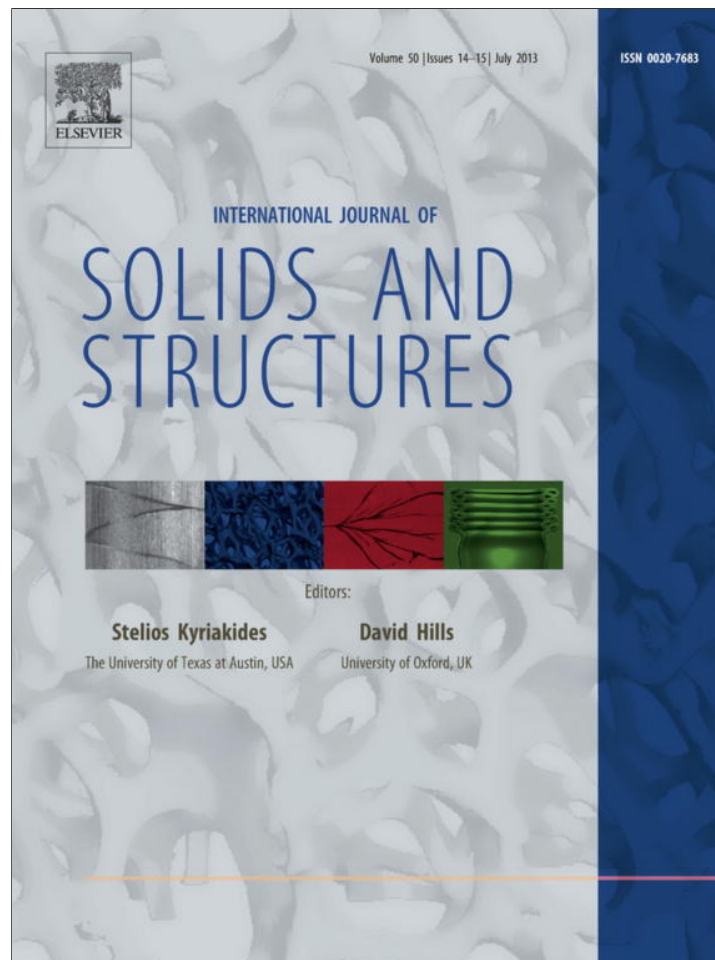


Provided for non-commercial research and education use.
Not for reproduction, distribution or commercial use.



This article appeared in a journal published by Elsevier. The attached copy is furnished to the author for internal non-commercial research and education use, including for instruction at the authors institution and sharing with colleagues.

Other uses, including reproduction and distribution, or selling or licensing copies, or posting to personal, institutional or third party websites are prohibited.

In most cases authors are permitted to post their version of the article (e.g. in Word or Tex form) to their personal website or institutional repository. Authors requiring further information regarding Elsevier's archiving and manuscript policies are encouraged to visit:

<http://www.elsevier.com/authorsrights>

Contents lists available at [SciVerse ScienceDirect](http://SciVerse.ScienceDirect.com)

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

Driving forces for interface kinetics and phase field models

R. Spatschek^{a,*}, B. Eidel^{b,c}^a Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany^b Institut für Mechanik, Universität Duisburg-Essen, D-45117 Essen, Germany^c Lehrstuhl für Numerische Mechanik, Universität Siegen, D-57068 Siegen, Germany

ARTICLE INFO

Article history:

Received 23 September 2012

Received in revised form 18 February 2013

Available online 3 April 2013

Keywords:

Phase field

Elasticity

Plasticity

Variational principles

ABSTRACT

Phase field models for applications in physics and materials science are typically written in variational form starting from a free energy functional, and sharp interface descriptions for moving boundary problems can be formulated similarly. Here we discuss why and under which circumstances this postulate for deriving the equations of motion is justified, and what are limitations for specific cases. We investigate this in particular for alloys, systems with elastic, viscoelastic and plastic effects, mainly based on analytical and numerical investigations in one dimension. We find that the naturally guessed equations of motion, as derived via partial functional derivatives from a free energy, are usually reasonable, only for materials with plastic effects this assumption is more delicate due to the presence of internal variables.

© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

The modeling of microstructure evolution has become a central topic in materials science and physics, since these pattern formation processes are not only essential phenomena in our day-to-day life but also important for the understanding and prediction of material behavior. In this respect the development of phase field models can be considered as a milestone, which triggered an enormous intensification of research activities in this direction (Steinbach, 2009; Chen, 2002; Karma et al., 2001; Boettinger et al., 2002; Provatas et al., 2010). Starting with pure curvature driven motion (Langer, 1978; Fix, 1983; Collins and Levine, 1985; Langer, 1986) phase field modeling experienced a first 'gold rush' by the investigation of diffusion limited solidification, in particular dendritic growth, and substantially contributed to a deeper understanding of this complex problem. Since then, it has become a routine toolkit for modeling interfacial pattern formation processes not only for highly idealized scientific investigations, but also for realistic simulations of kinetic processes in engineering materials (Tiaden, 1999). Later on, more and more phenomena have been investigated by the means of phase field modeling (Spatschek et al., 2011), and nowadays even applications in biology, medicine and soft matter science start to emerge (Travasso et al., 2011).

With the increasing knowledge about this modeling tool also the understanding of this method has reached a significantly deeper level. Initially, the method was considered purely as a mathe-

tical tool that avoids the complex tracking of interface during moving boundary problems. Instead, order parameters are introduced to discriminate between different 'phases', and at interfaces these order parameters change only gradually. The description of interface dynamics is then reduced to partial differential equations for the order parameters. The original idea is that in the sharp interface limit, where the lengthscale over which the order parameters are smeared out at the interfaces between the 'phases' is small in comparison to the relevant physical lengthscales, the dynamics effectively recovers the governing laws for the kinetics of the sharp interfaces. Although physically all interfaces have a finite thickness, this true physical width is negligibly small in comparison to the scales of the patterns, and therefore a sharp interface description is usually appropriate. The numerical lengthscale, which is introduced in phase field models, is usually a pure auxiliary parameter, and numerical efficiency demands to actually choose it much larger than the true interface thickness. For quantitative modeling it is therefore mandatory to check that the results are insensitive to a change of the numerical interface thickness. Typically, first order equations (in time) are constructed for the phase field evolution, and in this 'traditional picture' the choice of the right hand side of the equations is not restricted, as long as it recovers the proper sharp interface limit.

During the past years, the use of so called thermodynamically consistent models, where the evolution is expressed via a thermodynamic functional, has attracted a lot of interest. This is particularly useful in the generalization to multi-phase and -component systems, see e.g. (Nestler et al., 2005). In a special case, which is recurrent in descriptions of physical phenomena, this free energy functional contains at least two ingredients: a well or obstacle

* Corresponding author. Tel.: +49 0211 6792 684; fax: +49 0211 6792 465.

E-mail address: spatschek@mpie.de (R. Spatschek).

potential and a gradient square term, the latter being a Dirichlet-type energy; these two lead to the proper interfacial energy of the system, and the dynamical evolution corresponds to curvature driven motion. For the description of alloys, a term corresponding to the free energy change due to impurities is added. Also mechanical effects have been considered, which lead to an additional elastic energy term (see e.g. (Spatschek et al., 2006; Brener et al., 2007; Spatschek et al., 2007; Fleck et al., 2011)), and also other physical effects have been discussed in a similar way. There are also insights concerning the postulation of continuum field models and the related driving forces in a more fundamental mathematical and mechanical context, particularly related to variational and non-variational derivations, and we mention here in particular (Mariano, 2002) and references therein for more general setups. Here, balance equations of micro structural interaction can be derived from first principles involving the invariance of the external power of actions alone.

Based on the experience that these thermodynamically motivated models indeed lead to the correct equations of motion in the sharp interface limit, the paradigm has changed to use such extensions of free energy functionals and the derived phase field models in a predictive manner also for problems, where an established sharp interface description is not yet available. In fact, it is often easier to find proper energy functionals than to derive or guess the correct sharp interface equations.

Nevertheless, it should be pointed out that not all phase field models are based on such a thermodynamic approach. In fact, the generalization to a model with thin interface asymptotics typically introduces non-variational terms (Karma and Rappel, 1996; Karma and Rappel, 1998). These terms are justified by a higher order asymptotic analysis, and the generalization to other models than established solidification problems is far from being trivial; for that reason, frequently only the antitrapping current is taken into account. More recently, these models have been revisited under the aspect of Onsager symmetries, taking into account cross-coupling between different fields (off-diagonal terms in the Onsager matrix) (Brener and Boussinot, 2012).

The interplay of phase transformations and plasticity has been discussed already in several publications. Closely related to the present article is the work by Ostwald et al. (2011), who investigate a one-dimensional model. There, also the aspect that dislocations can be inherited or pushed away from the phase transformation front has been discussed, and the model is illustrated for shape memory alloys and TRIP steels. The underlying von Mises plasticity model and the probabilistic approach to the phase transformation rate already has a certain complexity, which allows to model realistic stress–strain curved. Bartel and Hackl studied martensitic transformations in shape memory alloys, taking into account inelastic and dissipative relaxation (Bartel and Hackl, 2009). In Bartel et al., 2011 the issue of plasticity inheritance, i.e. the question concerning the plastic state of a material that has undergone a phase transformation, is discussed. A Ginzburg–Landau model to capture hardening plasticity has been developed in Fabrizio (2012). Takaki et al. combined a phase field model with crystal plasticity to simulate the microstructure and dislocation density during the deformation process of a polycrystalline metal (Takaki et al., 2007). Martensitic transformations in polycrystals subject to elasto-plastic material behavior was studied in Yamanaka et al. (2010) where the influence of plasticity on lamellar microstructure formation is contrasted to the purely elastic case. A phase field model coupled to viscoplasticity for the investigation of rafting in superalloys is presented in Gaubert et al. (2010). In the present article we confine the analysis to elementary plasticity models and focus on the aspect of thermodynamic consistency and the relation to phase field models.

In view of the extension of phase field models by plasticity, we investigate several prototype models and inspect the equations of

motion, as motivated from a thermodynamic approach without reference to a sharp interface limit, from a physical point of view. As we will see, an extension to plasticity, which introduces the new aspect of “internal variables” which are not derived from the same free energy functional as the phase field equations, brings in aspects, which make it less obvious, whether the usual approach to derive equations of motion, is appropriate. We note that this issue is also relevant for plastic deformations in other materials like ferroelectrics, magneto elastic materials, quasicrystals, polymeric bodies etc.

To make this point more transparent, we will investigate different models as prototype for various problems. The phase field ϕ is assumed to follow an Allen–Cahn equation for a non-conserved order parameter

$$\frac{\partial \phi}{\partial t} = -\frac{\delta F}{\delta \phi}, \quad (1)$$

where time is renormalized such that a kinetic coefficient in front of the variational derivative has become 1. In case of an alloy model, this evolution equation is coupled to a diffusion equation for the concentration, which can be considered as a prototype of a conserved order parameter,

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(c \nabla \frac{\delta F}{\delta c} \right). \quad (2)$$

We mention a mathematically motivated discussion of these equations in a more general setting in Mariano (2005). Yet another case are additional elliptical equations, as e.g. in the case of a coupling to static elasticity. Here, the displacement field \mathbf{u} with components u_i obeys an equation of the type

$$\frac{\delta F}{\delta u_i} = 0. \quad (3)$$

In all cases, the variational derivative in the phase field equation is calculated such, that the other fields are kept constant during the “virtual variation” of the order parameter; we can therefore use the terminology of a “partial functional derivative”. To that end, the free energy is formally expanded up to first order in a variation $\phi \rightarrow \phi + \delta \phi$, and the difference is represented in the form

$$F[\phi + \delta \phi, c, \mathbf{u}] - F[\phi, c, \mathbf{u}] = \int \frac{\delta F}{\delta \phi} \delta \phi dV + \mathcal{O}(\delta \phi^2) \quad (4)$$

and the integral kernel on the right hand side defines the variational derivative of the functional. At this point, we mention in passing that the precise mathematical definition of the “vertical” functional derivative used here may raise questions concerning the function space, which are beyond the scope of this article on a general level. From a physical perspective, this issue is related to boundary conditions, which may also be derived variationally. We will briefly return to this point later.

