + 2\xi\eta_p \int c_{ijkl}\varepsilon^0_{kl}(p) e_i \Omega_{jm}(\mathbf{e}) \hat{\sigma}^0_{mn}(\mathbf{k}) e_n \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \frac{d^3\mathbf{k}}{(2\pi)^3}, \tag{1}$$

where the stress σ^0_{mn} is calculated as

$$\sigma^0_{mn}(\mathbf{r}) = c_{mnkl}\Big[\sum_{q=1}^{\nu} \varepsilon^0_{kl}(q)\left(\eta^2_q(\mathbf{r}) - \langle\eta^2_q\rangle\right) + \sum_{\beta=1}^{\mu} \varepsilon^d_{kl}(\beta)\left(h(\psi_\beta)(\mathbf{r}) - \langle h(\psi_\beta)\rangle\right)\Big] \tag{2}$$

and the Fourier transform of the stress $\hat{\sigma}^0_{mn}$ is calculated by

$$\hat{\sigma}^0_{mn}(\mathbf{k}) = \int_V \sigma^0_{mn}(\mathbf{r}) \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{r}. \tag{3}$$

Here c_{ijkl} are the components of the elastic modulus tensor, Ω_{jm} is the Green tensor, $\langle\eta^2\rangle$ and $\langle h(\psi)\rangle$ are the volume averaging functions, ν is the number of the martensitic variants and μ is the number of the slip systems, e_i are components of a unit vector $\mathbf{k}/k$ in reciprocal space. Furthermore, $\varepsilon^d(\beta) = \frac{1}{H^\beta}\mathbf{b}^\beta \otimes \mathbf{n}^\beta$ is the parameter which represents the plastic strain of dislocations, $\mathbf{b}^\beta$ is the Burgers vector, $\mathbf{n}^\beta$ is a normal to a slip plane and $H^\beta = 100$ is a hight of a dislocation band. The Green tensor is calculated as $\Omega_{jm} = \frac{\delta_{jm}}{G} - \frac{e_j e_m}{2G(1-\upsilon)}$, where G is the shear modulus and υ is the Poisson coefficient.

The first term on the right hand side of Eq. (1) is the gradient term, which forces interfaces to have a finite width. The second term is the derivative of the local specific free energy with respect to the order parameter. The free energy function is defined as the Landau polynomial expansion

$$f(\vec{\eta}) = \frac{1}{2}a_2 \sum_{p=1}^{3} \eta_p^2 - \frac{1}{3}a_3 \sum_{p=1}^{3} \eta_p^3 + \frac{1}{4}a_4 \left(\sum_{p=1}^{3} \eta_p^2\right)^2, \tag{4}$$

where $a_2 = 0.312$, $a_3 = 3a_2 + 12\Delta f$ and $a_3 = 2a_2 + 12\Delta f$ with Δf ss the chemical driving force of MT or the dimensionless undercooling.

The quadratic form of the order parameter function in eq. (2) is chosen because it produces a regular twinned structure. We will show that this model allows to simulate both the twinned region corresponding to the midrib in the lenticular martensite plate and the formation of untwinned region with the dislocations.

3 Evolution of phase field order parameters of dislocations

For the calculation of the evolution of the dislocation order parameters, we use the theory of the dislocation evolution developed in [10–12] and further extended in [17]. The phase-field kinetic equation for a slip system α in dimensionless form is similar to the martensitic phase transformation

$$\frac{\partial \psi_\alpha(\mathbf{r})}{\partial t} = \phi^d \left[\nabla^2 \psi_\alpha(\mathbf{r}) - (\mathbf{n}^\alpha \cdot \nabla)(\nabla\psi_\alpha \cdot \mathbf{n}^\alpha)\right] - 2A^d \psi_\alpha(1-\psi_\alpha)(1-2\psi_\alpha) + \xi^d h'_{\psi_\alpha} \int c_{ijkl}\varepsilon^d_{kl}(\alpha) e_i \Omega_{jm}(\mathbf{e}) \hat{\sigma}^0_{mn}(\mathbf{k}) e_n \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \frac{d^3\mathbf{k}}{(2\pi)^3}, \tag{5}$$

Table 1. Dimensionless material and phase-field model parameters used in the simulation

Parameter	Value
Shear modulus, G	1
Poisson coefficient, ν	0.374
Time step, Δt	0.125
Gradient coefficient, ϕ	0.0162
Gradient coefficient, ϕ^d	0.004
Lattice coefficient, A^d	0.005
Elastic energy coeff., ξ	9.0
Elastic energy coeff. of disl., ξ^d	9.0
Undercooling, Δf	0.02

where the stress σ^0_{mn} and the Fourier transform of the stress $\hat{\sigma}^0_{mn}(\mathbf{k})$ are calculated by eqs. (2) and (3). The second gradient term can be written in a component form as

$$(\mathbf{n}^\alpha \cdot \nabla)(\nabla\psi_\alpha \cdot \mathbf{n}^\alpha) = \frac{\partial^2\psi_\alpha}{\partial r_i \partial r_k} n_i^\alpha n_k^\alpha. \quad (6)$$

The model function is defined as $h(\psi_\alpha) = \psi_\alpha^2(3 - 2\psi_\alpha)$.

