

# Towards diffuse interface models with a nonlinear polycrystalline elastic energy

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## Abstract

Recently in [8], an extension of the Cahn-Hilliard model was derived that takes into account nonlinear elastic energies of the precipitates and includes composite laminates in the physical description. The aim of this work is to provide a basis for the further generalization of isothermal diffuse interface models, which we do by developing our methods exemplary for the Allen-Cahn/Cahn-Hilliard equations. Since segregated phases in typical physical applications are polycrystalline, it is natural to incorporate also effects present in polycrystals rather than in single crystals, leading to a polycrystalline lamination theory. To this end we recall some models and methods used in the context of polycrystalline materials and composites. Finally, we outline how the Allen-Cahn/Cahn-Hilliard model can be extended to polycrystalline geometrically linear elasticity.

## 1 INTRODUCTION

Diffuse interface models have been successfully applied to model segregation and precipitation phenomena in alloys and liquid mixtures. However, so far, elastic effects due to composite structures of the considered materials as well as effects due to polycrystalline structures of the considered materials have mostly been neglected. In this article we shall consider these effects and provide a basis for a generalization of the existing diffuse interface models.

We focus on three cases: (i) single crystalline materials which follow the linear elastic theory developed by Eshelby, [17], in the context of elastic inclusions and inhomogeneities, (ii) single crystalline materials which are described well by a geometrically

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linear theory of elasticity that takes phase fractions on the microscale into account and was developed in [14], and (iii) polycrystalline materials that are described well by a geometrically linear theory of elasticity that takes phase fractions on the microscale as well as the underlying texture of the polycrystal on a mesoscopic scale into account. This is very important for many applications where the classical single crystal theory is not general enough.

The first two cases are treated in Section 2.1. We develop the third case in Section 2.2, where we also provide a general introduction to the methods of composite materials and polycrystals and repeat concepts like texture of a material and homogenization as well as established bounds on the effective elastic energy of polycrystals. Furthermore we mention recent results for stress-induced phase transformations in polycrystalline materials, [7]. Starting from elasticity models for the three cases we then generalize diffuse interface models for precipitation and segregation phenomena, which is the topic of Section 3.

Our approach is quite general and can be applied to any of the established models, provided the temperature is conserved (for non-isothermal settings, the validity of the second law of thermodynamics requires further correction terms which are not studied here). For practical reasons and in order to have a concise presentation, we will discuss in this article the coupling of the afore-mentioned elastic lamination theories to the Allen-Cahn/Cahn-Hilliard equations (AC-CH equations for short). This model, first introduced in [13], contains both the Allen-Cahn equation and the Cahn-Hilliard equation as special cases, which are the two most-frequently used models to investigate segregation, precipitation, and phase change problems in materials science, engineering, theoretical physics, and biology, among others. The Allen-Cahn system with linear elasticity was studied before in [10], the Cahn-Hilliard system with linear elasticity in [19], [25] and [12]. An extension of the Cahn-Hilliard system with geometrically linear elasticity valid for single crystals was recently found in [8]. The coupling to elasticity changes significantly the morphology of the precipitates and the coarsening patterns, see, e.g., the classification in [18], which opens interesting research topics for the future.

Next to the generalization of the AC-CH equations we are interested in proving existence and uniqueness of the new systems of differential equations. In Section 3.1 we prove existence and uniqueness of weak solutions for a class of functionals inspired by Eshelby's linear theory of elasticity with lamination. In Section 3.2 we obtain similar results for materials falling in the second category, i.e., for single crystalline materials described by a geometrically linear elastic lamination theory. Section 3.3 is devoted to the generalization of the AC-CH equations to polycrystalline materials and provides the basis of further analytical and numerical research.

We end this work with an outlook and a discussion of our results.