Physically, such a variational expression would be interpreted as the energy change that would emerge from a variation of the phase field, and therefore the interface position, while all other fields are considered as being frozen in. If we look e.g. at diffusional growth during solidification, this would intuitively correspond to a situation where the diffusion of impurities is slow in comparison to the fast fluctuations of a rough interface: When the interface (or correspondingly the phase field) makes a “trial step”, the concentration field almost does not change, since it is assumed that this diffusion process is significantly slower, and therefore it is appropriate to assume in the above functional derivative that the concentration is unaffected by the “virtual” interface motion.

Let us contrast this extreme situation to the behavior of the electron density, which is typically of course not considered for the description of phase transition kinetics on this level. The electron density is for sure different in different phases (imagine

a bcc–fcc transition), and is “integrated out” in the free energy expression. Therefore, it is assumed that the electron density instantaneously adjusts to a modification of the lattice structure, which results here from a phase change (Born–Oppenheimer approximation). In this sense, the electron density n_e is a function of the local phase state, $n_e(\phi)$. Formally, it means that in the functional derivative for the calculation of the driving force an energy change would rather be calculated from the work variation $F[\phi + \delta\phi, c, \mathbf{u}, n_e(\phi + \delta\phi)] - F[\phi, c, \mathbf{u}, n_e(\phi)]$, and therefore it would also contain contributions from the variational derivative $\delta F/\delta n_e$. For this example, it would be very counterintuitive to keep the electron density fixed in a part of the system where the material is transformed from one phase to another – such a configuration would be far from equilibrium and therefore energetically highly unfavorable.

These two examples are intended to point out, that from a physical point of view it should not be obvious, which “variational derivative” is appropriate as expression for the driving force, whether it is a “partial derivative”, where only the phase field is adjusted, or whether in the sense of a “total derivative” also other fields have to follow and therefore potentially influence the energetic situation. We note that in more general cases of comparable timescales for the different physical phenomena, the driving force should be “in between” the two extreme situations of the partial and total derivative. We contrast here these two limiting cases, which are highly relevant for many applications, e.g. solidification, where diffusion in the solid phases can be neglected due to the much larger timescales, or slow solid state transformation, where elastic degrees of freedom can be considered as instantaneously relaxed. A counterexample is brittle fracture, where the crack front propagation occurs on the same velocity scale as the relaxation of the mechanical degrees of freedom. Nevertheless, there has been significant progress in phase field modeling, see (Spatschek et al., 2011) for a review.

It is the purpose of the present paper to shed light on this question, and this in view of the extension towards the incorporation of plastic effects and their influence on the kinetics of phase transformations. We note that this discussion is not at all restricted to phase field models, as also sharp interface methods require the knowledge of the correct thermodynamic driving force. For such descriptions, also the energy change upon a “virtual” shift of the interface position is calculated. Therefore, the same question, whether other fields should be kept constant or being “slaved” for the calculation of this energy change, appear. Technically, the calculation of driving forces is more cumbersome for sharp interface formulations, since for non-planar fronts differential geometrical aspects need to be taken into account, and therefore the development of a phase field model is typically much more straightforward. In this article we will also explicitly make use of sharp interface descriptions, but restrict the investigations to one-dimensional situations, where the tracking of the interface requires just the bookkeeping of a single, time dependent coordinate $L_1(t)$. The motion of the interfaces would then – in the spirit of the discussion above – be directly related to two different expressions for the chemical potential μ , which is the free energy change upon a variation of the interface position L_1 . Here, one candidate for the driving force is the “partial derivative expression” with the strain ε

$$\Delta\mu_p = \left(\frac{\partial F}{\partial L_1} \right)_{c, \varepsilon, \dots}, \quad (5)$$

where other fields are kept constant, whereas in the “total derivative expression”

$$\Delta\mu_t = \frac{dF}{dL_1}, \quad (6)$$

all fields do depend on the interface position, and therefore contribute to the total derivative. The analogy of an equation of motion (1) is in the sharp interface limit

$$\frac{dL_1}{dt} = -K\Delta\mu_p, \quad (7)$$

where the kinetic coefficient K is related to interfacial and kinetic properties of the corresponding phase field model.

We will address the question of the appropriate driving force here using the simplest models to highlight the essential points and not to obscure them by other effects. This means in particular that we will largely focus on one-dimensional geometries, consider only two distinct phases, equal elastic and plastic properties etc. Nevertheless, all statements can directly be transferred to more complex situations.

We point out that aside from the issues related to finding the correct expression for the driving force for interface motion, also other effects need to be considered, which are related to *configurational forces*. They arise when the shape of some material changes not only due to mechanical deformations (which lead to the usual mechanical forces) but by changing the amount of material, i.e. by creating or destroying surfaces without changing the lattice structures and properties. The role of such configurational forces have widely been discussed in the literature, see e.g. (Gurtin, 2000) for an overview in the field of continuum thermodynamics. A well known example is the role of interfacial energy, and its distinction from surface stress (Fischer et al., 2008; Spatschek and Fleck, 2007), but also the conservation of momentum at advancing interfaces in continuum models of fracture are cases where these concepts are applied (Freund, 1998; Brener and Spatschek, 2003). Thermodynamic forces can cause phenomena like grain boundary premelting, see (Sutton and Balluffi, 1995; Adland et al., 2013; Spatschek et al., 2013). In a more general sense we mention also frameworks for phase field models, sharp interface and related formulations, see (Gurtin, 1996; Maugin et al., 2010) for an overview. In this paper, we instead focus entirely on the aspect of the bulk driving force only. In contrast to more general considerations as in Gurtin (2000); Maugin et al. (2010) we study here only specific examples, which are frequently encountered in Materials Science applications, and discuss the models in view of fundamental physical perspectives.

The article is organized as follows: First, we revisit the case of a conserved order parameter model for the description of an alloy in Section 2. Section 3 discusses situations, where elastic effects are relevant. Sections 4 and 5 treat the more complex cases of plastic and viscoelastic effects. The results are summarized in Section 6.

2. Concentration coupling

Above we argued that in situations, where the interface motion is fast in comparison to the diffusion, the use of the partial functional derivative should give the appropriate driving force for the phase field evolution, as the concentration field reacts only slowly to interface fluctuations and can therefore be considered as fixed. Here we will investigate the opposite limit, that the diffusion is infinitely fast in comparison to the interface kinetics. Then the concentration field immediately adjusts to a motion of the interface (similar to the electron density), and we would expect that in this extreme case rather the total functional derivative

$$\frac{\mathcal{D}F}{\mathcal{D}\phi(\mathbf{r})} = \frac{\delta F[\phi, c[\phi]]}{\delta\phi(\mathbf{r})} = \frac{\delta F}{\delta\phi(\mathbf{r})} + \int \frac{\delta F}{\delta c(\mathbf{r}')} \frac{\delta c(\mathbf{r}')}{\delta\phi(\mathbf{r})} d\mathbf{r}' \quad (8)$$

should be the appropriate driving force. Here, the volume integrals are carried out over the whole system with positions \mathbf{r} and \mathbf{r}' . The integral term, which appears due to the chain rule, therefore seems

to give an additional contribution to the driving force in general. In this case the chemical potential μ must be homogeneous in the system,

$$\mu = \frac{\delta F}{\delta c} = \text{const}, \quad (9)$$

which follows from the stationary diffusion equation

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(Dc \nabla \frac{\delta F}{\delta c} \right) = 0, \quad (10)$$

under the assumption that the flux vanishes at infinity, thus $Dc \nabla (\delta F / \delta c) \equiv 0$. Notice that the constancy of the chemical potential holds also if the diffusion constant is different in the phases. Inversion of this relation formally gives $c = c[\phi]$, which is therefore slaved by the phase field.

It is important to take into account here the conservation of the total amount of the impurities,

$$\int c(\mathbf{r}) d\mathbf{r} = \bar{c}V = \text{const} \quad (11)$$

with a given average concentration \bar{c} . Notice that the conservation law is also related to the issue of a finite system size, here with volume V . In this sense, it is also the domain of integration in all the expressions here. Since boundary terms are suppressed in the variational derivatives, this implicitly assumes no-flux boundary conditions, in agreement with the aforementioned material conservation. We therefore introduce a new functional

$$\tilde{F} = F - \lambda \left(\int c(\mathbf{r}) d\mathbf{r} - \bar{c}V \right), \quad (12)$$

with a Lagrange multiplier, instead of incorporating explicitly the conservation constraint. Then by the equilibrium condition for the concentration field (minimization of the free energy F with respect to c under the conservation constraint) we have

$$\frac{\delta \tilde{F}}{\delta c} = \frac{\delta F}{\delta c} - \lambda = 0. \quad (13)$$

As a result, the Lagrange multiplier equals the chemical potential, $\lambda = \mu$. In this sense, the transition from F to \tilde{F} is a Legendre transformation. If the constraint is fulfilled, of course $\tilde{F} = F$. Therefore then also

$$\frac{\mathcal{D}F}{\mathcal{D}\phi(\mathbf{r})} = \frac{\mathcal{D}\tilde{F}}{\mathcal{D}\phi(\mathbf{r})} = \frac{\delta F}{\delta \phi(\mathbf{r})} - \lambda \int \frac{\delta c(\mathbf{r}')}{\delta \phi(\mathbf{r})} d\mathbf{r}' + \int \frac{\delta F}{\delta c(\mathbf{r}')} \frac{\delta c(\mathbf{r}')}{\delta \phi(\mathbf{r})} d\mathbf{r}' = \frac{\delta F}{\delta \phi(\mathbf{r})}, \quad (14)$$

since the last two terms cancel by the definition of the chemical potential. Interestingly, we can therefore conclude that the driving force expression, as it would emerge from a definition via the total derivative, equals the partial variational derivative, as it is routinely used in phase field modeling, which therefore justifies this approach. Notice that for the present case, that the diffusion is infinitely fast, would be the case where we would have expected the largest deviation from the partial work approach, but it turns out that both expressions are identical.

To make this situation more transparent, we use a simple phase field model in dimensionless units

$$f_{pf} = \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}\phi^2(1-\phi)^2 + Th(\phi), \quad (15)$$

$$f_c = c \ln c - c + h(\phi)c, \quad (16)$$

where the coupling function $h(\phi)$ interpolates between 0 and 1, e.g. $h(\phi) = \phi^2(3 - 2\phi)$. T is a reduced temperature deviation from the melting temperature for the pure materials. The term $h(\phi)c$ penalizes segregation in the solid phase and is responsible for the

partitioning. The resulting equilibrium phase diagram has straight solidus and liquidus lines. The free energy functional is

$$F = F_{pf} + F_c = \int (f_{pf} + f_c) dV. \quad (17)$$

The standard equations of motion are

$$\dot{\phi} = -\frac{\delta F}{\delta \phi}, \quad (18)$$

$$\dot{c} = \nabla \cdot \left(c \nabla \frac{\delta F}{\delta c} \right). \quad (19)$$

Here, the derivatives are treated in the sense of partial derivatives, which means that c is considered as frozen in during variation with respect to ϕ .

