Chapter 23

Properties of Phase Microstructures and Their Interaction with Dislocations in the Context of TRIP Steel Systems

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Abstract Transformation Induced Plasticity (TRIP) steels undergo a diffusionless phase transformation from austenite to martensite, resulting in a material exhibiting desirable material properties such as exceptional balance of strength and ductility as well as good fatigue behavior. Computational modeling at the mesoscale is potentially a suitable tool for studying how plastic deformation interacts with phase transformations and ultimately affects the bulk properties of these steels. We introduce models that represent the phase microstructure in a continuum approach and couple a time-dependent Ginzburg-Landau equation with discrete dislocation via their elastic strain energy densities. With this, the influence of several dislocation configurations are examined, namely a single dislocation, a “penny-shaped crack”, and a “dislocation cascade”. It is shown that the strain due to the presence of dislocations has a significant influence on the resultant martensitic microstructure. Furthermore, the importance of using a non-local elasticity approach for the dislocation stress fields is demonstrated.

23.1 Introduction

The solid-solid phase transformation in transformation induced plasticity (TRIP) steels leads to desirable properties for engineering applications. In the case of a Cr-Mn-Ni steel matrix, a high fault austenite phase is converted to α -martensite, and a high number of dislocations are active during the process of phase transformation, as also seen via in situ experiments, e.g., as in [1].

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Computer simulations and numerical modeling of TRIP-steels can be very beneficial for understanding the interaction of different microstructural phenomena, such as planar defects (e.g., phase transformations) and linear defects (dislocations), all of which may have significant influence on the mechanical properties of the bulk material. Dislocations are responsible for plastic deformation of metals; they may interact among themselves and can also be nucleated, e.g., during martensitic phase transformations. The combination of martensitic phase transformations and dislocation activity results in lattice distortions and may ultimately lead to increased work hardening.

Predictive modeling requires to spatially resolve the relevant physical phenomena and to describe their evolution in time. E.g., molecular dynamics (MD) simulations are inherently able to model both phase transformations and dislocations [2–4]. However, the computational cost for solving Newton’s equation of motion together with the interaction of *all* atoms for volumes and strain rates that are comparable to experimentally used ones is very high. As a consequence, typical MD simulations operate with strain rates that are several orders of magnitudes higher than the experimentally used strain rates and, at the same time, are also restricted to relatively small systems with typical sizes ranging from several nanometers to a few hundreds of nanometers.

Phenomenological continuum models of plasticity can reach relevant timescales and length scales, however, details regarding phase transformations or dislocations can only be incorporated indirectly and are generally not directly based on the underlying mechanisms. A macroscopic continuum model also cannot resolve the interface of two phases properly due to a highly coarsened resolution. Phase field models (PFMs) are based on the minimization of total energy and are “mesoscopic” methods in which individual atoms or their interactions are not explicitly represented, but in which microscopic effects are still able to be considered. However, this requires either input from lower scale methods or parameterization with experimental data.

The general phase field approach is based on a set of order parameters, $\phi_1, \dots, \phi_n$, continuous functions in space, which represent the different phases in the system. The time evolution of the order parameters is governed by the minimization of total energy. Based on this, the relevant physical properties are described as functions of the order parameters. The governing PFM equation is the time dependent Ginsburg-Landau (TDGL) evolution equation [5], first implemented for martensitic phase transformations by Khachaturyan [6].

In the following we will introduce a coupled phase field—dislocation framework that shows how dislocations or idealized cracks interact with phase boundaries between a martensitic and an austenitic phase. A second focus is then on a general approach in the context of non-local elasticity for representing the stress field of discrete dislocations.

The following nomenclature is employed throughout this chapter: We denote vectors by bold lower case latin $\mathbf{a}$ and greek α letters, and the dot operator “ $\cdot$ ” denotes the scalar product $\mathbf{a} \cdot \mathbf{b} \in \mathcal{R}$. We will, however, abuse this notation and use the dot “ $\cdot$ ” as well for inner products, whenever appropriate.

Second order tensors are denoted by bold uppercase latin letters $\mathbf{A}$. We introduce a scalar product between second order tensors denoted by “ $:$ ” as $\mathbf{A} : \mathbf{B} := \text{tr} \mathbf{A} \cdot \mathbf{B}^\top$,

where $\mathbf{B}^\top$ is the transpose of $\mathbf{B}$ and $\text{tr}(\cdot)$ denotes the trace operator. In an inner product space this product implies the norm $\|\mathbf{A}\| := \sqrt{\mathbf{A} : \mathbf{A}}$. Given an orthogonal tensor $\mathbf{R}$ and an arbitrary order tensor Φ , $\mathbf{R} * \Phi$ denotes the RAYLEIGH product of $\mathbf{R}$ and Φ ; for a second order tensor $\mathbf{A}$, we have $\mathbf{R} * \mathbf{A} = \mathbf{R} \cdot \mathbf{A} \cdot \mathbf{R}^\top$.

Third order tensors are denoted by bold calligraphic letters $\mathcal{A}$ and “ $\dot{\cdot}$ ” is the corresponding full contraction operator. Fourth order tensors are denoted by black board upper case letters $\mathbb{A}$.

23.2 Interaction Between Martensitic Phase Transformations and Dislocations

23.2.1 Phase Field Equations

The high strain induced via a phase transformation between face centered cubic (FCC) austenite and body centered cubic (BCC) martensite may trigger the nucleation of a large number of dislocations inside the material. Both dislocations and martensitic phase transformations affect the bulk properties of steels, and therefore, representing the interaction between dislocations and interfaces, and how this affects the phase transformation are essential for micromechanical modeling.

Thus, our computational model consists of two parts: the evolution of the phase microstructure is governed by the TDGL equation which minimizes the total energy in the system. The second part of the model considers discrete edge dislocations in a two-dimensional domain, for which an analytical solution of stress is available [7]. Such methods of coupling PFM and dislocations have been successfully applied for materials such as nickel-based superalloys [8, 9]. The modeling of the phase transformation will not consider any intermediate phases, and therefore only one order parameter, ϕ , is needed. It will also be assumed in the model that inside the martensitic phase, the dislocation mobility will approach zero, resulting in no movement of the dislocations inside the martensite phase. The TDGL requires the gradient energy at the phase boundary, the elastic strain energy, and a transformation potential. Here, contributions to the free energy arise from the elastic energy, W , the separation potential, f , and gradient energy. The time-dependent evolution of the order parameter is then given by

$$\frac{\partial \phi}{\partial t} = -M \left(\frac{\partial W}{\partial \phi} + G \left(\frac{\kappa_s}{L_{\text{char}}} \frac{\partial f}{\partial \phi} + \kappa_g L_{\text{char}} \Delta \phi \right) \right), \quad (23.1)$$

where ϕ is the order parameter describing the current phase at each point in space. The material specific parameters are mobility, M , interfacial energy density, G , characteristic length scale, L_{char} , and the calibration constants, κ_s and κ_g , which control the width of the interface between the two phases [10].

