

ЧЕБЫШЕВСКИЙ СБОРНИК
Том 18 Выпуск 3

УДК 539.3, 519.6

DOI 10.22405/2226-8383-2017-18-3-363-376

ПОДХОД ФАЗОВОГО ПОЛЯ
К ВЗАИМОДЕЙСТВИЮ МЕЖДУ
ФАЗОВЫМИ ПЕРЕХОДАМИ
И ПЛАСТИЧНОСТЬЮ
НА НАНОРАЗМЕРНОМ
УРОВНЕ ПРИ БОЛЬШИХ ДЕФОРМАЦИЯХ

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Аннотация

В статье рассматривается современный подход теории фазового поля (ПТФП) к взаимодействию между фазовыми переходами (ФП) и дислокациями на наноразмерном уровне. Он разрабатывается при больших деформациях как нетривиальное сочетание нового прогрессивного подхода теории фазового поля с мартенситными фазовыми переходами и эволюцией дислокаций. Выполняется моделирование на основе метода конечных элементов (МКЭ) для решения совместных уравнений теории фазового поля и теории упругости. Эволюция дислокаций и фазы высокого давления в наногранулированном материале, находящемся под действием давления и сдвига, изучается и используется для интерпретации экспериментальных результатов по фазовым переходам, вызванным пластической деформацией, под действием высокого давления в камере вращения алмазной наковальни.

Ключевые слова: подход теории фазового поля, фазовые переходы, дислокации, взаимодействие, наноразмерный уровень.

Библиография: 13 названий.

PHASE FIELD APPROACH TO
INTERACTION BETWEEN PHASE
TRANSFORMATIONS AND PLASTICITY AT
THE NANOSCALE AT LARGE STRAINS

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Abstract

In the paper, our recent phase field approach (PFA) to the interaction between phase transformations (PTs) and dislocations at the nanoscale is reviewed. It is developed at large strains as a nontrivial combination of our recent advanced PFAs to martensitic PTs and dislocation evolution. Finite element method (FEM) simulations are performed to solve the coupled phase-field and elasticity equations. The evolution of dislocations and high pressure phase in a nanograined material under pressure and shear is studied and utilized for interpretation of experimental results on plastic strain induce PTs under high pressure in rotational diamond anvil cell.

Keywords: phase field approach, phase transformations, dislocations, interaction, nanoscale.

Bibliography: 13 titles.

1. Introduction

Interaction between martensitic PTs and dislocations is of great importance for various applications such as transformation-induced plasticity [1], plastic shear induced PTs under high pressure [2, 3], martensite nucleation and growth [4, 5, 6], and heat and thermomechanical treatments of steels. The main focus of the current paper is to review our recent work on PFA to interaction between evolving martensitic PTs and discrete dislocations at the nanoscale and at large strains. A thermodynamically consistent PFA for the coupled PT and dislocation evolution at the nanoscale was developed in [7–10]. This theory synergistically combines fully geometrically nonlinear theory for martensitic PTs [11–14] and dislocations [7, 15, 16], with nontrivial interactions and inheritance of dislocations during PTs. Corresponding numerical approaches presented in [11, 17] for PTs, in [7, 18] for dislocations, and in [8, 9, 19, 20] for interaction of dislocations and PTs. Note that for PTs [11, 17], the Levin's method of multiple superposition of finite deformations [21–23] have been utilized.

2. Complete system of equations [10, 19]

Both parts of the theory that describe PT and dislocation evolution satisfy some important requirements related to the thermodynamic equilibrium and instability conditions as well as provide the stress- and temperature-independent thermodynamically equilibrium transformation deformation gradient and Burgers vector [13,16]. They also reproduce some important features of the stress-strain curves, and allow one to include all thermomechanical properties of both austenite and martensitic variants [13,16]. PFA to dislocation evolution also defines dislocation height by equations rather than by computational mesh, which was typical for the previous approaches. Thus, it leads to a well-posed formulation and mesh-independent dislocation height H for any dislocation orientation. The

gradient energy for dislocations contains an additional term, which excludes localization of dislocation within height smaller than H without producing interfacial energy. The interaction between dislocations and PT is included in terms of kinematics and dependence of all material parameters for dislocations on the order parameter for PT η . Interaction also occurs through stress fields and is determined by solution of coupled phase field and nonlinear mechanical problems.