For slow interface motion the conjecture would be that the evolution of the phase field should instead follow an equation of the sort

$$\dot{\phi} = -\frac{\mathcal{D}F}{\mathcal{D}\phi}, \quad (20)$$

where $\mathcal{D}/\mathcal{D}\phi$ symbolizes a “total derivative”, in the sense that the concentration field can adjust immediately.

For a fast equilibrating concentration field we have the condition

$$\frac{\delta F}{\delta c} = \ln c + h(\phi) = \mu = \text{spatially constant}, \quad (21)$$

and therefore the concentration field is slaved by the phase field

$$c(\phi) = \exp(\mu - h(\phi)). \quad (22)$$

The total derivative would thus be

$$\frac{\mathcal{D}F[\phi, c(\phi)]}{\mathcal{D}\phi} = \frac{\delta F}{\delta \phi} + \frac{\partial f_c}{\partial c} \frac{\partial c}{\partial \phi} = \frac{\delta F}{\delta \phi} - \mu h'(\phi)c(\phi), \quad (23)$$

where we used $\partial f_c / \partial c = \mu$. Here it seems that a new term appears which is not used in typical phase field formulations, and as we will see below, it is not correct here. First we note the interpretation of this term: Consider a planar front moving through the system, let's say during solidification. Then in each bulk phase the concentrations are (in this fast diffusion limit, where no solute trapping occurs) equal to the equilibrium values c_s and c_l . Only in the interface region we have a nontrivial transition between these two values. If the interface moves, therefore now excess solute $c_l - c_s$ has to be removed from the system against the “work” of the chemical potential μ , and this is exactly expressed through the new term in the variational derivative above. Since the removal takes place at the boundary of the system, this is a highly nonlocal process, and is intimately related to the fact that the concentration is a conserved quantity. However, this is the reason why the above total derivative is *not* the correct driving force. We used a free energy functional to derive the equations of motion. Thermodynamically, this is only the right functional for a system with fixed volume and number of particles, and therefore for the constraint

$$\int c dV = \text{constant in time}. \quad (24)$$

According to the interpretation given above, this constraint is so far not taken into account in the derivation above, and therefore, the above total derivative is *not* the correct driving force. The consideration of the correct thermodynamic potential is therefore mandatory for obtaining the correct driving force. Here we find that for the alloy example the definition of the correct variational procedure is less critical, as both lead to the same expression. However, this is not a general result, as will become more transparent later. We mention in passing that e.g. in situations with non-constant temperature in closed systems maximization entropy is the proper

thermodynamic principle, and therefore this potential is used in phase field models of alloys (Nestler et al., 2005) or applied electrical currents and Joule heating (Brush, 2003).

To correct the mistake of the improper material conservation, we need to take into account that the chemical potential is not constant during interface motion, but adopts according to the conservation law above. Therefore, it becomes a nonlocal functional of the phase field, and therefore leads to a contribution in the correct driving force term. The concentration has to obey the constraint

$$\int c dV = \bar{c}V, \quad (25)$$

with the average concentration \bar{c} and the system volume V . Therefore we get from Eq. (22) the value of the chemical potential

$$\mu = \ln \frac{\bar{c}V}{\int \exp(-h(\phi)) dV}. \quad (26)$$

Hence the concentration is a nonlocal functional of the phase field

$$c[\phi] = \frac{\bar{c}V \exp(-h(\phi))}{\int \exp(-h(\phi)) dV}. \quad (27)$$

We can calculate the total functional derivative of the free energy contribution F_c

$$\frac{\mathcal{D}F_c}{\mathcal{D}\phi(\mathbf{r})} = \frac{\delta F_c(\phi, c[\phi])}{\delta \phi} = \frac{\delta F_c(\phi, c)}{\delta \phi} + \int \frac{\partial f_c(\phi, c)}{\partial c} \frac{\delta c(\mathbf{r}')}{\delta \phi(\mathbf{r})} d\mathbf{r}', \quad (28)$$

where the first term is the usual one, and we do not consider it further; it is present also in the “partial work approach”. In the second term the variation of the concentration upon a change of ϕ is

$$\frac{\delta c(\mathbf{r}')}{\delta \phi(\mathbf{r})} = \frac{\bar{c}V \exp(-h(\phi(\mathbf{r}')))}{[\int \exp(-h(\phi)) dV]^2} \exp(-h(\phi(\mathbf{r}))) h'(\phi(\mathbf{r})) - \frac{\bar{c}V}{\int \exp(-h(\phi)) dV} h'(\phi(\mathbf{r})) \exp(-h(\phi(\mathbf{r}))) \delta(\mathbf{r} - \mathbf{r}')$$

Inserting this into the second integral term above gives

$$\int \frac{\partial f_c(\phi, c)}{\partial c} \frac{\delta c(\mathbf{r}')}{\delta \phi(\mathbf{r})} dV = 0, \quad (29)$$

where we used $\partial f_c(\phi, c)/\partial c = \mu$, which is spatially constant. Consequently, we obtain in this limit, where the concentration is slaved and conserved

$$\frac{\mathcal{D}F_c}{\mathcal{D}\phi} = \frac{\delta F_c(\phi, c)}{\delta \phi}. \quad (30)$$

The expectation was that in this case, where the concentration field adjust instantaneously to changes of the interface position, that here the deviation from the partial derivative (“partial work”) as driving force would be highest; however, now we see that even in this limit both approaches coincide.

In view of these result it is not surprising that the free energy is a Lyapunov functional even in the general case, where the concentration field is not slaved. From the equations of motion above we deduce after an integration by parts

$$\begin{aligned} \frac{dF}{dt} &= \int \left(\frac{\delta F(\phi, c)}{\delta \phi} \dot{\phi} + \frac{\delta F(\phi, c)}{\delta c} \dot{c} \right) dV \\ &= - \int \left[\left(\frac{\delta F(\phi, c)}{\delta \phi} \right)^2 + c \left(\frac{\delta F(\phi, c)}{\delta c} \right)^2 \right] dV \leq 0. \end{aligned} \quad (31)$$

3. Elasticity

Elastic effects are essential during many solid-state transformations, and their implementation in phase field models has been demonstrated repeatedly in the literature (see e.g. (Chen, 2002;

Spatschek et al., 2011)). In many cases, the assumption of static elasticity is legitimate, since the front velocities are often slow in comparison to the sound speed. Here, we would again expect that the elastic degrees of freedom adjust instantaneously during a “trial step” of the interface to explore the decay of the free energy as driving force. In contrast to what is usually used for phase field models we would therefore expect an equation of motion of the form

$$\frac{\partial \phi}{\partial t} = - \frac{\mathcal{D}F}{\mathcal{D}\phi}. \quad (32)$$

However, from the elastic equilibrium conditions for the displacement components u_i

$$\frac{\delta F}{\delta u_i} = 0 \quad (33)$$

follows immediately

$$\frac{\mathcal{D}F}{\mathcal{D}\phi} = \frac{\delta F}{\delta \phi} \quad (34)$$

by the chain rule,

$$\frac{\mathcal{D}F}{\mathcal{D}\phi(\mathbf{r})} = \frac{\delta F}{\delta \phi(\mathbf{r})} + \int \frac{\delta F}{\delta \mathbf{u}(\mathbf{r}')} \frac{\delta \mathbf{u}(\mathbf{r}')}{\delta \phi(\mathbf{r})} d\mathbf{r}'. \quad (35)$$

Again, both driving force expressions therefore give identical results. We note that no assumption about the elastic model had to be made, and the statement therefore holds equally for isotropic as for anisotropic, for linear as for nonlinear elasticity. We mention that upon integration by parts for the functional derivatives elastic boundary conditions naturally arise. This is illustrated explicitly in the one-dimensional formulation below, where we consider in particular fixed-volume scenarios, in agreement with the use of the Helmholtz free energy as thermodynamic potential (Landau, 1986).

Instead of a phase field formulation, also a sharp interface model can be used equivalently, as will be illustrated in the following. For simplicity, we consider the simplest case of a one-dimensional, linear elastic model, since there the interface tracking problem is reduced to the requirement to know just the (time-dependent) interface coordinate. Nevertheless, all steps can be transferred to more complicated situations, and the link to phase field models will be established below. The following example serves also as basis for the inclusion of plasticity later in the text.

The system is assumed to have the length L , and the interface is located at the position $0 < L_1(t) < L$. The free energy of the system is then

$$F_0[\varepsilon_1, \varepsilon_2, L_1] = \int_{x=0}^{L_1} f_1(\varepsilon_1(x)) dx + \int_{x=L_1}^L f_2(\varepsilon_2(x)) dx, \quad (36)$$

where interfacial energy terms are neglected, since they give only an additive constant (the surface “area” is constant in one dimension).

Since in the following it is more convenient to work with strains $\varepsilon = du/dx$ than with displacements, we have to fulfil additionally the constraint that the total displacement should equal the system elongation Δ , which we realize by a Lagrange multiplier λ_u

$$\begin{aligned} F[\varepsilon_1(x), \varepsilon_2(x), L_1] &= F_0[\varepsilon_1(x), \varepsilon_2(x), L_1] \\ &\quad - \lambda_u \left[\int_{x=0}^{L_1} \varepsilon_1(x) dx + \int_{x=L_1}^L \varepsilon_2(x) dx - \Delta \right]. \end{aligned} \quad (37)$$

The reason is that for the free energy as proper thermodynamic functional the system volume, which is here related to the total displacement Δ , has to be constant. As we will see below, the transition from F_0 to F corresponds to a change from the Helmholtz to the Gibbs free energy via a Legendre transformation by addition of “ pV ” (pressure times volume). The local stress is defined as

$$\sigma_i(x) = \frac{\partial f_i(\varepsilon_i(x))}{\partial \varepsilon_i(x)}. \quad (38)$$

Mechanical equilibrium requires that the functional (37) is minimized with respect to the strains, thus

$$\frac{\delta F}{\delta \varepsilon_1(x)} = \frac{\partial f_1}{\partial \varepsilon_1(x)} - \lambda_u = 0, \quad (39)$$

$$\frac{\delta F}{\delta \varepsilon_2(x)} = \frac{\partial f_2}{\partial \varepsilon_2(x)} - \lambda_u = 0, \quad (40)$$

which implies that the stresses in both phases are spatially constant and equal,

$$\sigma_1(x) = \sigma_2(x) = \lambda_u =: \sigma = const, \quad (41)$$

which also identifies the meaning of the Lagrange multiplier as the system stress. This also shows that the difference between F_0 to F corresponds to a “ pV term”.

The driving force which is related to a virtual shift of the interface position and fixed elastic fields (corresponding to the partial variational derivative in a phase field framework) is

$$\Delta \mu_p = \left(\frac{\partial F}{\partial L_1} \right)_{\varepsilon_1(x), \varepsilon_2(x)}. \quad (42)$$

This has to be contrasted with the “total” driving force

$$\Delta \mu_t = \frac{dF}{dL_1}, \quad (43)$$

where the strains are not frozen but taken as functions of L_1 .