Fig. 23.1 Potential of phase transition. The two wells signify martensite variants 1 and 2. The local maximum signifies a metastable austenite phase

W is the elastic strain energy density which takes the form

$$W(\varepsilon, \phi) = \mathbf{E}_{\text{el}} : \mathbf{S} \quad (23.2)$$

where $\mathbf{E}_{\text{el}}$ is the elastic strain tensor and $\mathbf{S}$ is the stress tensor.

The second term describes the potential of phase transformation. In our model, we use a so-called “2-4-6 potential” (see Fig. 23.1), given as

$$f(\phi) = \frac{(3A^2 - 1 - 2\phi^2)(1 - \phi^2)^2}{(3A^2 - 1)}, \quad (23.3)$$

where A is a fit parameter which can be obtained from lower scale simulation methods. The final term accounts for the gradient of the interface between the two phases [11].

23.2.2 Dislocations and Mechanical Equilibrium Conditions

The stress field around a dislocation follows—outside the core region—linear elasticity. Any solid body in static equilibrium obeys the mechanical equilibrium equation, i.e., the divergence of the stress tensor, $\mathbf{S}$, must be zero,

$$\nabla \cdot \mathbf{S} = 0. \quad (23.4)$$

While this follows from the conservation of linear momentum, the conservation of angular momentum is responsible for the symmetry of the stress tensor, $\mathbf{S} = \mathbf{S}^T \Leftrightarrow S_{ij} = S_{ji}$. Assuming linear elastic material, the stresses and strains are related by the

stiffness tensor, $\mathbb{C}$, as

$$\mathbf{S} = \mathbb{C} : \mathbf{E}_e(\mathbf{E}, \phi), \quad (23.5)$$

where, in a phase field ansatz, the elastic strain tensor, $\mathbf{E}_e(\mathbf{E}, \phi)$, is a function of the order parameter as well as of the total strain, $\mathbf{E}$. We assume a small strain context in our model, and therefore strains may be additively decomposed into their elastic and inelastic parts:

$$\mathbf{E}_e(\mathbf{E}, \phi) = \mathbf{E} - \mathbf{E}_{\text{inel}}. \quad (23.6)$$

The tensor of inelastic strains, $\mathbf{E}_{\text{inel}}$, consists of the transformation strain $\mathbf{E}_{\text{tr}}$ and the dislocation eigenstrain $\mathbf{E}_{\text{dis}}$. In the following we will only consider a horizontal slip system in a plane strain model. The plane components of the stress tensor for a single dislocation in an infinite, linear elastic medium then follow the following analytical solution [7]:

$$S_{11} = \frac{-\mu b}{2\pi(1-\nu)} \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2}, \quad (23.7)$$

$$S_{22} = \frac{-\mu b}{2\pi(1-\nu)} \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}, \quad (23.8)$$

$$S_{12} = \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}, \quad (23.9)$$

where b is the absolute value of the Burgers vector, μ is the shear modulus, and ν is Poisson's ratio. In order to avoid the unphysical diverging behavior close to the dislocation core, a numerical regularization approach as proposed in [12] is used; a physically more rigorous approach is presented in the subsequent section. The resulting stress components are shown in Fig. 23.2. The strain tensor, which governs the dislocation eigenstrain, can then be straightforwardly obtained from $\mathbf{E}_{\text{dis}} = \mathbb{C}^{-1} : \mathbf{S}$. Equation (23.2) couples the phase field model and the dislocation model through the eigenstrain of dislocations and the eigenstrain contribution due to the phase transformation. While in this work we only consider stationary dislocation configurations, in general, the equation of motion for the dislocations would be a second equation where the two models are coupled.

23.2.3 Simulation Setup and Boundary Conditions

In order to observe the interaction between the dislocation and the phase field interface, a martensitic phase transformation needs to be triggered first. In our first simulation setup this is done via a martensitic “seed”, which is an artificial inclusion of the martensite phase. The first simulation setup consists of a circular martensitic seed surrounded by an austenite matrix, as shown in Fig. 23.3a, with one dislocation placed inside the austenite phase. The entire domain measures 200 nm by 200 nm.

Fig. 23.2 Individual components to the stress tensor for a single dislocation, according to (23.7)–(23.9)

In our second simulation setup we use a penny-shaped crack, as shown in Fig. 23.3b, to initiate a phase transformation. The introduction of several stationary positive and negative dislocations on either ends of a crack mode II crack tip effectively mimics a small crack inside of a material. The equivalent dislocation distribution function of the crack is given by Weertman [13].

In both setups, free boundaries were considered. To avoid a rigid body motion, the domains were fixed in one corner, and in an adjacent corner, a zero displacement was prescribed in vertical direction only to avoid over-constraining the system. The two martensite variants are considered by one order parameter which is $\phi = 1$ for variant 1 and $\phi = -1$ for variant 2. The simulations progress by time integrating the TDGL, and we let them evolve until a quasi-static configuration is reached. The numerical implementation was done using the finite element method. We used quadratic shape functions and a rectangular mesh with 100 elements into each direction.

Fig. 23.3 Schematic of initial setups of the simulations showing **a** a martensitic seed surrounded by an austenite matrix, and **b** a penny-shaped crack in an austenite matrix

23.2.4 Simulation Results

23.2.4.1 Martensitic Seed and Edge Dislocation

Our first simulation set up considers the geometry and initial values shown in Fig. 23.3a. Figure 23.4 shows the order parameter, the S_{12} component of the stress tensor, and the elastic energy density at three distinct points in time. The initial configuration with the circular seed is an artificial and energetically highly unfavorable microstructural state. This is why immediately at the beginning of the simulation the horizontal and vertical martensitic bands originating from the location of the seed were created, as shown in the first snapshot. However, due to the spatially heterogeneous structure with changing transformation strains across the interfaces stresses and elastic strain energy are still high (Fig. 23.4 bottom and middle row) which show that equilibrium has not yet reached.

The TDGL minimizes total energy in the system, so as time progresses, the system will attempt to transform into a state where energy decreases. If there was no dislocation present, the system would be perfectly symmetric in the vertical and horizontal direction, and there would be no physical reason for one band to be preferred. The preferred band direction would only be decided based on numerical errors or other artifacts. However, the introduction of the dislocation breaks the symmetry (compare the right red region of the stress in Fig. 23.4 at $t = t_s$) and thereby determines the growth direction of the band. At the intermediate time step t_m , the horizontal band has already shrunk to nearly 50% of its original thickness, and the energy as well as the stress level have strongly decreased.