## 2 A POLYCRYSTALLINE LAMINATION THEORY

### 2.1 THE ELASTIC ENERGY IN SINGLE CRYSTALLINE COMPOSITES

Our main objective in this section is to study geometrically linear elasticity for composites in the context of isothermal phase transitions. For systematic reasons, we first recall the linear ansatz dating back to Eshelby, [17]. This allows us, as a byproduct of the existence theory proved in Section 3.1, to obtain a new existence result for the Allen-Cahn/Cahn-Hilliard equations with linear elasticity.

Throughout this paper let  $\Omega \subset \mathbb{R}^D$  for  $D \geq 1$  be a bounded domain with Lipschitz boundary which serves as the reference configuration. By  $u : \Omega \rightarrow \mathbb{R}^D$  we describe the displacement field, such that a material point  $x$  in the undeformed body  $\Omega$  is at  $x' = x + u(x)$  after the deformation. Then the (linearized) strain tensor is defined by

$$\varepsilon(u) := \frac{1}{2} (\nabla u + \nabla u^t), \quad (1)$$

where  $A^t$  denotes the transpose of a matrix  $A \in \mathbb{R}^{D \times D}$ . As usual,  $\cdot$  stands for the inner product in  $\mathbb{R}^D$ , i.e.,  $u \cdot v = \sum_{i=1}^D u_i v_i$ , and for  $A, B \in \mathbb{R}^{D \times D}$  we denote by  $A:B := \text{tr}(A^t B) = \sum_{i,j=1}^D A_{ij} B_{ij}$  the inner product in  $\mathbb{R}^{D \times D}$ .

The linear theory by Eshelby, [17], developed in the context of elastic inclusions and inhomogeneities, can be summarized in the following ansatz for the elastic energy of a composite

$$W_{\text{lin}}(d, \varepsilon) := \frac{1}{2} (\varepsilon - \underline{\varepsilon}(d)) : C(d) (\varepsilon - \underline{\varepsilon}(d)) \quad (2)$$

for all  $\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}$ ,  $d \in \mathbb{R}$ , and  $\underline{\varepsilon}(d) := d \underline{\varepsilon}$  with a constant  $\underline{\varepsilon} \in \mathbb{R}_{\text{sym}}^{D \times D}$ . The notion of  $d$  will become clear in Section 3. Here we only mention that  $d \in [0, 1]$  is a conserved or unconserved order parameter of a diffuse interface model that describes, e.g., segregation in a solid with reference configuration  $\Omega \subset \mathbb{R}^D$  with  $D \geq 1$ .

By  $C(d)$  we denote the symmetric, positive definite and concentration dependent elasticity tensor of the system that maps symmetric tensors in  $\mathbb{R}^{D \times D}$  to themselves. For the rest of this section we discuss the geometrically linear elasticity theory that takes the laminates of the material into account. As is shown in [8, Remark 1], the above-mentioned linear elasticity theory by Eshelby is a special case of this geometrically linear theory.

In the following we assume that two phases are present in the considered material which may form microstructures as e.g. displayed in Figures 7 and 8. We refer to the energy of each of the phases as microscopic energy, cf. (3), and to the energy  $\widehat{W}(d, \varepsilon(u))$  in (4), which reflects the effective behavior of the system with microstructures, as the mesoscopic energy. When we include polycrystalline structures, we

moreover consider a macroscopic scale, see Section 2.2.

To determine the energy  $\widehat{W}(d, \varepsilon(u))$  in the geometrically linear case we need to solve a local minimization problem, see (4) below, which we shall explain now.

Consider an open ball  $B := B_r(x_0) \subset \Omega$  containing a two-phase microstructure. We assume that the volumes occupied by each of the two phases in  $B$  are measurable sets. In particular, if  $\tilde{d}_1 \equiv \tilde{d}$ ,  $\tilde{d}_2 = 1 - \tilde{d}$  characterize the two phases on the microscale, we have  $\tilde{d}_i \in BV(B; \{0, 1\})$  and  $\tilde{d}_1 + \tilde{d}_2 = 1$  a.e. in  $B$ . The symbol  $BV$  denotes the space of functions of bounded variation, see, e.g., [1, 27]. By

$$\langle \tilde{m} \rangle := \oint_B \tilde{m}(x) dx := \frac{1}{|B|} \int_B \tilde{m}(x) dx$$

we denote the average of a function  $\tilde{m}$  in  $B$ , where  $|E|$  is the  $D$ -dimensional Lebesgue measure of a set  $E$ .