For an explicit model we assume linear elasticity with equal elastic constants E in the two phases, thus the energy densities are

$$f_1 = \frac{1}{2} E \varepsilon_1^2 + \Delta f, \quad (44)$$

$$f_2 = \frac{1}{2} E (\varepsilon_2 - \varepsilon_0)^2, \quad (45)$$

with eigenstrain ε_0 and a tilt term Δf , which reflects temperature deviations from phase equilibrium. Therefore the stress is $\sigma = E \varepsilon_1 = E (\varepsilon_2 - \varepsilon_0) = const$. From this follows in particular that the elastic strain in each phase is constant, and we obtain

$$\varepsilon_1 = \varepsilon_2 - \varepsilon_0 = \Delta/L - (1 - L_1/L) \varepsilon_0. \quad (46)$$

Therefore, the free energy becomes

$$F(L_1) = \frac{E}{2L} (-\Delta + (L - L_1) \varepsilon_0)^2 + \Delta f L_1, \quad (47)$$

from which we directly get the total work expression

$$\Delta \mu_t = \sigma \varepsilon_0 + \Delta f. \quad (48)$$

In contrast, the “partial” work expression is

$$\Delta \mu_p = \frac{1}{2} E \varepsilon_1^2 - \frac{1}{2} E (\varepsilon_2 - \varepsilon_0)^2 - \sigma (\varepsilon_1 - \varepsilon_2) + \Delta f. \quad (49)$$

By virtue of Eq. (46) we readily obtain the expected agreement with the total work expression

$$\Delta \mu_p = \sigma \varepsilon_0 + \Delta f. \quad (50)$$

The nonequilibrium front propagation is in this sharp interface model described by an evolution law of the kind

$$\frac{dL_1}{dt} = -K \Delta \mu \quad (51)$$

with a kinetic coefficient K . This simple problem can easily be solved analytically, and we obtain

$$L_1(t) = L_1^{(eq.)} + c_1 \exp \left[-\frac{KE \varepsilon_0^2 t}{L} \right] \quad (52)$$

with

$$c_1 = L_1(t=0) + \frac{\Delta}{\varepsilon_0} - L + \frac{L \Delta f}{E \varepsilon_0^2} \quad (53)$$

and the equilibrium width of phase 1

$$L_1^{(eq.)} = -\frac{\Delta}{\varepsilon_0} + L - \frac{L \Delta f}{E \varepsilon_0^2}. \quad (54)$$

Whenever $L_1^{(eq.)}/L$ is in the range (0, 1) we get phase coexistence in equilibrium. This is shown in Fig. 1, together with a numerical integration of the equation of motion (51). For this, at each time step the partial or total energy change for interface motion in both directions is computed (they are equal up to the sign for the present problem), and then the interface is advanced accordingly. From Eqs. (46) and (52) follows then the stress evolution, which is shown in Fig. 2.

If we call phase 1 the austenite and phase 2 the martensite, we get the “martensite start temperature”

$$M_s(\Delta) = -\frac{E \varepsilon_0 \Delta}{L} \quad (55)$$

and the “finish temperature”

$$M_f(\Delta) = E \varepsilon_0^2 - \frac{E \varepsilon_0 \Delta}{L}. \quad (56)$$

Notice that both of them depend on the external displacement Δ , which shifts the temperatures linearly (Clausius–Clapeyron effect).

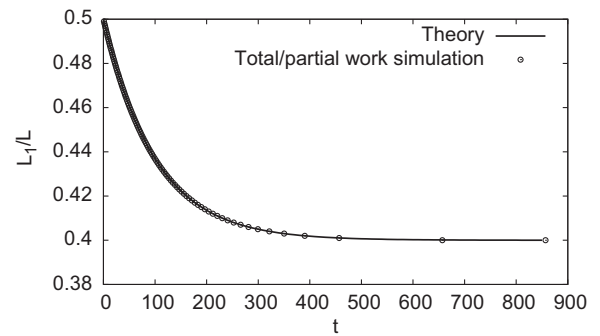


Fig. 1. Interface evolution for a purely elastic case. The exponential relaxation towards the equilibrium interface position agrees well between the theoretical prediction (using either the total or partial work as driving force), and the numerical simulation. Parameters are $E = 1$, $\varepsilon_0 = 0.1$, $\Delta = 0.01L$, $\Delta f = 0.005$ and $K = 1$.

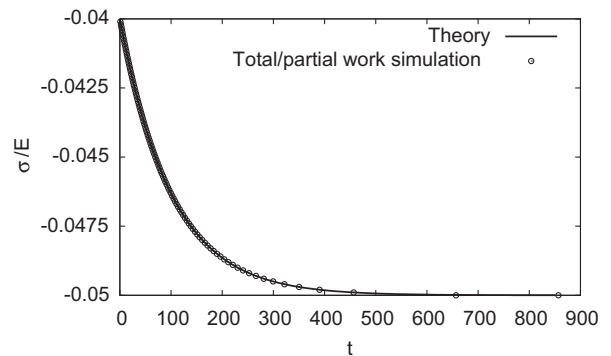


Fig. 2. Stress evolution as function of time for the purely elastic case, corresponding to the interface motion in Fig. 1. During the growth of the less dense phase 2 the compressive stress in the clamped system increases and hampers further phase transformation, until the elastic driving force balances the undercooling and the process asymptotically comes to rest.

The width of the coexistence region is $M_f - M_s = E\varepsilon_0^2$. In between, the martensite volume fraction varies linearly with temperature, see Fig. 3. Notice that within this one-dimensional model we do not have an elastic hysteresis, therefore the martensite start and austenite finish temperature coincide, as well as the martensite finish and austenite start temperature. Corresponding stress–strain curves are shown in Fig. 4. In the single phase regimes the stress increases linearly with strain, but stays constant in the two-phase region.

This case shows in particular the duality of phase field and sharp interface descriptions. The fact, that total and partial work coincide holds both for the phase field as well as the sharp interface description. To make the link more explicit, we can use for a one-dimensional phase field description the functional

$$F[\phi, u] = \int_0^L (f_s + f_{dw} + f_{el} + f_T) dx \quad (57)$$

with the Landau free energy density

$$f_s = \frac{3\gamma\xi}{2} \left(\frac{d\phi}{dx} \right)^2 \quad (58)$$

with the interface thickness ξ and the interfacial energy γ . Notice, that although we do not need the latter parameter in the sharp interface description, since the interface is just a point in a

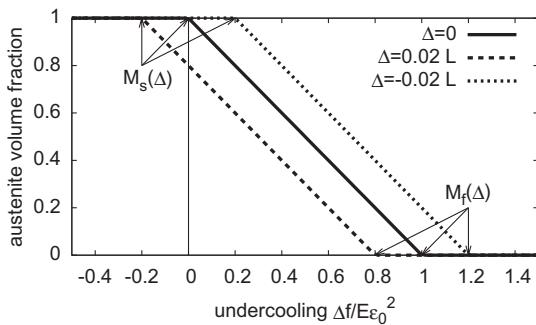


Fig. 3. Austenite volume fraction as function of undercooling for different applied strains. The martensite start temperature M_s and finishing temperature M_f depend on the total system displacement. For a lower density martensite, $\varepsilon_0 = 0.1 > 0$ here, the conversion to martensite is favored for tensile strain, and therefore the transition starts already at higher temperatures (dashed curve), for compressive strain the coexistence region is shifted towards lower temperatures (dotted curve). In the coexistence regime the volume fraction changes linearly with temperature. For a stress free system without mechanical constraint coexistence is only possible at the nominal phase equilibrium temperature $\Delta f = 0$. Parameters are the same as in Fig. 1.

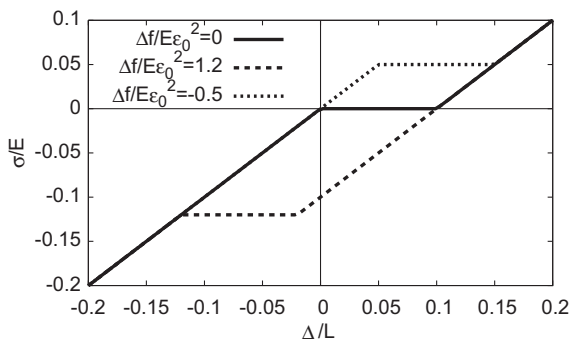


Fig. 4. Stress–strain curve for different temperatures in the linear elastic regime. During the elastically induced phase transformation the stress remains constant. Parameters are the same as in Fig. 1.

one-dimensional situation and therefore the surface “area” cannot change, it still appears in a phase field description and is required for the interface stabilization. However, its choice is not crucial here, but a proper choice may stabilize in particular moving interfaces. The double well potential is

$$f_{dw} = \frac{6\gamma}{\xi} \phi^2 (1 - \phi)^2, \quad (59)$$

and the elastic energy density in agreement with the sharp interface model

$$f_{el} = h(\phi) \frac{1}{2} E \varepsilon^2 + [1 - h(\phi)] \frac{1}{2} E (\varepsilon - \varepsilon_0)^2, \quad (60)$$

with an interpolating function $h(\phi) = \phi^2(3 - 2\phi)$. Notice that now we do not have to explicitly discriminate between the strains in the two phases, $\varepsilon = u'$. Hence $\phi = 1$ corresponds to phase 1 and $\phi = 0$ to phase 2. Finally, we add the thermal tilt

$$f_T = h(\phi) \Delta f. \quad (61)$$

The equation of motion is

$$\frac{\partial \phi}{\partial t} = - \left(\frac{\delta F}{\delta \phi} \right)_u = - \frac{DF}{D\phi}, \quad (62)$$

where the time scale has been renormalized such that no additional kinetic coefficient appears in front of the variational derivative. The latter identity follows from the static mechanical equilibrium condition

$$\left(\frac{\delta F}{\delta u} \right)_\phi = 0. \quad (63)$$

A planar front solution is

$$\phi(x, t) = \frac{1}{2} \left(1 - \tanh \frac{x - L_1(t)}{\xi} \right), \quad (64)$$

with front velocity

$$\dot{L}_1 = 3\xi\Delta\mu, \quad (65)$$

in the sharp interface limit, and hence we identify for this model $K = 3\xi$.

4. Elasto-viscoplasticity

Typical (visco-) plasticity models bring in a new aspect into phase transition modeling, as they contain internal variables, with evolution laws that are not derived from the same functional as the other dynamical equations. The main message of this paper is, that due to this property, the driving force expressions as derived from different variational derivatives give different results, and therefore one should postulate evolution equations with care. To underline this statement and some consequences, we use in the following a simple, one-dimensional von Mises-type model. Isotropic strain hardening is considered in the following (except of in the simulations). We refrain here from discussing more complex models, which may be used for realistic modeling, in order not to obscure the result; nevertheless, it should be pointed out that the same question for the correct driving force appears also in these cases.

We will start the discussion again with a one-dimensional sharp interface model, since this allows an analytical treatment, and also for numerical investigations it is easier to switch between the ‘partial’ and ‘total’ work for interface motion.