Fig. 23.4 Temporal evolution of order parameter, elastic energy density, and S_{12} with one dislocation. t_s is an early point in time, t_m is an intermediate time, and at t_e the quasi-static state is reached

At the quasi-stationary time, a fully formed, vertical martensitic band structure is observed, and a minimized energy and stress is reached. The band structure is at equilibrium because the total strain is exactly the eigenstrain (except for the dislocation contribution), resulting in a deformed but stress-free state. However, the stress around the dislocation will not change because the dislocation is fixed in place. The “try” to relax this further causes a slight distortion from the original straight interface, as seen in Fig. 23.4. The shear stress at t_e still shows very slight remnants of the vertical phase microstructure; the reason is that the interface of the martensite band is not perfectly straight but has small fluctuations due to the used finite element approximation. Reducing the element size would remedy this effect.

23.2.4.2 Penny Shaped Crack in Austenitic Matrix

The introduction of a penny shaped crack induces enough eigenstrain in the system to trigger a phase transformation and is therefore an interesting way to get rid of the artificial initial seed. Similar as in the previous example, at the first snapshot in time, two perpendicular martensite bands can be observed (Fig. 23.5, left). Here, the stress field of the crack is responsible for the symmetry breaking. Again, the heterogenous microstructure causes a high stress and high strain energy density, which also decreases during the time integration of the TDGL equation. At the intermediate time step, one can additionally observe that the interfaces of the vertical band are pinned into place by the stress field of the crack, compare the slightly wavy structure of the band in Fig. 23.5. This “bump” is then progressing towards the top and the bottom such that at the stationary state the band stretches into vertical direction and has a thickness that is dictated by the crack length as shown in the right column in Fig. 23.5. At this point on time, a relaxed state with a minimum energy and a minimized stress is reached.

Fig. 23.5 Evolution in time of order parameter, elastic energy density, and S_{12} with a penny-shaped crack

23.3 On the Interaction of Planar Defects with Dislocations Within the Phase-Field Approach

23.3.1 Introduction

Phase field approaches have proven to be a very powerful tool for the investigation of the formation and evolution of microstructures due to solid-solid phase transformations and twinning. This appears to be the natural framework for the investigation of the interaction of planar crystal defects such as phase- or twin-boundaries with line defects (dislocations, disclinations). A typical phase field model for diffusionless (martensitic) transformations comprises of an evolution equations of ALLEN-CAHN-type for the order parameters ϕ_β

$$M_\beta \dot{\phi}_\beta = \alpha \Delta \phi_\beta - \rho \partial_{\phi_\beta} \psi, \quad (23.10)$$

where M_β and α are constants, ρ denotes the mass density, and ψ is a bulk free energy density. Assuming a small perturbation setting, the linear strain tensor $\mathbf{E}$ can be additively decomposed into elastic $\mathbf{E}_e$ and inelastic (i.e., eigenstrain) $\mathbf{E}_{tr}$ contributions, such that $\mathbf{E}_e(\mathbf{E}, \phi_\beta) = \mathbf{E} - \mathbf{E}_{tr}(\phi_\beta)$. Assuming linear elasticity, the stress $\mathbf{S}$ is given by $\mathbf{S} = \mathbb{C} : \mathbf{E}_e(\mathbf{E}, \phi_\beta)$, and the free energy density takes the form

$$\psi(\mathbf{E}, \phi_\beta, \theta) = \frac{1}{2} \mathbf{E}_e(\mathbf{E}, \phi) : \mathbb{C} : \mathbf{E}_e(\mathbf{E}, \phi) + \psi_b(\phi_\beta, \theta). \quad (23.11)$$

As a consequence, the evolution equation (23.10) can be rewritten as

$$M_\beta \dot{\phi}_\beta = \alpha \Delta \phi_\beta + \mathbf{S} : \partial_{\phi_\beta} \mathbf{E}_{tr} - \rho \partial_{\phi_\beta} \psi_b. \quad (23.12)$$

In classical elasticity theory the stresses diverge as the defect line is approached. In particular for dislocations the singularity is of $1/r$ -type. As per (23.12), this results in singular driving forces for the evolution of the order parameters, effectively negating the concepts such as a nucleation barrier or a pile-up stress. Different approaches to regularize the stress in the core region exist in literature based either on the concept of a distributed BURGER's vector [12, 14–16] or generalized continuum theories [17–20]. However, the first strain gradient approach advocated by Po et al. [20] has the advantage that the obtained regularization is independent of the type of defect in question and therefore does not require any defect-specific information for the determination of model parameters. In principle, these parameters can directly be obtained from atomistic interaction potentials [21].

The purpose of this work is to follow a micromorphic approach and to derive a framework which consistently couples first strain gradient elasticity to ALLEN-CAHN-type microstructure evolution ensuring non-singular driving forces on the order parameters in the presence of line defects.

23.3.2 Balance Equations and Boundary Conditions

The principle of virtual power (PVP) provides a systematic way of deriving field equations and boundary conditions for arbitrary mechanical and coupled problems (cf. [22–24]). In the present work it is used in the following form: The virtual power of the inertia forces $\mathcal{P}_a^*$ balances the virtual power $\mathcal{P}_{\text{int}}^*$ of the internal and $\mathcal{P}_{\text{ext}}^*$ of the external forces acting on any sub-domain $\mathcal{S}$ of the material body $\mathcal{B}$ for any admissible virtual velocity field $\mathbf{v}^*$ and virtual rate of order parameter field $\dot{\phi}^*$, i.e.,

$$\mathcal{P}_a^* = \mathcal{P}_{\text{int}}^* + \mathcal{P}_{\text{ext}}^*. \quad (23.13)$$

For the sake of simplicity we disregard any higher order inertia terms [25] as well as inertial forces acting on the order parameter, resulting in

$$\mathcal{P}_a^* = \int_{\mathcal{S}} \rho \dot{\mathbf{v}} \cdot \mathbf{v}^* \, dV. \quad (23.14)$$