2.1. Kinematics

The following multiplicative decomposition of the deformation gradient $\mathbf{F}$ into elastic $\mathbf{F}_e$, transformational U_t , and plastic F_p parts is justified [10]:

$$\mathbf{F} = \mathbf{F}_e \cdot U_t \cdot F_p. \quad (1)$$

The expression for U_t vs. the order parameter η for a single martensitic variant, which satisfy thermodynamic equilibrium and instability conditions, is derived [13]:

$$U_t = \mathbf{I} + [a\eta^2(1 - \eta)^2 + (4\eta^3 - 3\eta^4)] \varepsilon_t; 0 < a < 6, \quad (2)$$

where ε_t is the transformation strain tensor and $\mathbf{I}$ is the unit tensor. For the austenite, $\eta = 0$; for the martensite, $\eta = 1$.

An additivity of the plastic velocity gradients for different slip systems is postulated, similar to the crystal plasticity:

$$l_p := \dot{F}_p \cdot F_p^{-1} := \sum_{\alpha=1}^p \frac{1}{H^\alpha} b^\alpha \otimes n^\alpha \dot{\Upsilon}(\xi_\alpha) = \sum_{\alpha=1}^p \gamma_\alpha m^\alpha \otimes n^\alpha \dot{\Upsilon}(\xi_\alpha);$$

$$\Upsilon = (\bar{\xi}_\alpha)^2 (3 - 2\bar{\xi}_\alpha) + \text{Int}(\xi_\alpha). \quad (3)$$

Here ξ_α is the order parameter for a dislocation in a slip system α , which varies between $n - 1$ and n when $n - 1$ complete dislocations exist and the n_{th} dislocation appears; $\text{Int}(\xi_\alpha)$ and $\bar{\xi}_\alpha$ are the integer and the fractional parts of ξ_α , respectively; b^α is the Burgers vector of the slip system α , H^α is the height of dislocation band, n^α is the unit vector normal to the slip system, m^α is the unit vector in the direction of b^α , and $\gamma_\alpha = \frac{|b^\alpha|}{H^\alpha}$ is the plastic shear strain.

2.2. Helmholtz free energy

The Helmholtz free energy per unit mass can be expressed as the sum of elastic energy ψ^e , thermal energy for PT ψ_η^θ , crystalline energy for dislocations ψ_ξ^c , the energy of interaction of dislocation cores belonging to different slip systems ψ_ξ^{int} , and gradient energies related to martensitic PT ψ_η^∇ and dislocations ψ_ξ^∇ as follows

$$\psi = J_t \psi^e + \psi_\eta^\theta + \psi_\xi^c + \psi_\xi^{int} + \psi_\eta^\nabla + \psi_\xi^\nabla; J_t = \det U_t. \quad (4)$$

The simplest finite-strain elastic energy is

$$\rho_0 \psi^e = \frac{1}{2} E_e : C : E_e, \quad (5)$$

where ρ_0 is the mass density in the reference configuration, $\mathbf{C}$ is the fourth-rank elastic moduli tensor, and $E_e = \frac{1}{2}(F_e^T \cdot F_e - I)$ is the Lagrangian elastic strain tensor. The thermal energy is derived as

$$\rho_0 \psi_\eta^\theta = A_0 (\theta - \theta_c) \eta^2 (1 - \eta)^2 - \Delta s (\theta - \theta_e) (4\eta^3 - 3\eta^4), \quad (6)$$

where θ_c is the critical temperature at which stress-free austenite loses its stability, θ_e is the phase equilibrium temperature, Δs is the change in the entropy, and A_0 is a material parameter.