For convenience, we replace the rate-independent elasto-plasticity model by a rate-dependent viscoplasticity model according to

decomp. of deformation $\varepsilon = \varepsilon_{el} + \varepsilon_{vpl}$ (66)

closure of elastic domain $\mathbb{E}_\sigma := \{(\sigma, \alpha) \in \mathbb{R} \times \mathbb{R}_+ | f(\sigma, \alpha) \leq 0\}$ (67)

yield function $f(\sigma, \alpha) := |\sigma| - [\sigma_y + K\alpha]$ (68)

flow rule(Duvaut-Lions) $\dot{\varepsilon}_{vpl} = \begin{cases} \frac{E^{-1}}{\tau} [\sigma - \mathbf{P}\sigma] & \text{if } f(\sigma, \alpha) > 0 \\ 0 & \text{else} \end{cases}$ (69)

hardening law $\dot{\alpha} = |\dot{\varepsilon}_{vpl}|$ (70)

where $\mathbf{P} : \mathbb{R} \rightarrow \partial\mathbb{E}_\sigma$ is the closest point projection onto $\partial\mathbb{E}_\sigma$, i.e. the boundary of the elastic range. Furthermore, the yield stress is denoted by σ_y and the viscoplastic relaxation timescale is τ . Notice, that in the limit $\tau \rightarrow 0$ the case of rate-independent plasticity is restored.

The present model exhibits the visco-plastic strain ε_{vpl} and the equivalent plastic strain α driving isotropic strain hardening. The previously introduced eigenstrain can be understood as a special case of a plastic deformation, with the only difference that the eigenstrain can there change only due to the phase transition, but not as a result of plastic flow.

The previous results can therefore also be interpreted as the phase transition between two materials, with one of them previously being loaded beyond the elastic limit, such that a plastic strain $\varepsilon_{vpl,2} = \varepsilon_0$ remains, and, consecutively, purely elastic deformations. However, the preceding analysis suggests that a qualitatively different behavior can occur if plastic deformations occur during the phase transformation process.

The first example that we use here is a case where the initial state is still in the elastic regime, i.e. initially the stress is below the yield stress. For simplicity we assume again that the two elastic constants are equal, and that phase 1 has in the beginning a vanishing plastic strain, whereas $\varepsilon_{vpl,2} = \varepsilon_0$ in the beginning e.g. due to prior plastic deformations or a density difference in comparison to phase 1.

In contrast to the elastic case, where we have a unique link between phase and eigenstrain, this is not necessarily the case for phase transitions involving plastic deformations. The plastic strain is a dynamical quantity, and it is usually not homogeneous within one phase, but may change there even discontinuously. This will be discussed in more detail below, and for the moment we assume that the plastic strain is homogeneous in each phase, which simplifies the theoretical analysis.

As long the system remains in the elastic state, the stress in the two-phase region for the equilibrium interface position is

$$\sigma = -\frac{\Delta f}{\varepsilon_0}, \quad (71)$$

which follows from Eqs. (50) and (51). Depending on the initial phase fractions and temperature the stress can increase or decrease during the interface motion. In case that it grows we expect a deviation from the previous exponential relaxation to the equilibrium phase fractions if the stress exceeds the yield stress σ_y . For a situation in which the absolute value of the stress grows monotonically during the evolution, we get a transition from the purely elastic to a plastic regime if $|\Delta f/\varepsilon_0| > \sigma_y$.

The noticeable effect is that at the moment when the yield stress is reached, the martensite volume fraction changes fast and linearly in time. Intuitively spoken, the reason for this abrupt change of the material behavior is that the stress remains constant in the plastic regime, and therefore the driving force does not change. Consequently the phase transformation velocity is constant in our one-dimensional example. In the following, we will analyze this behavior analytically.

Let t_p be the time when the yield stress is reached. At that moment the interface is located at $L_1(t_p)$. From then on the stress must stay at the level of the yield stress if the relaxation timescale τ is

short, $\tau \rightarrow 0$. At $t = t_p$ we start with known values of $\varepsilon_{vpl,1}(t_p)$ and $\varepsilon_{vpl,2}(t_p)$. If phase 1 grows, this would create a stress overshoot $\sigma_y + \delta\sigma$ with $\delta\sigma = -E(\varepsilon_{vpl,1} - \varepsilon_{vpl,2})\Delta x$, along with a plastic strain rate following from the flow rule

$$\dot{\varepsilon}_{vpl,i} = \frac{1}{\tau E} \delta\sigma, \quad i = 1, 2 \quad (72)$$

which is equal for both phases. Therefore, we get equally the same inelastic strain increment $\Delta\varepsilon_{vpl}(t)$ in both phases

$$\varepsilon_{vpl,i}(t) = \varepsilon_{vpl,i}(t_p) + \Delta\varepsilon_{vpl}(t), \quad i = 1, 2 \quad (73)$$

The decomposition of deformation reads

$$\varepsilon_{vpl,1}(t) = \varepsilon_i(t) - \varepsilon_{el}, \quad i = 1, 2. \quad (74)$$

Together with the compatibility condition, i.e. the displacements at $x = L$ obeying

$$u(x = L) = \varepsilon_1 L_1 + \varepsilon_2 (L - L_1) = \Delta, \quad (75)$$

we have five equations for the five unknowns $\varepsilon_1(t)$, $\varepsilon_2(t)$, $\varepsilon_{vpl,1}(t)$, $\varepsilon_{vpl,2}(t)$ and $\Delta\varepsilon_{vpl}(t)$ for known interface position $L_1(t)$.

Next, we assume that the free energy density has the form

$$f_1(\varepsilon_1, \varepsilon_{vpl,1}) = \frac{1}{2} E \varepsilon_{el,1}^2 + f_{vpl,1}(\varepsilon_{vpl,1}) + \Delta f, \quad (76)$$

$$f_2(\varepsilon_2, \varepsilon_{vpl,2}) = \frac{1}{2} E \varepsilon_{el,2}^2 + f_{vpl,2}(\varepsilon_{vpl,2}), \quad (77)$$

in agreement with the stress-strain relation used before. The term $f_{vpl,i}$, $i = 1, 2$ is a function of the local plastic strain state and represents a “defect energy” of the material, which typically leads to the phenomenological effect of strain hardening. In Eq. (68) a simple linear isotropic strain hardening was assumed to hold, following from a quadratic form of the plastic potential $f_{vpl,i} = 1/2K\alpha^2$.

Concerning the definition of the different candidates for driving force terms, more care should be used here. As mentioned before, the reason is that e.g. for the elastic case the eigenstrain is directly linked to the “phase state” and homogeneous in each phase. The plastic strain, however, can be inhomogeneous in each phase, since it obeys a separate dynamical evolution. A simple example would be a cylindrical hole, which acts as a stress concentrator, and then the material can be still fully elastic far away from the whole but plastic with a nonvanishing plastic strain close to the defect (Fleck et al., 2010). Furthermore, the motion of a phase boundary can influence the plastic state: if one phase is converted into another, it is not a priori clear in which “defect state” the new phase will grow. On the one hand it is possible that in the newly transformed phase many misfit dislocations are generated, therefore leading to a high plastic strain in this region, but on the other hand it is also conceivable that the new phase can grow defect free although the mother phase contains many dislocations. In particular, it is therefore possible that the newly grown phase has a very different plastic strain than parts of the same phase. This implies that within each phase the material properties, here the plastic strain, can change discontinuously, and therefore also in the calculation of the driving forces all functions have to be evaluated with care. In fact, we find that the choice of the variational procedure does matter here, which is a central message of the present paper. This is illustrated in the following in more detail.

4.1. Total work expression

For the calculation of the total work one therefore gets in general different driving forces for the growth of the two phases, one for a interface trial step $\delta L_1 > 0$ and another for $\delta L_1 < 0$. To discriminate between the different states for the internal variables before

and after the interface motion step, we therefore use superscripts (old) and (new) and obtain

$$\Delta\mu_t^{\delta L_1 > 0} = f_1^{(new)}|_{int} - f_2^{(old)}|_{int} - \sigma(\varepsilon_1^{(new)}|_{int} - \varepsilon_2^{(old)}|_{int}) + \int_0^{L_1} \frac{\partial f_1}{\partial \varepsilon_{vpl,1}} \frac{\partial \varepsilon_{vpl,1}(x, L_1)}{\partial L_1} dx + \int_{L_1^+}^L \frac{\partial f_2}{\partial \varepsilon_{vpl,2}} \frac{\partial \varepsilon_{vpl,2}(x, L_1)}{\partial L_1} dx. \quad (78)$$

Here, the term $f_1^{(new)}|_{int} - f_2^{(old)}|_{int}$ accounts for the work to replace the material consisting of phase 2 at the interface (in the plastic state before the trial step) by the newly grown phase 1 in the new state. The second term, $\sigma(\varepsilon_1^{(new)}|_{int} - \varepsilon_2^{(old)}|_{int})$, is the mechanical work that is necessary to maintain the coherency, since the previous phase 2 before the transformation has a new strain than the new phase 1 after the transformation. The last two terms are the nonlocal terms which result from plastic bulk dissipation ($\Delta\mu_{nl}$). Here it is assumed that the plastic strain changes smoothly in these regions. In the second integral the lower integration bound is L_1^+ , i.e. it has to be evaluated in phase 2 only, despite the fact that an (infinitesimally small) part of this phase at the interface is converted to phase 1 at the interface.

For growth of phase 2, $\delta L_1 < 0$, the expression is similarly

$$\Delta\mu_t^{\delta L_1 < 0} = f_1^{(old)}|_{int} - f_2^{(new)}|_{int} - \sigma(\varepsilon_1^{(old)}|_{int} - \varepsilon_2^{(new)}|_{int}) + \int_0^{L_1^-} \frac{\partial f_1}{\partial \varepsilon_{vpl,1}} \frac{\partial \varepsilon_{vpl,1}(x, L_1)}{\partial L_1} dx + \int_{L_1}^L \frac{\partial f_2}{\partial \varepsilon_{vpl,2}} \frac{\partial \varepsilon_{vpl,2}(x, L_1)}{\partial L_1} dx. \quad (79)$$

For the “partial” work as driving force, all fields have to be evaluated in the old state, since the fields are frozen during the trial step. This means in particular that there is no distinction between the different directions of interface growth, and no nonlocal terms appear. Hence we obtain

$$\Delta\mu_p = f_1^{(old)}|_{int} - f_2^{(old)}|_{int} - \sigma(\varepsilon_1^{(old)}|_{int} - \varepsilon_2^{(old)}|_{int}). \quad (80)$$

For the presently considered case that the material grows in the same plastic state as the same adjacent already existing phase and continuous functions f_i , the distinction between (old) and (new) is not necessary, and therefore the only relevant difference between total and partial work expression is the appearance of the nonlocal terms. Furthermore, the “partial work expression” does not depend on the direction of interface motion.