The power of internal forces is given by

$$\mathcal{P}_{\text{int}}^* = - \int_{\mathcal{S}} \left(\mathbf{S}^\top : \mathbf{L}^* + \mathcal{T} : \text{grad } \mathbf{L}^* - \pi \dot{\phi}^* + \boldsymbol{\xi} \cdot \text{grad } \dot{\phi}^* \right) dV, \quad (23.15)$$

with $\mathbf{L}^* := \text{grad } \mathbf{v}^*$. Here $\mathbf{S}$ and $\mathcal{T}$ are the CAUCHY and higher order stresses, respectively, while π and $\boldsymbol{\xi}$ are thermodynamic forces that directly correspond to the internal microforce and microstress introduced by Gurtin [26]. We note that the invariance requirement of $\mathcal{P}_{\text{int}}^*$ with respect to superimposed rigid body motions results in $\mathbf{S} = \mathbf{S}^\top$. For the power of external forces we consider the very simple case of no body or contact forces acting on $\mathbf{L}^*$ and $\text{grad } \dot{\phi}^*$, and only a contact (micro)force ζ acting $\dot{\phi}^*$

$$\mathcal{P}_{\text{ext}}^* = \int_{\mathcal{S}} \mathbf{f} \cdot \mathbf{v}^* \rho \, dV + \int_{\partial \mathcal{S}} (\mathbf{t} \cdot \mathbf{v}^* + \zeta \dot{\phi}^*) \, da. \quad (23.16)$$

In order to obtain the consequences of the PVP, the integrals in (23.15) are transformed using the following identities

$$\text{div}(\mathbf{S} \cdot \mathbf{v}^*) = (\text{div } \mathbf{S}) \cdot \mathbf{v}^* + \mathbf{S} : \mathbf{L}^*, \quad (23.17)$$

$$\text{div}(\mathcal{T} : \mathbf{L}^*) = (\text{div } \mathcal{T}) : \mathbf{L}^* + \mathcal{T} : \text{grad } \mathbf{L}^*, \quad (23.18)$$

$$\text{div}((\text{div } \mathcal{T}) \cdot \mathbf{v}^*) = (\text{div div } \mathcal{T}) \cdot \mathbf{v}^* + (\text{div } \mathcal{T}) : \mathbf{L}^*, \quad (23.19)$$

$$\text{div}(\boldsymbol{\xi} \dot{\phi}^*) = (\text{div } \boldsymbol{\xi}) \dot{\phi}^* + \boldsymbol{\xi} \cdot \text{grad } \dot{\phi}^*, \quad (23.20)$$

and the divergence theorem, resulting in

$$\begin{aligned}
\mathcal{P}_{\text{int}}^* = & \int_{\mathcal{S}} (\operatorname{div} \mathbf{S} - \operatorname{div} \operatorname{div} \mathcal{T}) \cdot \mathbf{v}^* \, dV - \int_{\partial \mathcal{S}} \mathbf{n} \cdot (\mathbf{S}^\top - \operatorname{div} \mathcal{T}) \cdot \mathbf{v}^* \, da \\
& - \int_{\partial \mathcal{S}} \mathbf{n} \cdot \mathcal{T} : \mathbf{L}^* \, da + \int_{\mathcal{S}} (\pi + \operatorname{div} \boldsymbol{\xi}) \dot{\phi}^* \, dV - \int_{\partial \mathcal{S}} \mathbf{n} \cdot \boldsymbol{\xi} \dot{\phi}^* \, da. \quad (23.21)
\end{aligned}$$

Introducing the surface gradient operator

$$\operatorname{grad}_S(\cdot) = \operatorname{grad}(\cdot) - \partial_{\mathbf{n}}(\cdot) \otimes \mathbf{n}, \quad (23.22)$$

where $\partial_{\mathbf{n}}$ is the directional derivative in the direction of the outward normal $\mathbf{n}$, the third integral in expression (23.21) can be rewritten as

$$\int_{\partial \mathcal{S}} \mathbf{n} \cdot \mathcal{T} : \mathbf{L}^* \, da = \int_{\partial \mathcal{S}} \mathbf{n} \cdot \mathcal{T} : \operatorname{grad}_S \mathbf{v}^* \, da + \int_{\partial \mathcal{S}} \mathbf{n} \cdot \mathcal{T} : \partial_{\mathbf{n}} \mathbf{v}^* \otimes \mathbf{n} \, da \quad (23.23)$$

$$\begin{aligned}
& = \int_{\partial \mathcal{S}} \operatorname{div}_S(\mathbf{n} \cdot \mathcal{T} \cdot \mathbf{v}^*) \, da - \int_{\partial \mathcal{S}} \operatorname{div}_S(\mathbf{n} \cdot \mathcal{T}) \cdot \mathbf{v} \, da + \\
& \quad + \int_{\partial \mathcal{S}} \mathbf{n} \cdot \mathcal{T} : \partial_{\mathbf{n}} \mathbf{v}^* \otimes \mathbf{n} \, da. \quad (23.24)
\end{aligned}$$

Finally, applying the surface divergence theorem and, for the sake of simplicity, neglecting any wedge line and corner contributions, we find

$$\int_{\partial \mathcal{S}} \operatorname{div}_S(\mathbf{n} \cdot \mathcal{T} \cdot \mathbf{v}^*) \, da = \int_{\partial \mathcal{S}} (\operatorname{div}_S \mathbf{n}) \mathbf{n} \otimes \mathbf{n} : \mathcal{T} \cdot \mathbf{v}^* \, da. \quad (23.25)$$

Enforcing (23.13) we arrive after a number of straightforward algebraic manipulations at the following field equations on $\mathcal{B}$

$$\rho \dot{\mathbf{v}} = \operatorname{div}(\mathbf{S} - \operatorname{div} \mathcal{T}) + \rho \mathbf{f}, \quad (23.26a)$$

$$0 = \operatorname{div} \boldsymbol{\xi} + \pi, \quad (23.26b)$$

and boundary conditions on $\partial \mathcal{B}$

$$\mathbf{t} = (\mathbf{S} - \operatorname{div} \mathcal{T}) \cdot \mathbf{n} - \operatorname{div}_S(\mathbf{n} \cdot \mathcal{T}), \quad (23.26c)$$

$$\zeta = \boldsymbol{\xi} \cdot \mathbf{n}. \quad (23.26d)$$

We note that, introducing the total stress

$$\mathbf{S}_t := \mathbf{S} - \operatorname{div} \mathcal{T}, \quad (23.27)$$

the balance of linear momentum (23.26a) regains its standard form for simple materials

$$\rho \dot{\mathbf{v}} = \operatorname{div} \mathbf{S}_t + \rho \mathbf{f}, \quad (23.28)$$

which is convenient for the numerical implementation.

23.3.3 Constitutive Equations

The following equations are formulated assuming the small perturbation hypothesis, i.e., both the displacement $\mathbf{u}$ as well as the displacement gradient can be considered small, $\mathbf{u} \ll L$ and $\|\operatorname{grad} \mathbf{u}\| \ll 1$. In this case the deformation is characterized by the linear strain tensor $\mathbf{E} = \frac{1}{2} (\operatorname{grad} \mathbf{u} + (\operatorname{grad} \mathbf{u})^\top)$. Its gradient will be denoted $\mathcal{Y} := \operatorname{grad} \mathbf{E}$.