In the following, we assume that the dislocations will form and evolve only in the austenite. Furthermore, the growth of the opposite orientation variant in the dislocation loop is not allowed. We consider a single crystal system of the austenite, i.e. a system which contains in initial state only one grain without boundaries.

4 Numerical results and discussion

Equations (1) and (5) are solved for a 3D system by using the fast Fourier transform technique. We simulate two orientation variants of the martensitic phase { ε_3^0, ε_2^0, ε_1^0 } and { ε_1^0, ε_3^0, ε_2^0 } with eigenstrains, as for Fe-Ni alloys, $\varepsilon_1^0 = \varepsilon_2^0 = 0.1322$, $\varepsilon_3^0 = -0.1994$. One slip system in the austenite is chosen with the slip plane $(\bar{1}11)$ and the slip direction $[\bar{1}10]$. The material parameters and phase-field model parameters used in the simulations are listed in Table 1. The discretization grid size corresponds to $\Delta x = 2.5$ nm that corresponds to the twin thickness of 10 nm.

One nucleus containing 2 martensitic variants is generated in the center of a box of size $64 \times 64 \times 64$. Periodic boundary conditions are applied for all sides.

The simulated microstructure during MT at the time $2400\Delta t$ is shown in Fig. 1 in the 2D cross-sections perpendicular to axises [100], [010] and [001]. The final microstructure consists of one martensitic plate of two martensitic variants in the austenitic matrix.

In the next step of the procedure, 4 nuclei of dislocations were inserted equidistantly on the top of the box near the martensitic plate to see the difference of the evolution of the martensitic variants on the top and on the bottom of the simulation box, i.e. with and without dislocations. All dislocations belong to one slip system and therefore we use only one order parameter ψ. In the second case, 4 nuclei of dislocations were inserted on the top and 4 nuclei on the bottom of the box near the martensitic plate to produce a symmetric substructure. The simulation box is elongated in z-direction in order to give space for the dislocation evolution.

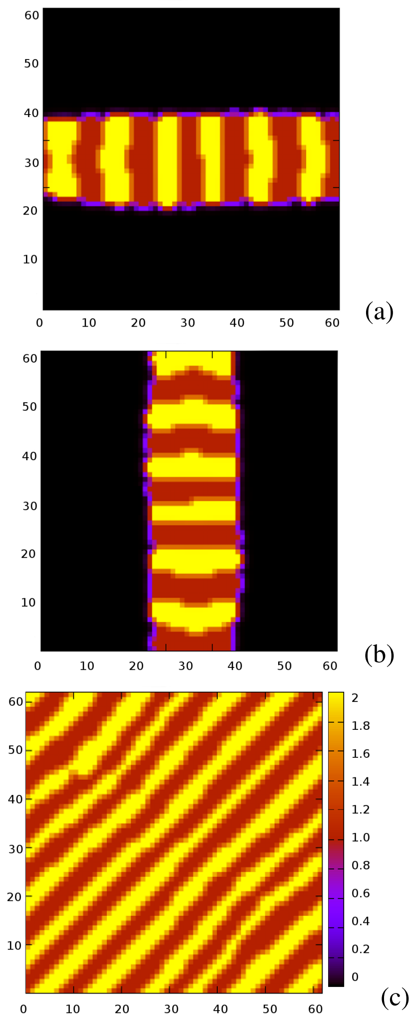

Figure 1. 2D cross-sections of simulated microstructure of the martensitic plate perpendicular to the axises [010] (a), [101] (b) and [001] (c) at $2400\Delta t$ without dislocations. Two martensitic variants are indicated by red and yellow color.

In Fig. 2 the 2D cross-sections of the simulated microstructure perpendicular to the axis [010] are shown for the box of size $64\times64\times96$ with 4 dislocations (a) and with 8 dislocation (b) at $4800\Delta t$. Two martensitic variants are indicated by red and yellow color. During the microstructure evolution, the dislocations are inherited by the MT front of one martensitic variants and thereby a slip region of lenticular martensite can be formed. It can be seen in Fig. 2 (a) that on the top of the simulation box one martensitic variant (which is indicated by yellow color) evolves together with the dislocation order parameter but on the bottom of the simulation box the martensitic variants does not grow essentially after 3600 time steps. In Fig. 2 (c) the order parameter of dislocations, which evolve in the substructure, is shown, where one dislocation loop forms for one dislocation nucleus.