The crystalline energy for dislocations is accepted as follows

$$\rho_0 \psi_\xi^c = \sum_{\alpha=1}^p A_\alpha (\eta, \bar{y}^\alpha) (\bar{\xi}_\alpha)^2 (1 - \bar{\xi}_\alpha)^2; A_\alpha (\eta) = A_\alpha + (A_\alpha^M - A_\alpha^A) \eta^2 (3 - 2\eta);$$

$$A_\alpha (\bar{y}^\alpha) = \begin{cases} \bar{A}_\alpha & \bar{y}^\alpha \leq H^\alpha; \\ k \bar{A}_\alpha & \bar{y}^\alpha > H^\alpha; \end{cases} \quad \bar{y}^\alpha = y^\alpha - \text{Int} \left(\frac{y^\alpha}{H^\alpha + d^\alpha} \right) (H^\alpha + d^\alpha), \quad (7)$$

in which PTs and the inheritance of slip systems during PTs are taken into account. The coefficient $A_\alpha (\eta, \bar{y}^\alpha)$ characterizes the phase dependent theoretical yield strength. $A_\alpha (\eta, \bar{y}^\alpha)$ is a periodic step-wise function of the coordinate y^α along the normal to the corresponding slip plane α . The parameter A_α is equal to its normal value $\bar{A}_\alpha$ within each dislocation band of the height H^α and $k \bar{A}_\alpha$ ($k \gg 1$) in a thin boundary layer between dislocations of the width d^α . Thus, it excludes the spreading of the dislocation outside the desired dislocation band.

The energy of interaction of dislocation cores belonging to different slip systems is expressed in the following form

$$\rho_0 \psi_\xi^{int} = \sum_{\alpha=1}^p A_{\alpha k} (\eta) (\bar{\xi}_\alpha)^2 (1 - \bar{\xi}_\alpha)^2 (\bar{\xi}_k)^2 (1 - \bar{\xi}_k)^2; A_{\alpha\alpha} = 0;$$

$$A_{\alpha k} (\eta) = A_{\alpha k}^A + (A_{\alpha k}^M - A_{\alpha k}^A) \eta^2 (3 - 2\eta), \quad (8)$$

where $A_{\alpha k}^A$ and $A_{\alpha k}^M$ are the coefficients of the energy of interaction of dislocation cores in the austenite and martensite, respectively. The interaction energy penalizes simultaneous presence of dislocations belonging to different slip systems at the same material point. For PTs with only one martensitic variant, the gradient energy is

$$\rho_0 \psi_\eta^\nabla = \frac{\beta_\eta}{2} |\nabla \eta|^2, \quad (9)$$

where β_η is the coefficient of the gradient energy for PT. For dislocations, the gradient energy takes into account variation of the gradient energy coefficients $\beta_\xi (\eta)$ during PTs:

$$\rho_0 \psi_\xi^\nabla = \frac{\beta_\xi(\eta)}{2} \sum_{\alpha=1}^p ((\nabla^m \xi_\alpha)^2 + M (1 - \bar{\xi}_\alpha)^2 (\nabla^n \xi_\alpha)^2);$$

$$\beta_\eta(\eta) = \beta_\xi^A + (\beta_\xi^M - \beta_\xi^A) \eta^2 (3 - 2\eta), \quad (10)$$

where β_ξ^A and β_ξ^M are the coefficient of the gradient energy for dislocations in austenite and martensite, respectively; M is the ratio of the coefficients for the gradient energy normal to and along the slip plane; ∇^m and ∇^n are the gradient operators along and normal to the slip system α , respectively.

2.3. The first Piola-Kirchhoff P and Cauchy σ stresses

$$P = \rho_0 J_t F_e \cdot \frac{\partial \psi}{\partial E_e} \cdot U_t^{-1} \cdot F_p^{T-1}; \sigma = \rho J_t F_e \cdot \frac{\partial \psi}{\partial E_e} \cdot F_e^T, \quad (11)$$

where ρ is the mass density in the current (actual) configuration.