23.3.3.1 Laws of State

We choose the following ansatz for the free energy density and thermodynamic forces

$$\begin{aligned} \psi &= \psi(\mathbf{E}, \mathcal{Y}, \phi, \operatorname{grad} \phi, \theta), & \xi &= \xi(\mathbf{E}, \mathcal{Y}, \phi, \operatorname{grad} \phi, \theta), \\ \mathbf{S} &= \mathbf{S}(\mathbf{E}, \mathcal{Y}, \phi, \operatorname{grad} \phi, \theta), & \pi &= \pi(\mathbf{E}, \mathcal{Y}, \phi, \operatorname{grad} \phi, \theta, \dot{\phi}), \\ \mathcal{T} &= \mathcal{T}(\mathbf{E}, \mathcal{Y}, \phi, \operatorname{grad} \phi, \theta), \end{aligned}$$

The second law of thermodynamics in the form of the CLAUSIUS-DUHEM inequality is given for the isothermal case by

$$\begin{aligned} (\mathbf{S} - \rho \partial_{\mathbf{E}} \psi) : \dot{\mathbf{E}} + (\mathcal{T} - \rho \partial_{\mathcal{Y}} \psi) : \dot{\mathcal{Y}} - (\pi + \rho \partial_{\phi} \psi) \dot{\phi} + \\ + (\xi - \rho \partial_{\operatorname{grad} \phi} \psi) \cdot \operatorname{grad} \dot{\phi} \geq 0 \end{aligned} \quad (23.29)$$

an can be exploited using the classical COLEMAN-NOLL procedure to arrive at the laws of state

$$\mathbf{S} = \rho \partial_{\mathbf{E}} \psi, \quad \mathcal{T} = \rho \partial_{\mathcal{Y}} \psi, \quad \xi = \rho \partial_{\operatorname{grad} \phi} \psi \quad (23.30)$$

and the residual dissipation inequality

$$-\pi_d \dot{\phi} \geq 0, \quad \text{with} \quad \pi_d := \pi + \rho \partial_{\phi} \psi. \quad (23.31)$$

23.3.3.2 Free Energy and Dissipation Potential

As customary in phase field models for solid-solid transformations, the free energy density can be split into an elastic-, a bulk chemical- and an interface-contribution

$$\psi = \psi_e(\mathbf{E}, \mathbf{y}, \phi, \theta) + \psi_b(\phi, \theta) + \psi_i(\phi, \text{grad } \phi, \theta). \quad (23.32)$$

In our formulation, the elastic free energy is of HELMHOLTZ-type, i.e.,

$$\begin{aligned} \rho \psi_e(\mathbf{E}, \mathbf{y}, \phi, \theta) &= \frac{1}{2} \mathbf{E}_e(\mathbf{E}, \phi) : \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) \\ &+ \frac{1}{2} (\mathbb{C}(\phi) : \mathbf{y} \cdot \mathbf{\Lambda}(\phi)) : \mathbf{y}, \end{aligned} \quad (23.33)$$

where $\mathbf{E}_{tr}(\phi)$ is the inelastic strain, $\mathbf{E}_e(\mathbf{E}, \phi) := \mathbf{E} - \mathbf{E}_{tr}(\phi)$ is the elastic strain, $\mathbb{C}$ the stiffness tensor and $\mathbf{\Lambda}(\phi)$ a gradient length scale tensor (cf. [20]). The specific choice of functional dependence of $\mathbf{E}_{tr}(\phi)$, $\psi_b(\phi, \theta)$ and $\psi_i(\phi, \text{grad } \phi, \theta)$ on the order parameter ϕ is of no relevance at this point, we will assume that the interface energy is of the form

$$\rho \psi_i(\phi, \text{grad } \phi, \theta) := \frac{\alpha}{2} \|\text{grad } \phi\|^2 + g(\phi, \theta). \quad (23.34)$$

Using the laws of state (23.30) we immediately find

$$\mathbf{S} = \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) = \mathbb{C}(\phi) : (\mathbf{E} - \mathbf{E}_{tr}(\phi)), \quad (23.35a)$$

$$\mathcal{T} = \mathbb{C}(\phi) : \mathbf{y} \cdot \mathbf{\Lambda}(\phi), \quad (23.35b)$$

$$\xi = \alpha \text{grad } \phi, \quad (23.35c)$$

and combining the first two equations

$$\mathcal{T} = \mathbb{C}(\phi) : \text{grad} (\mathbb{C}^{-1}(\phi) : \mathbf{S}) \cdot \mathbf{\Lambda}(\phi) + \mathbb{C}(\phi) : \text{grad } \mathbf{E}_{tr}(\phi) \cdot \mathbf{\Lambda}(\phi). \quad (23.36)$$

Equation (23.27) can now be used in two ways: In conjunction with the laws of state (23.35a) and (23.35b) it is a constitutive equation for the total stress $\mathbf{S}_t$, which enters the balance of linear momentum (23.28)

$$\mathbf{S}_t(\mathbf{E}, \mathbf{y}, \phi) = \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) - \text{div} [\mathbb{C}(\phi) : \mathbf{y} \cdot \mathbf{\Lambda}(\phi)]. \quad (23.37)$$

When combined with (23.36), (23.27) can be used to determine the true stress $\mathbf{S}$ from the total stress $\mathbf{S}_t$

$$\begin{aligned} \mathbf{S} - \operatorname{div}[\mathbb{C}(\phi) : \operatorname{grad}(\mathbb{C}^{-1}(\phi) : \mathbf{S}) \cdot \mathbf{\Lambda}(\phi)] \\ = \mathbf{S}_t + \operatorname{div}(\mathbb{C}(\phi) : \operatorname{grad} \mathbf{E}_{\text{tr}}(\phi) \cdot \mathbf{\Lambda}(\phi)). \end{aligned} \quad (23.38)$$

In order to complete the phase field formulation we require a constitutive equation for π_d , which is obtained in the spirit of classical irreversible thermodynamics as

$$\dot{\phi} = -\partial_{\pi_d} \Omega(\pi_d) \quad (23.39)$$

from a dissipation potential $\Omega(\pi_d)$ that is homogeneous of degree two

$$\Omega(\pi_d) := \frac{1}{2} M^{-1} \pi_d^2, \quad (23.40)$$

where M is the so called mobility constant. Combining (23.26b), (23.31), (23.35c), (23.39) and (23.40) we find the classical ALLEN-CAHN equation

$$M \dot{\phi} = \alpha \Delta \phi - \rho \partial_{\phi} \psi, \quad (23.41)$$

or, specifically,

$$\begin{aligned} M \dot{\phi} = & \alpha \Delta \phi + \mathbf{S} : \partial_{\phi} \mathbf{E}_{\text{tr}} - \frac{1}{2} \mathbf{E}_e(\mathbf{E}, \phi) : \partial_{\phi} \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) \\ & - \frac{1}{2} (\mathbb{C}(\phi) : \mathcal{Y} \cdot \partial_{\phi} \mathbf{\Lambda}(\phi)) - \frac{1}{2} (\partial_{\phi} \mathbb{C}(\phi) : \mathcal{Y} \cdot \mathbf{\Lambda}(\phi)) : \mathcal{Y} \\ & - \rho \partial_{\phi} \psi_b(\phi, \theta) - \partial_{\phi} g(\phi, \theta). \end{aligned} \quad (23.42)$$

Note that all terms that appear in the driving force, and as per [17] the CAUCHY stress $\mathbf{S}$ in particular, are non-singular even in the presence of dislocations.