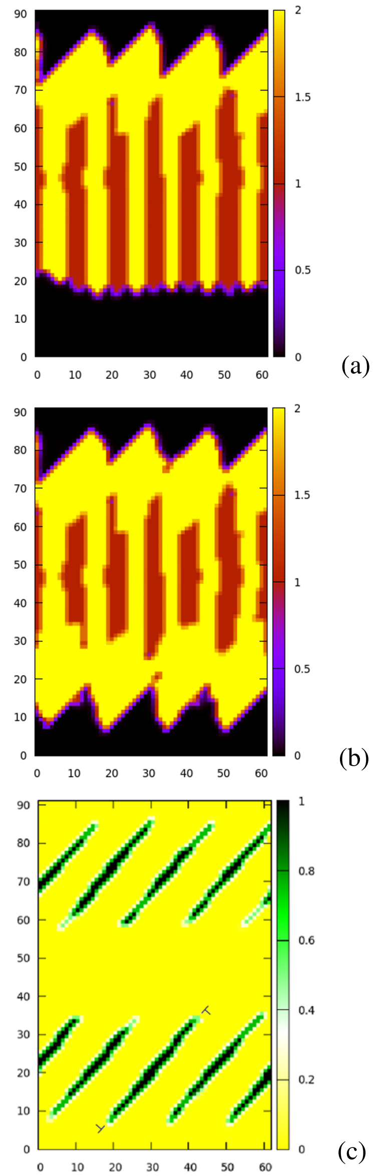

Figure 2. 2D cross-sections of simulated microstructure of MT at $4800\Delta t$: (a) phases in the box of size 64x64x96 with 4 dislocations; (b) phases in the box of size 64x64x96 with 8 dislocations; (c) the order parameter of 8 dislocations. The dislocations of the slip system $\mathbf{n} = (\bar{1}11)$, $\mathbf{b} = [\bar{1}10]$ are initialized on the top and the bottom side of the martensitic plate and evolve during the simulation. Two martensitic variants are indicated by red and yellow color.

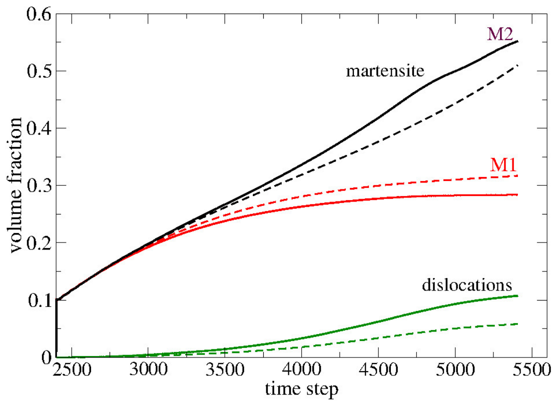

Figure 3. Time evolution of the volume fraction of the martensite f_m and the volume density of the order parameter of dislocations f_d. The dashed and solid lines are responsible for 4 and 8 dislocations in the system respectively. M1 and M2 indicate two martensitic variants.

The evolution of the volume fraction of martensitic phases f_m and the volume density of dislocations f_d for two cases are plotted in Fig. 3. The volume density of dislocations is calculated as the space averaged order parameter. This value can be recalculated to the dislocation line density by $\rho = 2\sqrt{\pi f_d / V\Delta x}$; for $f_d = 0.1$, $\rho \approx 3 \cdot 10^{14}$ 1/m^2. The evolution is shown for two cases: with 4 and 8 dislocations.

For different slip systems, the kinetic behavior of the dislocations will be different. For example, for the slip system $(\bar{1}11)$, [101] the dislocation loops previously developed in the austenite will collapse while attracting the transformation front and can not be inherited in the martensite. There is also a possibility to include a random nucleation of dislocations of various slip systems and investigate the influence of the dislocation density on the dislocation inheritance. We can expect that the systematic study of the dislocation/front interaction by means of the presented model in the future studies will contribute to the evaluation of the phenomenological parameters for the dislocation inheritance in the continuous dislocation approach [23].

5 Conclusion

In this work, we study the effect of individual dislocations evolving in the austenite near the transformation front on the formation of the substructure of a single plate of lenticular martensite as well as the effect of MT on the dislocation evolution. For this study, we have chosen the lenticular martensite as a representative complex system with dislocations. The elasto-plastic phase-field model for the evolution of individual dislocations is used to study more precisely the mechanism of the interaction of the MT front with the accommodation dislocations in comparison to the previously developed continuum dislocation field approach. The kinetics of MT and the evolution of dislocations are combined together by coupling terms in evolution equations. We simulated the evolution of the thin martensitic plate with and without dislocations and showed the transition from twinned to slip regions in the presence of dislocations of a specific slip system. In the untwinned region, a single martensitic variant grows due to the interaction with the plastic strain of the dislocations. Correspondingly, the growth of the dislocation order parameter is accelerated due to the interaction with the transformation elastic strain.

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