Let  $\varepsilon_i^T \in \mathbb{R}_{\text{sym}}^{D \times D}$ ,  $i = 1, 2$ , be the stress-free strain of the  $i$ -th phase relative to the chosen reference configuration and  $\alpha_i$  be its elasticity tensor. Then the elastic energy density of phase  $i$  subject to a strain  $\tilde{\varepsilon}$  is given by

$$W_i(\tilde{\varepsilon}) := \frac{1}{2} \alpha_i (\tilde{\varepsilon} - \varepsilon_i^T) : (\tilde{\varepsilon} - \varepsilon_i^T) + w_i \quad (3)$$

for constants  $w_i \geq 0$ .

Under the assumption that the elastic energy adapts infinitely fast and that the surface energy between laminates of the microstructure can be neglected, the effective elastic energy is, [14],

$$\widehat{W}(d, \varepsilon) := \inf_{\langle \tilde{d} \rangle = d} \inf_{\tilde{u}|_{\partial B} = \varepsilon x} \oint_B \tilde{d} W_1(\tilde{\varepsilon}) + (1 - \tilde{d}) W_2(\tilde{\varepsilon}) dx, \quad (4)$$

where we write for short  $\tilde{\varepsilon} = \tilde{\varepsilon}(\tilde{u}) = \frac{1}{2}(\nabla \tilde{u} + \nabla \tilde{u}^t)$ . The infimum over  $\tilde{d}$  is the result of homogenization subject to the constraint that the volume fraction of the selected phase is preset by  $d$ , see [16]. The other infimum in (4) is the result of relaxation theory, see [15], [20], which is now outlined. If for prescribed  $d = a + b$  the microscopic elastic energy density is  $W_d(\tilde{\varepsilon})$ , then

$$\widehat{W}_d(\varepsilon) := \inf_{\tilde{u}|_{\partial B} = \varepsilon x} \oint_B W_d(\tilde{\varepsilon}(\tilde{u})) dx \quad (5)$$

is the elastic energy density of the material with mesoscopic strain  $\varepsilon$  after microstructure has formed. As is shown in [15], this definition of  $\widehat{W}_d$  does not depend on  $B$ . Likewise, (4) is independent of  $B = B_r(x_0)$  as long as  $B \subset \Omega$ . We mention that there exist explicit analytic formulas for  $\widehat{W}$  if  $D = 2, 3$ , [14]. The representation for  $D = 2$  will be recalled in Section 3.2. Next we discuss a polycrystalline lamination theory before we come to the formulation of extended Allen-Cahn/Cahn-Hilliard models.

## 2.2 A POLYCRYSTALLINE LAMINATION THEORY

The Allen-Cahn/Cahn-Hilliard system is an established model for describing precipitation in solids, segregation phenomena, and more general phase change problems, among others. Very often, the actual physical phenomenon is very complicated, as it additionally depends on the morphology of the material on the small scale, or on plastic effects like the formation and movement of dislocations and hardening. In this article, we do not focus on the description of the later, but focus on the morphology of the material. Besides the lamination microstructure, also the polycrystalline nature of the solid is of importance.

A polycrystalline material is a solid which is composed of many grains with a lattice subsequently assumed to be identical, but with different orientations. Each grain behaves like a single crystal, at least this is what we shall assume in the following, where we neglect all effects resulting from grain boundaries. We are interested in materials that form microstructures within the grains. Such composites can for instance be laminates of order one and two as indicated in Figure 1.