For the specific model above we obtain

$$\frac{\partial f_i}{\partial \varepsilon_{vpl,i}} = -E\varepsilon_{el,i} + f'_{vpl,i}(\varepsilon_{vpl,i}) = -\sigma_y + f'_{vpl,i}(\varepsilon_{vpl,i}). \quad (81)$$

The local contribution to the chemical potential difference (partial work) is given by

$$\begin{aligned} \Delta\mu_p &= f_1(\varepsilon_1, \varepsilon_{vpl,1}) - f_2(\varepsilon_2, \varepsilon_{vpl,2}) - \sigma_y(\varepsilon_1 - \varepsilon_2) \\ &= \frac{\sigma_y^2}{2E} + f_{vpl,1} - \frac{\sigma_y^2}{2E} - f_{vpl,2} \\ &\quad - \sigma_y \left(\frac{\sigma_y}{E} + \varepsilon_{vpl,1}(t) - \frac{\sigma_y}{E} - \varepsilon_{vpl,2}(t) \right) + \Delta f \\ &= f_{vpl,1} - f_{vpl,2} - \sigma_y [\varepsilon_{vpl,1}(t_p) - \varepsilon_{vpl,2}(t_p)] + \Delta f. \end{aligned} \quad (82)$$

The nonlocal contribution is

$$\begin{aligned} \Delta\mu_{nl} &= \frac{\partial f_1}{\partial \varepsilon_{vpl,1}} \frac{d\varepsilon_{vpl,1}}{dL_1} L_1 + \frac{\partial f_2}{\partial \varepsilon_{vpl,2}} \frac{d\varepsilon_{vpl,2}}{dL_1} (L - L_1) \\ &= [-\sigma_y + f'_{vpl,1}] \frac{d\Delta\varepsilon_{vpl}}{dL_1} L_1 + [-\sigma_y + f'_{vpl,2}] \frac{d\Delta\varepsilon_{vpl}}{dL_1} (L - L_1) \\ &= \frac{d\Delta\varepsilon_{vpl}}{dL_1} [-\sigma_y L + f'_{vpl,1} L_1 + f'_{vpl,2} (L - L_1)] \end{aligned} \quad (83)$$

From the above equations we get

$$\Delta\varepsilon_{vpl} = \frac{\Delta - \varepsilon_{vpl,1}(t_p)L_1 - L_1\sigma_y/E}{L} - \frac{L - L_1}{L} \left(\frac{\sigma_y}{E} + \varepsilon_{vpl,2}(t_p) \right) \quad (84)$$

and therefore

$$\frac{d\Delta\varepsilon_{vpl}}{dL_1} = -\frac{\varepsilon_{vpl,1}(t_p)}{L} + \frac{\varepsilon_{vpl,2}(t_p)}{L}. \quad (85)$$

This means that the “total” driving force $\Delta\mu_t = \Delta\mu_p + \Delta\mu_{nl}$ is

$$\begin{aligned} \Delta\mu_t &= [\varepsilon_{vpl,2}(t_p) - \varepsilon_{vpl,1}(t_p)] \\ &\quad \times \left[f'_{vpl,1}(\varepsilon_{vpl,1})L_1 - f'_{vpl,2}(\varepsilon_{vpl,2})(L - L_1) \right] / L + f_{vpl,1}(\varepsilon_{vpl,1}) \\ &\quad - f_{vpl,2}(\varepsilon_{vpl,2}) + \Delta f. \end{aligned} \quad (86)$$

To simplify and illustrate the behavior, we assume $f_{vpl,i} = 0$, which means that the free energy of the defects is assumed to be negligibly small. It is quite remarkable that all mechanical effects completely drop out of the driving force term. Then $\Delta\mu_t = \Delta f$ becomes constant, which, together with the evolution equation $\dot{L}_1 = -K\Delta\mu_t$ leads to a constant interface velocity in the plastic regime, see Fig. 5. The time evolution of the stress and the plastic strain are shown in Figs. 6 and 7. The equilibrium austenite volume fraction as function of temperature, depending on the yield stress and external deformation, are shown in Figs. 8 and 9 respectively.

4.2. Partial work expression

Let us contrast this with a model where the interface motion is driven by the partial work expression. Again, for the case of negligible defect energy, $f_{vpl,i} = 0$, the driving force becomes constant in the plastic regime, $\Delta\mu_p = -\sigma_y [\varepsilon_{vpl,1}(t_p) - \varepsilon_{vpl,2}(t_p)] + \Delta f$, and therefore also here the interface velocity becomes constant. The process therefore stops only when the material is completely converted into a single phase. In contrast to the total work case, the interface velocity changes here continuously at the transition point between the elastic and plastic regime, see Fig. 5, since the strain difference at the plastification time t_p is exactly equal to the eigenstrain difference in the elastic regime, and therefore the driving force after this point matches the elastic expression (50).

The existence of the two-phase region is a consequence of the total volume constraint; in the purely elastic case phase coexistence would exist only for one specific temperature if instead of the total displacement the stress is given. The presence of plastic effects acts in some sense like a modification of the boundary conditions in closed systems, as the stress remains at the yield stress even if the interface moves. It is therefore consistent that the coexistence region becomes smaller through the presence of plastic effects. On the other hand it is quite remarkable, that with plastic

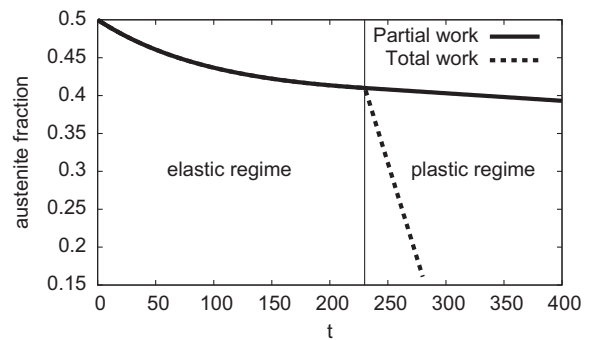


Fig. 5. Interface position as function of time. Initially, the system is in a purely elastic state, i.e. $\varepsilon_{vpl,1} = 0$ and $\varepsilon_{vpl,2} = \varepsilon_0 = 0.1$. During the evolution the absolute value of the stress increases, until it reaches the yield stress. At this moment, the interface starts to move linear in time until it hits the boundary, i.e. the equilibrium state is a single phase. This means that the martensite start and finish temperatures are changed through the plastic effects. Parameters are $E = 1, \sigma_y = 0.049, L = 1, \Delta = 0.01, \Delta f = 0.005, K = 1, f_{vpl,1} = f_{vpl,2} = 0$.

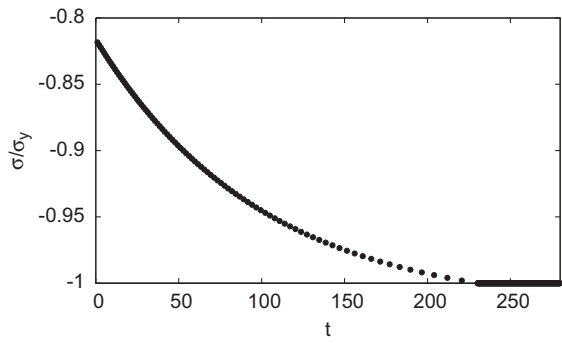


Fig. 6. Stress as function of time for the simulation in Fig. 5. The graph is valid for both the total and the partial work as driving force. The parameters are the same as in Fig. 5.

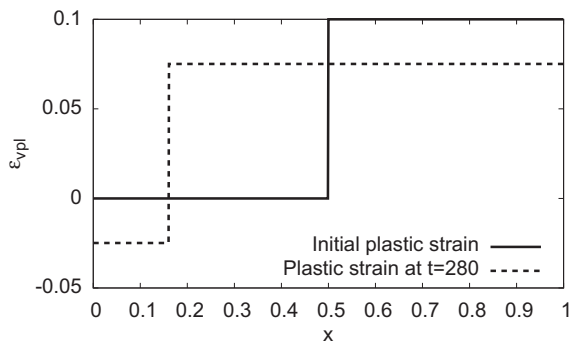


Fig. 7. Plastic strain at the beginning of the simulation and after the transition to the plastic growth regime. Note that at the given time the simulation is still in the two-phase region. In each phase the plastic strain is spatially homogeneous. The position of the jump in the plastic strain denotes the interface position. The parameters are the same as in Fig. 5.

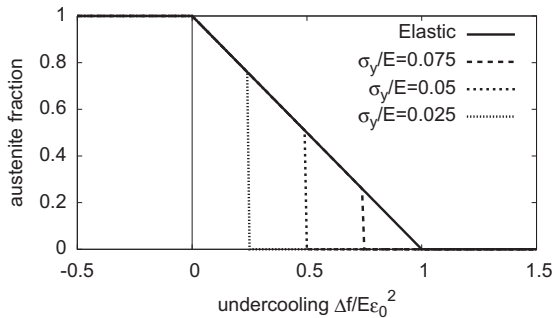


Fig. 8. Austenite volume fraction as function of undercooling, for different values of the yield stress. For high yield stresses, the behavior is the same as in the elastic case. For lower yield stresses plastic effects set in as soon the yield stress is exceeded, and then the remaining austenite is fully transformed into martensite. In this regime the knowledge of the full history is relevant, as a plastic stress could already be present in the initial state. Here we start with complete austenite at each temperature. No additional displacement is applied to the clamped system, therefore the purely austenitic system is stress free, and hence the transition sets in at the nominal coexistence temperature $\Delta f = 0$. The parameters are the same as in Fig. 5.

effects, i.e. with an additional dissipative effect (in the bulk), the interface moves even faster and with a constant velocity.

4.3. Energy dissipation

Let us consider also the time evolution of the free energy. For $f_{vpl,i} = 0$ we get in the first elastic regime according to Eq. (47) for equal elastic constants

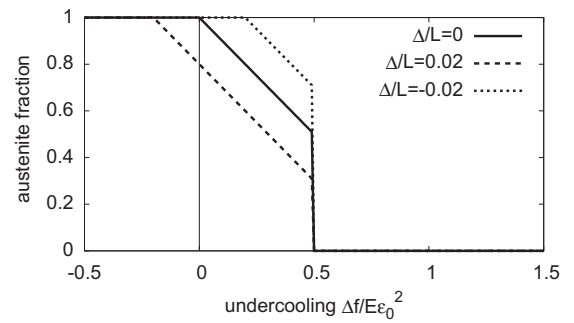


Fig. 9. Austenite volume fraction as function undercooling, for different values of the applied displacement Δ . In all cases the yield stress is $\sigma_y/E = 0.05$. Each simulation is started with austenite only, which means that for each temperature the material is initialized in a defect-free austenitic state. Due to the external load the martensite start temperature is shifted, whereas the finishing temperature remains the same. The parameters are the same as in Fig. 5.

$$F(L_1) = \frac{1}{2} E \frac{(\Delta - (L - L_1)\epsilon_0)^2}{L} + L_1 \Delta f, \quad (87)$$

where we added already the temperature contribution. The exponential relaxation of the interface position has already been calculated above.

In the plastic regime, we can obtain the above results also easily by a direct calculation of the free energy. Then in both phases $\sigma = \sigma_y$, with a free energy density

$$f_i = \frac{\sigma_y^2}{2E} \quad (88)$$

(without tilt and defect energy, $f_{vpl,i} = 0$), and thus the total free becomes (with tilt)

$$F(L_1) = \frac{\sigma_y^2}{2E} L + L_1 \Delta f, \quad (89)$$

from which we directly get

$$\Delta \mu_t = \frac{dF}{dL_1} = \Delta f. \quad (90)$$

Therefore, with the linear evolution of L_1 in the plastic regime, also the free energy decays linearly. The velocity is given by $\dot{L}_1 = -K \Delta \mu_t = -K \Delta f$, and therefore

$$\dot{F} = \frac{dF}{dL_1} \frac{dL_1}{dt} = -K(\Delta f)^2 < 0. \quad (91)$$

Both the elastic and the plastic regime are shown in Fig. 10.