2.4. The Ginzburg-Landau equations for PTs and dislocations

The Ginzburg-Landau equations for PTs and dislocations represent linear kinetic relationship between the rates of the order parameters and conjugate driving forces:

$$\dot{\eta} = L^\eta \left(\frac{1}{\rho_0} P^T \cdot F_e : \frac{\partial U_t}{\partial \eta} \cdot F_p + \nabla \cdot \left(\frac{\partial \psi}{\partial \nabla \eta} \right) - \frac{\partial \psi}{\partial \eta} \right);$$

$$\dot{\xi}_\alpha = L_\alpha^\xi(\eta) \left(\frac{1}{\rho_0} \tau_\alpha \gamma_\alpha \frac{\partial \Upsilon}{\partial \xi_\alpha} + \nabla \cdot \left(\frac{\partial \psi}{\partial \nabla \xi_\alpha} \right) - \frac{\partial \psi}{\partial \xi_\alpha} \right);$$

$$L_\alpha^\xi(\eta) = L_\alpha^A + (L_\alpha^M - L_\alpha^A) \eta^2 (3 - 2\eta); \tau_\alpha = n^\alpha \cdot F_p \cdot P^T \cdot F_e \cdot U_t \cdot m^\alpha, \quad (12)$$

where L_α^A and L_α^M are the kinetics coefficients for dislocations in the austenite and martensite, respectively. Momentum balance equation is expressed as $\nabla \cdot P = 0$. The boundary conditions for PTs and dislocations are $\nabla \eta \cdot k = 0$ and $\nabla \xi_\alpha \cdot b^\alpha = 0$, respectively, where k is the unit normal to the external surface. For some problems, periodic boundary conditions are applied.

FEM algorithms for the formulated system of equations have been implemented in code COMSOL.

3. Evolution of dislocations and high pressure phase in a nanograined material under pressure and shear

Application of high pressure to materials is a well-known way to discover new high pressure phases (HPPs) and phenomena. It is known from numerous

experiments that superposition of large plastic shear in rotational Bridgman or rotational diamond anvil cell (RDAC) [2,3,24-29] can lead to new phases that were not obtained under hydrostatic conditions and significantly reduces PT pressure. For example, a new high-density amorphous phase of SiC was observed in situ under pressure of 30 GPa and large shear [26] but no PTs were obtained under hydrostatic pressure up to 130 GPa. There are many examples that application of plastic straining reduces PT pressure by a factor of 2 to 10 for some PTs, including PTs to superhard phases of BN [25,29].

A basic understanding of the physics responsible for such drastic reduction in PT pressure is still in the development. It was demonstrated [2,3,9] that a simple addition of the work of shear stress along the transformation shear strain to the macroscopic mechanical driving force (which is minus pressure times volumetric transformation strain) does not change transformation pressure significantly. This is because macroscopic shear stress is limited by the yield strength in shear (~ 1 GPa), which is small in comparison to the applied pressure, e.g., 10-50 GPa.

The fundamental difference between the *plastic strain-induced* PTs under high pressure and *pressure-induced or stress-induced* PTs was first formulated in [2,3]. Pressure-induced or stress-induced PTs initiate at pre-existing defects at stress below the yield strength, while plastic strain-induced PTs occur by nucleation at new defects (e.g., dislocation pile-ups) produced during plastic straining, which cause stronger stress concentrations than the pre-existing defects. That is why plastic strain-induced PTs require completely different thermodynamic and kinetic treatment and experimental characterization, which is coupled to generation of defects and stress concentrators. To describe strain-induced PTs under high pressure at the nanoscale, a simple analytical model of nucleation at the tip of a dislocation pile-up in infinite space was developed in [2,3]. Despite the simplicity, this model explained many experimental results on PTs in RDAC and developed our intuition on the interaction between PTs and plasticity at the nanoscale.