23.3.4 Special Cases

For phase transformations the crystal lattice on both sides of the interface will, in general, be different leading to different elastic properties and a different dislocation core structure. In this case the (23.28), (23.37), (23.38) and (23.42) retain their full complexity. In the following, we consider a number of scenarios for which this is not the case.

23.3.4.1 Homogeneous Bulk Material

In the bulk phase the order parameter does not vary in space, i.e., $\operatorname{grad} \phi = \mathbf{0}$, $\mathbb{C}(\phi) = \mathbb{C}$, $\mathbf{\Lambda}(\phi) = \mathbf{\Lambda}$, $\mathbf{E}_{\text{tr}}(\phi) = \mathbf{0}$. The ALLEN-CAHN equation is fulfilled automatically and

(23.38), (23.37) recover the form derived by Po et al. [20]

$$\begin{aligned} \mathbf{S} - \operatorname{div}((\operatorname{grad} \mathbf{S}) \cdot \boldsymbol{\Lambda}) &= \mathbf{S}_t, \text{ with} \\ \mathbf{S}_t(\mathbf{E}, \mathbf{y}) &= \mathbb{C} : [\mathbf{E} - \operatorname{div}(\mathbf{y} \cdot \boldsymbol{\Lambda})]. \end{aligned} \quad (23.43a)$$

For materials with cubic symmetry the gradient length scale tensor $\boldsymbol{\Lambda}$ is isotropic, i.e., $\boldsymbol{\Lambda} = \ell^2 \mathbf{I}$, and the above expressions can be further simplified to the form derived by Lazar et al. [17]

$$\begin{aligned} \mathbf{S} - \ell^2 \Delta \mathbf{S} &= \mathbf{S}_t, \text{ with} \\ \mathbf{S}_t(\mathbf{E}, \mathbf{y}) &= \mathbb{C} : (\mathbf{E} - \ell^2 \operatorname{div} \mathbf{y}) = \mathbb{C} : (\mathbf{E} - \ell^2 \Delta \mathbf{E}). \end{aligned} \quad (23.43b)$$

23.3.4.2 Grain Boundaries as Planar Defects

The crystal lattices on both sides of a grain boundary differ only by a rotation $\mathbf{Q}(\phi)$. Hence, we assume that the chemical bulk energy is independent of the order parameter, i.e., $\psi_b(\phi, \theta) = \psi_b(\theta)$. Then the elastic stiffness $\mathbb{C}(\phi)$ and the gradient length scale tensor $\boldsymbol{\Lambda}(\phi)$ can be expressed as $\mathbb{C}(\phi) = \mathbf{Q}(\phi) * \mathbb{C}$ and $\boldsymbol{\Lambda}(\phi) = \mathbf{Q}(\phi) * \boldsymbol{\Lambda}$, respectively. Furthermore, without loss of generality, $\mathbf{E}_{tr}(\phi) = \mathbf{0}$. For this case (23.38), (23.37) and (23.42) take the form

$$\mathbf{S} - \operatorname{div}[(\mathbf{Q}(\phi) * \mathbb{C}) : \operatorname{grad}((\mathbf{Q}(\phi) * \mathbb{C}^{-1}) : \mathbf{S}) \cdot (\mathbf{Q}(\phi) * \boldsymbol{\Lambda})] = \mathbf{S}_t, \quad (23.44a)$$

with

$$\mathbf{S}_t(\mathbf{E}, \mathbf{y}, \phi) = \mathbb{C}(\phi) : \mathbf{E} - \operatorname{div}[(\mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{y} \cdot (\mathbf{Q}(\phi) * \boldsymbol{\Lambda})], \quad (23.44b)$$

and

$$\begin{aligned} M\dot{\phi} &= \alpha \Delta \phi - \frac{1}{2} \mathbf{E} : (\partial_\phi \mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{E} - \frac{1}{2} ((\mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{y} \cdot (\partial_\phi \mathbf{Q} * \boldsymbol{\Lambda})) - \\ &\quad - \frac{1}{2} ((\partial_\phi \mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{y} \cdot (\mathbf{Q}(\phi) * \boldsymbol{\Lambda})) : \mathbf{y} - \partial_\phi g(\phi, \theta). \end{aligned} \quad (23.44c)$$

The isotropy of the gradient length scale tensor $\boldsymbol{\Lambda}$ for cubic crystals implies that $\mathbf{Q}(\phi) * \boldsymbol{\Lambda} = \boldsymbol{\Lambda} = \ell^2 \mathbf{I}$, which simplifies (23.44) to the following form

$$\mathbf{S} - \ell^2 \operatorname{div}[(\mathbf{Q}(\phi) * \mathbb{C}) : \operatorname{grad}((\mathbf{Q}(\phi) * \mathbb{C}^{-1}) : \mathbf{S})] = \mathbf{S}_t, \quad (23.45a)$$

with

$$\mathbf{S}_t(\mathbf{E}, \mathbf{y}, \phi) = \mathbb{C}(\phi) : \mathbf{E} - \ell^2 \operatorname{div}[(\mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{y}], \quad (23.45b)$$

and

$$M\dot{\phi} = \alpha \Delta \phi - \frac{1}{2} \mathbf{E} : (\partial_{\phi} \mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{E} - \frac{1}{2} \ell^2 ((\partial_{\phi} \mathbf{Q}(\phi) * \mathbb{C}) : \mathcal{Y}) : \mathcal{Y} - \partial_{\phi} g(\phi, \theta). \quad (23.45c)$$