If, in contrast, we used the partial work as driving force for the interface motion, we would have

$$\Delta \mu_p = \sigma_y \epsilon_0 + \Delta f. \quad (92)$$

With the equation of motion $\dot{L}_1 = -K \Delta \mu_p$ we would therefore get

$$\frac{dF}{dt} = \frac{dF}{dL_1} \frac{dL_1}{dt} = -K \Delta f (\Delta f + \sigma_y \epsilon_0), \quad (93)$$

which can (in principle) be, depending on the eigenstrain, positive or negative. This seems to indicate a violation of the second law of thermodynamics, but in fact the situation is more complicated. Obviously, this problem could occur only in the plastic regime. If the process is started in the elastic regime, the necessary condition for entering the plastic regime is $|\Delta f/\epsilon_0| > \sigma_y$. Let us assume that $\epsilon_0 > 0$. The condition for a violation of the second law of thermodynamics is $\Delta f (\Delta f + \sigma_y \epsilon_0) < 0$. If $\Delta f > 0$, we would need $\Delta f < -\sigma_y \epsilon_0$, which is impossible for the chosen signs. In the opposite case, $\Delta f < 0$, the condition would be $\Delta f > -\sigma_y \epsilon_0$ or equivalently $|\Delta f|/\epsilon_0 < \sigma_y$, which contradicts the above requirement for being in the plastic regime.

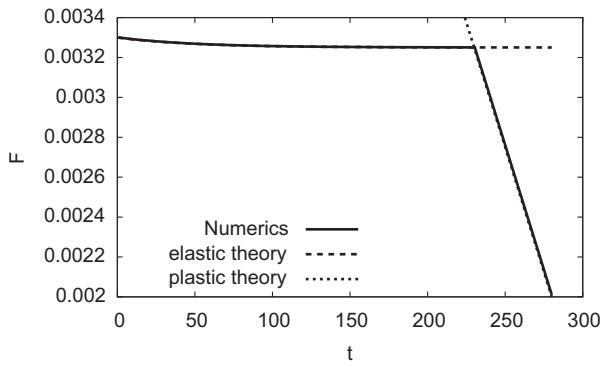


Fig. 10. Time evolution of the free energy, based on the total work expression. The parameters are the same as in Fig. 5.

Physically, the dissipation rate should be higher if we use the total free energy change as driving force. It consists of the local “transformation energy” plus the bulk dissipation due to plastic relaxation. Since the latter also reduces the free energy, it gives an additional contribution for the driving force. With the partial work ansatz, the system also relaxes plastically, but the bulk contribution to the free energy reduction is not taken into account in the interface equation of motion, and therefore the interface moves more slowly. As a consequence, the decay of the free energy is slower, too.

4.4. Discussion

On the level of a continuum modeling, equations of motion can only be postulated. Since we have encountered here a case where total and partial work approach lead to different results, the proper choice for realistic modeling needs to be discussed. On the hand side, the approach via the total work seems to be appealing, since it considers in particular the instantaneous relaxation of the elastic degrees of freedom, which can often be assumed to be fast. On the other hand, this approach also takes bulk dissipation far away from the interface into account as a driving force for interface motion. The motion of the interface leads to localized dissipation in this region as well as to bulk dissipation everywhere due to plastic flow if the yield stress is exceeded. This is counterintuitive, since energy losses far away, which do not lead to any changes of the atomic configuration at the interface, may still influence its motion. A similar situation is encountered for viscous materials, which are considered in the next section. One would expect that only the material behavior in the immediate interface region can be related to its motion. Also, the acceleration of the interface in the moment that the plastic regime is entered, is questionable.

This suggests another model for the choice of the driving force, which is in some sense between these two extreme cases,

$$\Delta\mu_{it}^{\delta L_1 > 0} = f_1^{(new)}|_{int} - f_2^{(old)}|_{int} - \sigma(\varepsilon_1^{(new)}|_{int} - \varepsilon_2^{(old)}|_{int}) \quad (94)$$

and

$$\Delta\mu_{it}^{\delta L_1 < 0} = f_1^{(old)}|_{int} - f_2^{(new)}|_{int} - \sigma(\varepsilon_1^{(old)}|_{int} - \varepsilon_2^{(new)}|_{int}). \quad (95)$$

It takes into account the full relaxation of the trial states, but only the dissipation in the interfacial region is relevant for the interface motion. For the situation, that we have considered so far, where the material grows in the same defect state as its adjacent “substrate phase”, the expressions become the same as the partial driving force. This suggests that also here the use of the virtual variation (or partial functional derivative in a phase field model) leads to reasonable interface dynamics.

Nevertheless, this new model also allows get a different behavior, as it includes the possibility to have different driving forces for

both growth directions. To illustrate this, we consider a case where phase 2 grows from phase 1 preserving the defect state, i.e. in the newly grown material the plastic strain remains as it was before. In the other direction we assume that the newly created phase 1 has the same plastic strain as the already existing phase 1. This growth behavior is sketched in Fig. 11. To keep the situation as simple as possible, we consider now only cases where the stress always remains below the yield stress, thus the plastic strain never changes via the back projection onto the yield surface but only via the phase transition. Nevertheless, the behavior is different than the purely elastic case, because the material possesses now a “memory” of a defect state, i.e. an internal variable. In contrast to the purely elastic case the eigenstrain of the material is not uniquely connected with the notion of the phase.

Starting from the phase and plastic strain distribution as depicted in Fig. 11a and considering the growth of phase 2, the elasto-plastic situation does not change from (a) to (b), and therefore the driving force becomes

$$\Delta\mu_{it}^{\delta L_1 < 0} = \Delta f. \quad (96)$$

For the interface motion in opposite direction, i.e. the transition (a) to (c), the behavior is the same as the previously discussed elastic problem, and therefore the driving force is

$$\Delta\mu_{it}^{\delta L_1 > 0} = \sigma\varepsilon_0 + \Delta f. \quad (97)$$

The discrepancy between these two expression has the following consequences. First, growth of phase 2 demands $\Delta\mu_{it}^{\delta L_1 < 0} > 0$, and conversely growth of phase 1 requires $\Delta\mu_{it}^{\delta L_1 > 0} < 0$. Now it is possible that none of these conditions is satisfied, and then the interfaces are pinned. Or, if both conditions hold, the interface becomes unstable, since different parts (in more than one dimension) may move in opposite directions; in this case short wave corrugations may still be hampered by interfacial energy. Second, according to Eq. (96) the material would be completely converted to phase 2 (martensite) as soon as $\Delta f > 0$, and the front velocity is constant. For this case martensite start and finishing temperature would therefore

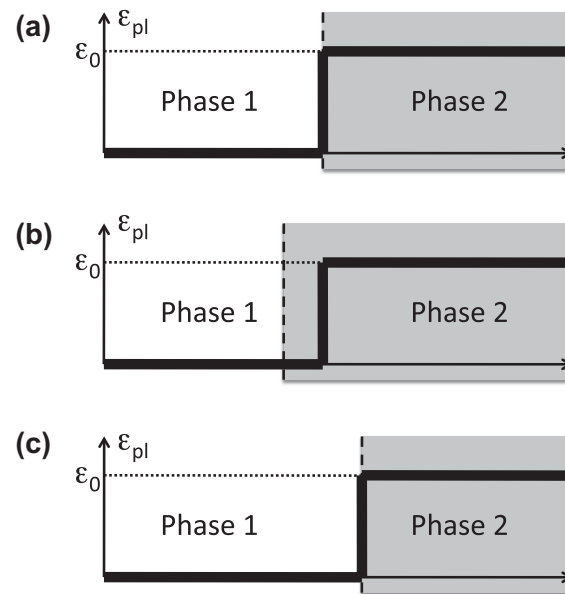


Fig. 11. Asymmetric growth scenario. Starting from configuration (a), where the dashed vertical line depicts the interface between phase 1 and 2, in (b) phase 2 has grown. However, in the newly converted phase the plastic strain is adopted from the mother phase, i.e. the plastic strain is now inhomogeneous in phase 2. For growth in the other direction (c), it is assumed that phase 1 stays in a homogenous plastic strain state.

coincide, since elastic deformations do occur. For the reverse transformation, however, the formation of austenite starts at $\Delta f = -\sigma\varepsilon_0$, and therefore the austenite start temperature differs from the martensite finish temperature. Consequently, such a simple model could be used as a starting point to describe systems with a transformation hysteresis.

In a phase field simulation this would require to use different evolution equations for growth and shrinkage, i.e. for the different signs of $\partial\phi/\partial t$. A similar concept has previously been used in the phase field modeling of irreversible fracture, where a crack is only allowed to grow but not to shrink, and this is implemented by the requirement $\partial\phi/\partial t \leq 0$, where $\phi = 0$ represents the broken material inside the crack (Henry, 2010).

A central conclusion from the inspection of plastic effects is therefore that model formulations should be chosen with care, since the presence of internal variables can lead to different behaviors depending on the choice of the driving force. This ambiguity therefore calls for further investigations, also e.g. with atomistic methods, to obtain further insights into this problem.

5. Viscoelasticity

Let us briefly comment on another material class with a complementary behavior to the plastic case. There, we had an additive decomposition into an elastic and a plastic strain, but stresses are only induced by the elastic strain. Furthermore, we considered the limit where plastic relaxation is fast, i.e. no timescale is present in this case. For a viscoelastic material, the situation is opposite: There, we have both an elastic ‘equilibrium’ stress and a viscous overstress, which additively give the total stress. Also, the process naturally contains a timescale in contrast to rate-independent elastoplasticity.

We consider again a one-dimensional situation, where the elastic stresses are

$$\sigma_{el,1} = E\varepsilon_1, \quad (98)$$

$$\sigma_{el,2} = E(\varepsilon_2 - \varepsilon_0). \quad (99)$$

The viscous stresses are related to the strain rates, and in a simple Kelvin model they are (Landau, 1986)

$$\sigma_{vis,i} = \eta\dot{\varepsilon}_i, \quad i = 1, 2. \quad (100)$$

The total stress

$$\sigma = \sigma_{el} + \sigma_{vis} \quad (101)$$

is homogeneous by the force balance condition $\partial\sigma/\partial x = 0$, where inertial terms are ignored, since we assume that the relaxation and interface motion is slow in comparison to the sound speed. This gives, together with the total displacement condition

$$L_1\varepsilon_1 + (L - L_1)\varepsilon_2 = \Delta, \quad (102)$$

the strain evolution equation

$$E\varepsilon_1 + \eta\dot{\varepsilon}_1 = E(\varepsilon_2 - \varepsilon_0) + \eta\dot{\varepsilon}_2 \\ = E\left(\frac{\Delta - L_1\varepsilon_1}{L - L_1} - \varepsilon_0\right) - \eta\frac{d}{dt}\left(\frac{\Delta - L_1\varepsilon_1}{L - L_1}\right), \quad (103)$$

where both the strain ε_1 and the interface position L_1 are time-dependent. Notice that – as in the elastic case – there is no ambiguity of how the strain evolves, since the eigenstrain is uniquely linked to the phase state. Also, since we ignore inertial effects, the strain is homogeneous in each phase. The evolution of the strain is uniquely determined through Eq. (103), as soon as the interface motion $L_1(t)$ is known; notice that here also the interface velocity plays a role.

A simple solution for Eq. (103) is

$$\varepsilon_1 \equiv \varepsilon_2 - \varepsilon \quad (104)$$

and this is the case, if the material is initially in static equilibrium, i.e. the viscous stresses vanish. Therefore, then and also at all later times $\sigma_{el,1} = \sigma_{el,2}$ and $\sigma_{vis,1} = \sigma_{vis,2}$. In the following we assume this physically reasonable situation.