Below, we review much more advanced results of studying HPP nucleation and evolution at the tip of a dislocation pile-up in a bicrystal under uniaxial compression and shear [9,20]. All size and time parameters are normalized by 1nm and 1ps, respectively. Plane strain problems and straight edge dislocations are considered. For the chosen material parameters, the phase equilibrium pressure between low and high pressure phases is 10 GPa; the critical pressure for the instability of the low pressure phase 20 GPa. With a single dislocation as a nucleation site, PT starts and almost completes at hydrostatic pressure of $p_h = 15\text{GPa}$. A rectangular sample with the size of 50×20 is considered which includes two nanograins surrounded by two areas at the top and bottom of the sample, each with the size of 50×5 , which play role as elastic accommodators (Fig. 1). A horizontal dislocation band is located in the middle of the left grain. Two dislocation systems inclined at $\pm 30^\circ$ from the horizontal line are located in the right grain. The lower side of the sample is fixed in both directions, the periodic boundary conditions are applied at the lateral sides, and a vertical stress is applied to the upper side in the deformed state. The upper side is also subjected

to a horizontal displacement u (which is given in terms of prescribed macroscopic shear $\gamma = u/h$, with the height of grains $h = 20$). In the first problem, dislocation activity in the right grain is forbidden. Under the applied shear, dislocations of opposite signs are nucleated from both grain boundaries in the left grain and create dislocation pile ups. The pile-ups produce strong concentration of the stress tensor near their tips, which significantly increase the local transformation work. Thus, the external pressure required for PT can be drastically decreased. For example, in this problem due to the generation of 3 dislocation piled ups due to applied $\gamma = 0.2$, the PT pressure is reduced from $P_h = 15\text{GPa}$ to 1.2GPa (an averaged pressure over grains after PT). This explains drastic reduction of the PT pressure due to applied shear in experiments for various materials [2,3,24,25,29]. Figs. 2a and b show the coupled solutions for PT and dislocations at some initial stage ($t=0.5$) and the stationary solution in the right grain, respectively. The phase concentration, i.e. the ratio of the transformed area to the initial total area in the right grain, reaches $c=0.51$. Such a significant transformation progress is due to the small distance between stress concentrators, which leads to a coalescence of nuclei and corresponding morphological transition.

When dislocations in the right grain are included, besides the promoting effect of plasticity on PT, it also suppresses PT by relaxing stresses at other concentrators. The solutions for PT and dislocations with two dislocation systems in the transformed grain are presented in Figs. 2c and d. Several dislocations nucleated at the tip of the pile up and propagated through the right grain. Due to stress relaxation, almost no high pressure phase appears at the left side of the right grain. For the same reason, PT is also suppressed in the right side of the right grain and the transformed region (Fig. 2c) is smaller than that in Fig. 2b. Therefore, while the number of dislocations increases, coalescence does not occur and the stationary solution is reached with $c=0.19$ and 6 and 3 dislocations in the lower and the upper dislocation systems, respectively.

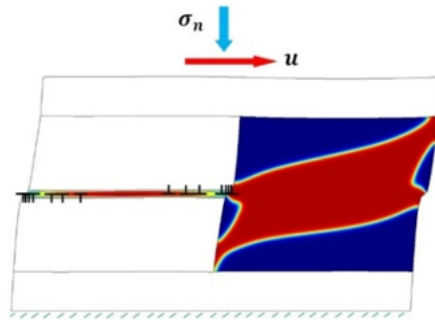


Fig. 1. Schematics of the sample under pressure and shear and stationary solution. Dislocations in the left grain cause transformation from the low-pressure (blue) to the high (red) pressure phases [9].

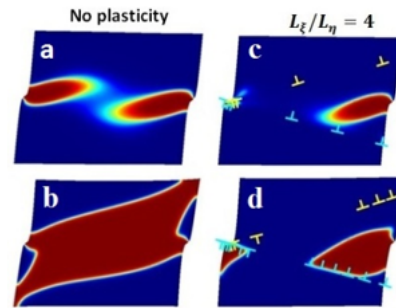


Fig. 2. The solution for PT without plasticity in the right grain at $t=0.5$ (a) and for the stationary state (b). The coupled PT and dislocation solutions at $t=0.5$ (c) and for the stationary state (d) [9].

Thus, dislocations play a dual role: in addition to creating stress concentrators and promoting PTs, they may relax stresses at other concentrators, thus

competing with PT. Some combinations of the applied normal and shear stresses have been found for which PT wins the competition, see Fig. 3.