23.3.4.3 Twin Boundaries as Planar Defects

Since the twin variants on both sides of the boundary are related by mirror and/or rotational symmetry transformations between the unit cells, we can—as in the case of grain boundaries—assume that the bulk chemical energy remains unchanged, i.e., $\psi_b(\phi, \theta) = \psi_b(\theta)$, and the elastic stiffness $\mathbb{C}(\phi)$ and the gradient length scale tensor $\mathbf{\Lambda}(\phi)$ can be expressed using an orthogonal tensor $\mathbf{Q}(\phi)$ as $\mathbb{C}(\phi) = \mathbf{Q}(\phi) * \mathbb{C}$ and $\mathbf{\Lambda}(\phi) = \mathbf{Q}(\phi) * \mathbf{\Lambda}$, respectively. Under these assumptions we find

$$\begin{aligned} \mathbf{S} - \operatorname{div} \left[(\mathbf{Q}(\phi) * \mathbb{C}) : \operatorname{grad} \left((\mathbf{Q}(\phi) * \mathbb{C}^{-1}) : \mathbf{S} \right) \cdot (\mathbf{Q}(\phi) * \mathbf{\Lambda}) \right] \\ = \mathbf{S}_t + \operatorname{div} [\mathbb{C}(\phi) : \operatorname{grad} (\mathbf{E}_{\text{tr}}(\phi)) \cdot \mathbf{\Lambda}(\phi)], \end{aligned} \quad (23.46a)$$

with

$$\mathbf{S}_t(\mathbf{E}, \mathcal{Y}, \phi) = \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}) - \operatorname{div} [(\mathbf{Q}(\phi) * \mathbb{C}) : \mathcal{Y} \cdot (\mathbf{Q}(\phi) * \mathbf{\Lambda})], \quad (23.46b)$$

and

$$\begin{aligned} M\dot{\phi} = \alpha \Delta \phi + \mathbf{S} : \partial_{\phi} \mathbf{E}_{\text{tr}} - \frac{1}{2} \mathbf{E}_e(\mathbf{E}, \phi) : (\partial_{\phi} \mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{E}_e(\mathbf{E}, \phi) \\ - \frac{1}{2} ((\mathbf{Q}(\phi) * \mathbb{C}) : \mathcal{Y} \cdot (\partial_{\phi} \mathbf{Q} * \mathbf{\Lambda})) \\ - \frac{1}{2} ((\partial_{\phi} \mathbf{Q}(\phi) * \mathbb{C}) : \mathcal{Y} \cdot (\mathbf{Q}(\phi) * \mathbf{\Lambda})) : \mathcal{Y} - \partial_{\phi} g(\phi, \theta). \end{aligned} \quad (23.46c)$$

For cubic lattices these expressions simplify to

$$\mathbf{S} - \ell^2 \operatorname{div} \left[(\mathbf{Q}(\phi) * \mathbb{C}) : \operatorname{grad} \left((\mathbf{Q}(\phi) * \mathbb{C}^{-1}) : \mathbf{S} \right) \right] \quad (23.47a)$$

$$= \mathbf{S}_t + \ell^2 \operatorname{div} [\mathbb{C}(\phi) : \operatorname{grad} \mathbf{E}_{\text{tr}}(\phi)], \quad (23.47b)$$

with

$$\mathbf{S}_t(\mathbf{E}, \mathcal{Y}, \phi) = \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) - \ell^2 \operatorname{div} [(\mathbf{Q}(\phi) * \mathbb{C}) : \mathcal{Y}], \quad (23.47c)$$

and

$$\begin{aligned} M\dot{\phi} = \alpha \Delta \phi + \mathbf{S} : \partial_{\phi} \mathbf{E}_{\text{tr}} - \frac{1}{2} \mathbf{E}_e(\mathbf{E}, \phi) : (\partial_{\phi} \mathbf{Q}(\phi) * \mathbb{C}) : \mathbf{E}_e(\mathbf{E}, \phi) - \\ - \frac{1}{2} \ell^2 ((\partial_{\phi} \mathbf{Q}(\phi) * \mathbb{C}) : \mathcal{Y}) : \mathcal{Y} - \partial_{\phi} g(\phi, \theta). \end{aligned} \quad (23.47d)$$

23.3.4.4 Phase Boundaries Between Cubic Phases

In the case of phase boundaries between different cubic phases the gradient length scale tensor $\mathbf{\Lambda}$ is isotropic on both sides of the interface, even though not necessarily constant across the interface, i.e., $\mathbf{\Lambda} = \ell(\phi)^2 \mathbf{I}$. This allows us to reduce (23.38), (23.37) and (23.42) to the following form

$$\begin{aligned} \mathbf{S} - \operatorname{div}[\ell(\phi)^2 \mathbb{C}(\phi) : \operatorname{grad}(\mathbb{C}^{-1}(\phi) : \mathbf{S})] \\ = \mathbf{S}_t + \operatorname{div}(\ell(\phi)^2 \mathbb{C}(\phi) : \operatorname{grad} \mathbf{E}_{\text{tr}}(\phi)), \end{aligned} \quad (23.48a)$$

with

$$\mathbf{S}_t(\mathbf{E}, \mathbf{y}, \phi) = \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) - \operatorname{div}(\ell(\phi)^2 \mathbb{C}(\phi) : \mathbf{y}), \quad (23.48b)$$

and

$$\begin{aligned} M\dot{\phi} = \alpha \Delta \phi + \mathbf{S} : \partial_{\phi} \mathbf{E}_{\text{tr}} + \frac{1}{2} \mathbf{E}_e(\mathbf{E}, \phi) : \partial_{\phi} \mathbb{C}(\phi) : \mathbf{E}_e(\mathbf{E}, \phi) \\ - \ell(\phi) \partial_{\phi} \ell(\phi) (\mathbb{C}(\phi) : \mathbf{y}) : \mathbf{y} - \frac{\ell(\phi)^2}{2} (\partial_{\phi} \mathbb{C}(\phi) : \mathbf{y}) : \mathbf{y} \\ - \rho \partial_{\phi} \psi_b(\phi, \theta) - \partial_{\phi} g(\phi, \theta). \end{aligned} \quad (23.48c)$$

23.3.5 Examples

This section contains a number of examples that demonstrate basic properties of the proposed model.

23.3.5.1 Regularization in the Dislocation Core

As shown in Sect. 23.3.4.1, the present model reduces to the set of equations proposed by Po et al. [20] in the homogeneous bulk phase. Figure 23.6 shows the shear stress component S_{12} in the glide plane of a single edge dislocation with and without regularization ($\ell = 2$ nm). In the classical case, the stress in the dislocation core is singular, whereas it is well defined for the regularized solution.