The partial work approach suggests here as driving force

$$\Delta\mu_p = \frac{1}{2}E\varepsilon_1^2 - \frac{1}{2}E(\varepsilon_2 - \varepsilon_0)^2 - \sigma_{el}(\varepsilon_1 - \varepsilon_2) + \Delta f. \quad (105)$$

As before, the term $\sigma_{el}(\varepsilon_1 - \varepsilon_2)$ is the coherency work, here against the elastic stress σ_{el} , which is equal in both phases. This means that we assume that the viscous stresses are not relevant also for the coherency work, and this expectation will be justified in the following. The first two terms can also be written as $\sigma_{el,1}\varepsilon_1/2$ and $\sigma_{el,2}(\varepsilon_2 - \varepsilon_0)/2$, which means that only the reversible elastic work is taken into account, in agreement with sharp interface and phase field models of fracture (Spatschek et al., 2008; Spatschek et al., 2011). As before, the coherency term appears automatically in a phase field model that operates with the displacements. For the fracture models, there is no density difference at the interface, hence the coherency term vanishes even in a sharp interface description, and also the energy density inside the crack is zero, if the elastic and viscous constants are zero there.

Together with the interface velocity expression

$$\dot{L}_1 = -K\Delta\mu_p. \quad (106)$$

Eqs. (98)–(106) form a closed set of equations for the time evolution.

We can justify the above partial work expression by noting that it agrees again with the dissipation at the interface. Notice that similar to a plastic model also bulk dissipation is present here. We first start with the free energy expression

$$F = \frac{1}{2}L_1E\varepsilon_1^2 + \frac{1}{2}(L - L_1)E(\varepsilon_2 - \varepsilon_0)^2 + \Delta f L_1 \quad (107)$$

and therefore its time derivative is

$$\dot{F} = \left(\frac{1}{2}E\varepsilon_1^2 - \frac{1}{2}E(\varepsilon_2 - \varepsilon_0)^2 + \Delta f\right)\dot{L}_1 + L_1E\varepsilon_1\dot{\varepsilon}_1 \\ + (L - L_1)E(\varepsilon_2 - \varepsilon_0)\dot{\varepsilon}_2. \quad (108)$$

At a first glance it seems that the first term $\sim \dot{L}_1$ is an interface term, whereas the rest comes from the bulk; however, this is not true, as it contains also the coherency work term (notice that the calculation is generic so far, and no use of viscoelasticity has been made so far). For the specific solution (104) we get from Eq. (102)

$$\varepsilon_1 = \frac{\Delta - (L - L_1)\varepsilon_0}{L} \quad (109)$$

and therefore

$$\dot{\varepsilon}_1 = \dot{\varepsilon}_2 = \frac{\dot{L}_1}{L}\varepsilon_0. \quad (110)$$

Hence for the feigned bulk term

$$L_1E\varepsilon_1\dot{\varepsilon}_1 + (L - L_1)E(\varepsilon_2 - \varepsilon_0)\dot{\varepsilon}_2 = \sigma_{el}\varepsilon_0\dot{L}_1, \quad (111)$$

which is exactly the coherency work term. Hence we get

$$\dot{F} = \Delta\mu_p\dot{L}_1. \quad (112)$$

Therefore, the partial work gives the correct driving force.

6. Summary and conclusion

In this article we analyzed various phase field and sharp interface models for the description of moving boundary problems

concerning the physical meaning of the driving forces. We contrasted the difference between a partial work expression and a total work expression. The first one is typically used in variational phase field models, where a virtual energy change is calculated while all other physical fields are kept constant. In the latter approach of total work, all physical fields are adjusted instantaneously even for the trial move of the interfaces. Although the latter is typically not used in phase field modeling, we argued that it should be the proper driving force in cases where the interface motion is slow in comparison to the kinetics of the other fields.

We demonstrated, that in cases of coupling to fast diffusion and static elasticity the two driving force expressions, which can be considered as limiting cases, coincide, and therefore the usual approach of the partial variational derivative should be appropriate. The equality of the two approaches does no longer hold for elasto-plastic material models, since they additionally contain internal variables which follow separate dynamics. These are usually not derived from the same free energy functional as the evolution equations for the other fields. Consequently, the partial and total work approach lead to different expressions for the driving forces. One central difference is that the latter contains also nonlocal terms which result from plastic bulk dissipation. The usual assumption is, however, that only the interface dissipation should play a role for the front propagation, and therefore it seems unlikely that bulk terms can be relevant. We therefore generalized the expression by proposing the true interface dissipation (where all other fields are slaved by the phase field) as driving force. It turns out, that this physically motivated expression coincides again with the partial work expression, provided that the material does not grow in different defect states than the underlying substrate phase. Otherwise, interface pinning and destabilization effects may occur, as well as the splitting of the direct and inverse transition curves, that is relevant for many solid-state transformations.

Acknowledgement

R.S. acknowledges financial support through the DFG program SPP 1296. B.E. acknowledges financial support through the Heisenberg program of the DFG.

References

- Adland, A., Karma, A., Spatschek, R., Buta, D., Asta, M., 2013. Phase-field-crystal study of grain boundary premelting and shearing in bcc iron. *Phys. Rev. B* 87, 024110.
- Bartel, T., Hackl, K., 2009. A micromechanical model for martensitic phase-transformations in shape-memory alloys based on energy-relaxation. *Z. Angew. Math. Mech.* 89, 792.
- Bartel, T., Menzel, A., Svendsen, B., 2011. Thermodynamic and relaxation-based modeling of the interaction between martensitic phase transformations and plasticity. *J. Mech. Phys. Solids* 59, 1004.
- Boettinger, W.J., Warren, J., Beckermann, C., Karma, A., 2002. Phase-field simulation of solidification. *Annu. Rev. Mater. Res.* 32, 163.
- Brener, E., Boussinot, G., 2012. Kinetic cross coupling between nonconserved and conserved fields in phase field models. *Phys. Rev. E* 86, 060601R.
- Brener, E.A., Spatschek, R., 2003. Fast crack propagation by surface diffusion. *Phys. Rev. E* 67, 016112.
- Brener, E., Marchenko, V., Spatschek, R., 2007. Influence of strain on the kinetics of phase transitions in solids. *Phys. Rev. E* 75, 041604.
- Brush, L.N., 2003. A phase field model with electrical current. *J. Crystal Growth* 247, 587.
- Chen, L., 2002. Phase-field models for microstructure evolution. *Annu. Rev. Mater. Res.* 32, 113.
- Collins, J.B., Levine, H., 1985. Diffuse interface model of diffusion-limited crystal growth. *Phys. Rev. B* 31, 6119.
- Fabrizio, M., 2012. Plasticity, internal structure and phase field model. *Mech. Res. Commun.* 43, 29.
- Fischer, F., Waitz, T., Vollath, D., Simha, N., 2008. On the role of surface energy and surface stress in phase-transforming nanoparticles. *Prog. Mater. Sci.* 53, 481.
- Fix, G., 1983. Phase field problems for free boundary problems. In: Primicerio, M., Fasano, A. (Eds.), *Free Boundary Problems: Theory and Applications*, vol. II. Pitman, Boston, p. 580.
- Fleck, M., Brener, E.A., Spatschek, R., Eidel, B., 2010. Elastic and plastic effects on solid state transformations: A phase field study. *Int. J. Mater. Res.* 101, 462.
- Fleck, M., Pilipenko, D., Spatschek, R., Brener, E.A., 2011. Brittle fracture in viscoelastic materials as a pattern-formation process. *Phys. Rev. E* 83, 046213.
- Freund, L.B., 1998. *Dynamic Fracture Mechanics*. Cambridge University Press.
- Gaubert, A., Le Bouar, Y., Finel, A., 2010. Coupling phase field and visco-plasticity to study rafting in Ni-base superalloys. *Philos. Mag.* 90, 375.
- Gurtin, M.E., 1996. Generalized Ginzburg–Landau and Cahn–Hilliard equations based on a microforce balance. *Phys. D* 92, 178.
- Gurtin, M.E., 2000. *Configurational Forces as Basic Concepts of Continuum Physics*. Springer.
- Henry, H., 2010. Study of three-dimensional crack fronts under plane stress using a phase field model. *Europhys. Lett.* 92, 46002.
- Karma, A., Rappel, W.-J., 1996. Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetics. *Phys. Rev. E* 53, R3017.
- Karma, A., Rappel, W.-J., 1998. Quantitative phase-field modeling of dendritic growth in two and three dimensions. *Phys. Rev. E* 57, 4323.
- Karma, A., Phase-field methods, in: Buschow, K.H.J. et al. (Ed.), *Encyclopedia of Materials Science and Technology*, Elsevier, Oxford, 6873, 2001.
- Landau, L.D., 1986. *Theory of Elasticity*, third ed. Butterworth Heinemann.
- Langer, J.S., 1986. Models of pattern formation in first-order phase transitions. In: Grinstein, G., Mazenko, G. (Eds.), *Directions in Condensed Matter Physics*. World Scientific, 165.
- Langer, J.S., unpublished notes.
- Mariano, P., 2002. Multifield theories in mechanics of solids. *Adv. Appl. Mech.* 38, 1.
- Mariano, P.M., 2005. Migration of substructures in complex fluids. *J. Phys. A: Math. Gen.* 38, 6823.
- Maugin, G.A., 2010. *Configurational Forces: Thermomechanics, Physics, Mathematics, and Numerics*. Chapman and Hall/CRC.
- Nestler, B., Garcke, H., Stinner, B., 2005. Multicomponent alloy solidification: phase-field modeling and simulations. *Phys. Rev. E* 71, 041609.
- Ostwald, R., Bartel, T., Menzel, A., 2011. A one-dimensional computational model for the interaction of phase-transformations and plasticity. *Int. J. Struct. Chem. Solids* 3, 63.
- Provatas, N., Elder, K., 2010. *Phase field methods in Materials Science and Engineering*. Wiley-VCH, Weinheim, Germany.
- Spatschek, R., Fleck, M., 2007. Influence of stress on interface kinetics. *Philos. Mag. Lett.* 87, 909.
- Spatschek, R., Hartmann, M., Brener, E., Müller-Krumbhaar, H., Kassner, K., 2006. Phase field modeling of fast crack propagation. *Phys. Rev. Lett.* 96, 015502.
- Spatschek, R., Müller-Gugenberger, C., Brener, E., Nestler, B., 2007. Phase field modeling of fracture and stress-induced phase transitions. *Phys. Rev. E* 75, 066111.
- Spatschek, R., Brener, E., Pilipenko, D., 2008. Crack growth by surface diffusion in viscoelastic media. *Phys. Rev. Lett.* 101, 205501.
- Spatschek, R., Brener, E., Karma, A., 2011. Phase field modeling of crack propagation. *Philos. Mag.* 91, 75.
- Spatschek, R., Adland, A., Karma, A., 2013. Structural short-range forces between solid-melt interfaces. *Phys. Rev. B* 87, 024109.
- Steinbach, I., 2009. Phase-field models in materials science. *Model. Simul. Mater. Sci. Eng.* 17, 073001.
- Sutton, A.P., Balluffi, R.W., 1995. *Interfaces in Crystalline Materials*. Clarendon Press, Oxford.
- Takaki, T., Yamanaka, A., Higa, Y., Tomita, Y., 2007. Phase-field model during static recrystallization based on crystal-plasticity theory. *J. Comp. Aided Mater. Des.* 14, 75.
- Tiaden, J., 1999. Phase field simulations of the peritectic solidification of Fe-C. *J. Crystal Growth* 198/199, 1275.
- Travasso, R., Castro, M., Oliveira, J., 2011. The phase-field model in tumor growth. *Philos. Mag.* 91, 183.
- Yamanaka, A., Takaki, T., Tomita, Y., 2010. Elastoplastic phase-field simulation of martensitic transformation with plastic deformation in polycrystal. *Int. J. Mech. Sci.* 52, 245.