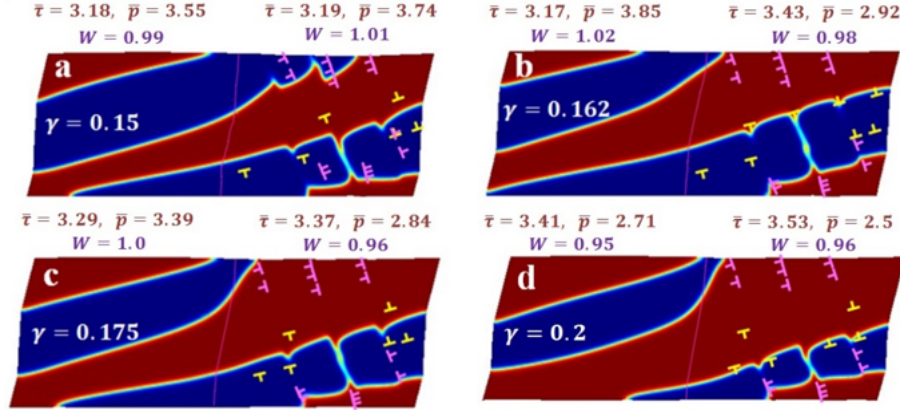


Fig. 3. Stationary phase and dislocation microstructures for different applied shears [9].

While nucleation is determined by the strong stress concentration, the stationary martensite morphology is determined by the equilibrium values of transformation work, i.e., by the simplest phase equilibrium condition. Indeed, the interface positions perfectly coincide with the lines corresponding to the equilibrium transformation work, both with and without plasticity (Fig. 4).

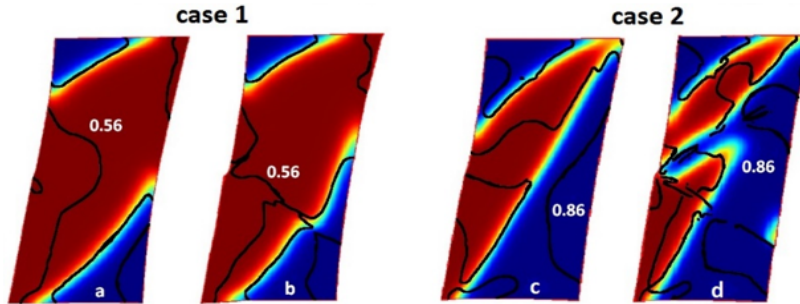


Fig. 4. Stationary phase state and contour line of the equilibrium transformation work for

case 1 without (a) and with plasticity (b), and for case 2 without (c) and with plasticity (d) [19]. Cases 1 and 2 differ by some material parameters.

Various parametric studies of this problem, as well as various other problems can be found in [9,19,20].

4. Concluding remarks

To summarize, a PFA to the interaction between PTs and dislocations at large strains is presented, which includes the following main features of the interaction event:

- (a) multiplicative kinematic decomposition of the deformation gradient into elastic, transformational, and plastic contributions;
- (b) inheritance of dislocations of austenite in martensite during martensitic PT and dislocations of martensite in austenite during reverse PT;

(c) dependence of all material parameters for dislocations on the order parameters for PT.

Problems for temperature and stress-induced PTs interacting with dislocation evolution are solved and several effects including the dual effect of plasticity on PT, athermal interface resistance caused by dislocations, and inheritance of dislocations of martensite in austenite for stress-induced PT are found [9,19,20]. Important next step should be inclusion of partial dislocations and dislocation reactions, in particular, for dislocations inherited by the growing phase. A similar approach can be developed for the interaction of dislocations with twins and diffusive PTs, as well as electromagnetic and reconstructive PTs. For multivariant martensitic PTs, the thermodynamic potentials developed in [30,31] can be utilized.

5. Acknowledgements

The support of NSF (CMMI-1536925 and DMR-1434613), ARO (W911NF-17-1-0225), and Iowa State University (Schafer 2050 Challenge Professorship) is gratefully acknowledged.

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Получено 19.05.2017

принято в печать 14.09.2017