23.3.5.2 Effect of the Regularization on the Interaction of Dislocations with a Phase Boundary

The following scenario considers a two-phase material with an initially flat interface between the austenite (A) and martensite (M) phases (see Fig. 23.7, left figure) and an immobile dislocation structure within the austenite. The material is cooled below the martensite start temperature, i.e., the interface will move to the right, interacting with the dislocation structure. This interaction significantly varies depending on the

Fig. 23.6 Shear stress component S_{12} in the glide plane of a single edge dislocation

Fig. 23.7 Phase evolution for $\ell = 2$ nm

choice of the regularization. For a large regularization length ($\ell = 2$ nm) the stress in the dislocation core is relatively low, which enables the chemical driving force to pull the interface across the dislocation structure, resulting in a fully martensitic material (Fig. 23.7). With decreasing regularization length ($\ell = 1$ nm) the stress in the dislocation core increases, which leads to a stronger interaction with the interface, which, as a consequence, is arrested at the rightmost dislocation (Fig. 23.8). After the interface is immobile, the second martensitic variant is formed, which consumes the austenite. For an even smaller regularization length ($\ell = 0.5$ nm) the interface is arrested earlier in its progress (Fig. 23.9).

If, however, no regularization is present, this trend does not continue. The stress singularity in the dislocation core triggers the formation of martensite well ahead of the initial interface, enabling it to “overrun” the immobile dislocation structure

Fig. 23.8 Phase evolution for $\ell = 1$ nm

Fig. 23.9 Phase evolution for $l = 0.5$ nm

Fig. 23.10 Phase evolution without regularization

(Fig. 23.10). The result in this case is mesh sensitive, since the computed stress magnitude depends on the choice of discretization and therefore is unsuitable for quantitative investigations of the interaction of planar defects with dislocations.

23.4 Conclusions

In order to model the interaction of phase transformations and dislocations, we have coupled a time-dependent Ginzburg-Landau equation with the stress/strain fields of stationary configurations of discrete dislocations. This allowed us to study the effect that dislocations have on the resulting evolution of the microstructure. Coupling two simulation models for different deformation mechanisms is usually more involved than just the simulation of one phenomenon. However, the present work also showed that such a “multiphysical” approach might show a particular promise since, e.g., the artificial initial seed for the phase microstructure becomes superfluous, which makes our simulations more realistic.

However, only using stationary dislocation configurations is clearly not realistic: these dislocations would usually move and interact among themselves. Thus, future work will consider such behavior where the evolution of the phase microstructure is governed by the TDGL and the dislocation dynamics is governed by an equation of motion, both of which are coupled.

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References

1. A. Weidner, H. Biermann, J. Mech. **67**(8), 1729 (2015). <https://doi.org/10.1007/s11837-015-1456-y>
2. B. Li, X.M. Zhang, P.C. Clapp, J.A. Rifkin, J. Appl. Phys. **95**(4), 1698 (2004). <https://doi.org/10.1063/1.1638609>
3. J. Shim, Y. Cho, S. Kwon, W. Kim, B. Wirth, Appl. Phys. Lett. **90**(2), 021906 (2007). <https://doi.org/10.1063/1.2429902>
4. A. Ibarra, D. Caillard, J. San Juan, M.L. Nó, Appl. Phys. Lett. **90**(10), 101907 (2007). <https://doi.org/10.1063/1.2710076>
5. L.D. Landau, Zh. Eksp. Teor. Fiz. **7**, 19 (1937). [Ukr. J. Phys. **53**, 25 (2008)]
6. A. Khachaturyan, *Theory of Structural Transformations in Solids* (Wiley, New York, 1983)
7. J.P. Hirth, J. Lothe, *Theory of Dislocations* (McGraw-Hill, New York, 1967)
8. R. Wu, S. Sandfeld, Scripta Mater. **123**, 42 (2016). <https://doi.org/10.1016/j.scriptamat.2016.05.032>
9. R. Wu, M. Zaiser, S. Sandfeld, Int. J. Plastic. **95**, 142 (2017). <https://doi.org/10.1016/j.iijplas.2017.04.005>
10. D. Schrade, B. Xu, R. Müller, D. Gross, *Proceedings of the ASME Conference on Smart Materials, Adaptive Structures and Intelligent Systems*, vol. 1 (2008), p. 299. <https://doi.org/10.1115/SMASIS2008-411>
11. R. Schmitt, C. Kuhn, R. Müller, K. Bhattacharya, Technische Mechanik **34**(1), 23 (2014). <https://doi.org/10.24352/UM.OVGU-2017-051>
12. W. Cai, A. Arsenlis, C.R. Weinberger, V.V. Bulatov, J. Mech. Phys. Solids **54**(3), 561 (2006). <https://doi.org/10.1016/j.jmps.2005.09.005>
13. J. Weertman, *Dislocation Based Fracture Mechanics* (World Scientific Pub Co Inc, 1996), pp. 2–5
14. R. Peierls, Proc. Phys. Soc. **52**(1), 34 (1940). <https://doi.org/10.1088/0959-5309/52/1/305>
15. F.R.N. Nabarro, Proc. Phys. Soc. **59**(2), 256 (1947). <https://doi.org/10.1088/0959-5309/59/2/309>
16. J. Lothe, *Elastic Strain Fields and Dislocation Mobility, Modern Problems in Condensed Matter Sciences*, vol. 31, ed. by V.L. Indenbom, J. Lothe (Elsevier, 1992), pp. 175–235. <https://doi.org/10.1016/B978-0-444-88773-3.50008-X>
17. M. Lazar, G.A. Maugin, E.C. Aifantis, Phys. Status Solidi B **242**(12), 2365 (2005). <https://doi.org/10.1002/pssb.200540078>
18. M. Lazar, G.A. Maugin, E.C. Aifantis, Int. J. Solids Struct. **43**(6), 1787 (2006). <https://doi.org/10.1016/j.ijsolstr.2005.07.005>
19. M. Lazar, G. Po, Phys. Lett. A **379**(24), 1538 (2015). <https://doi.org/10.1016/j.physleta.2015.03.027>
20. G. Po, M. Lazar, N.C. Admal, N. Ghoniem, Int. J. Plastic. **103**, 1 (2018). <https://doi.org/10.1016/j.iijplas.2017.10.003>
21. N.C. Admal, J. Marian, G. Po, J. Mech. Phys. Solids **99**, 93 (2017). <https://doi.org/10.1016/j.jmps.2016.11.005>
22. G. Maugin, Acta Mech. **35**(1–2), 1 (1980)
23. P. Germain, SIAM J. Appl. Math. **25**(3), 556 (1973). <https://doi.org/10.1137/0125053>
24. G. Del Piero, J. Mech. Mater. Struct. **4**(2), 281 (2009). <https://doi.org/10.2140/jomms.2009.4.281>
25. R. Mindlin, Arch. Ration. Mech. An. **16**(1), 51 (1964)
26. M. Gurtin, Physica D **92**(3–4), 178 (1996)

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