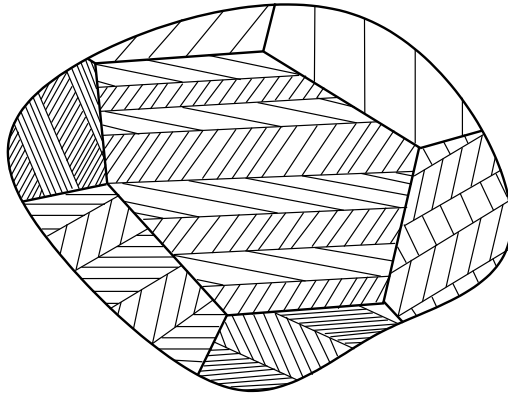


Figure 1: Part of a polycrystal showing laminates of order one and two in its grains.

The texture of polycrystalline materials is described by a matrix-valued function  $R : \Omega \rightarrow SO(3)$  which is constant on each grain (we assume that every grain has full Lebesgue measure in  $\mathbb{R}^D$ ). Here,  $SO(D)$  denotes the set of all rotations about the origin of  $\mathbb{R}^D$  (characterized by  $R^t R = \text{Id}$  and  $\det(R) = 1$ ). Thus the function  $R$  describes the number and shapes of the grains as well as their orientations. In Figure 2 we give a simple mathematical example of a polycrystal which shows the structure of a chessboard. This texture can for instance form if the lattice structure in the light squares is the reference configuration, i.e.,  $R = \text{Id}$ , whereas the lattice structure in the dark squares is obtained by a rotation,  $R = R_{\frac{\pi}{4}}$ . Another typical

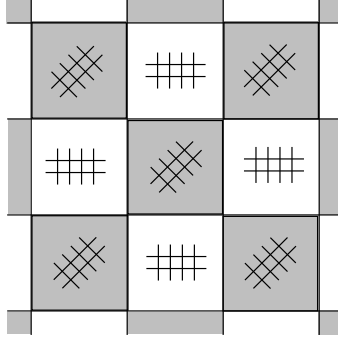


Figure 2: Part of a polycrystal prototype forming a chessboard structure.

example is the isotropic or random texture in which all rotations  $R \in SO(3)$  occur in the polycrystal identically distributed.

In the following we again consider a general polycrystal. Let us pick one grain with reference configuration  $G \subset \mathbb{R}^D$  and choose its orientation as the reference. Analogous to (5), the elastic energy of this grain obtained by relaxation is then

$$\widehat{W}(\varepsilon) = \min_{\tilde{u}|_{\partial G} = \varepsilon x} \int_G W(\tilde{\varepsilon}(\tilde{u})) dx,$$

where  $\varepsilon$  denotes again the symmetrized strain gradient given by (1), i.e., as before we work in the framework of geometrically linearized elasticity and  $W$  is the microscopic elastic energy having multiple wells related to different compatible phases.

The relaxed elastic energy of a grain rotated by  $R$  with respect to the reference grain is  $\widehat{W}(R^t \varepsilon R)$ . The macroscopic behavior of a polycrystal is obtained by nonlinear homogenization (see, e.g., [4]),

$$\overline{W}(\bar{\varepsilon}) = \min_{u|_{\partial \Omega} = \bar{\varepsilon} x} \int_{\Omega} \widehat{W}(R^t(x) \varepsilon(u(x)) R(x)) dx. \quad (6)$$

The mathematical structure of the definitions of  $\widehat{W}$  and  $\overline{W}$  looks similar, but they take into account different issues: while the relaxation of the multi-well energy  $W$  involves averages over composites on a subgrain length scale, the passage from  $\widehat{W}$  to  $\overline{W}$  involves averages over grains and thus depends on the texture of the material. In other words, here we consider composites on different length scales: there is the lamination on a microscopic scale, i.e., within the grains, and there is the polycrystalline structure on a mesoscopic scale, i.e., on the scale of the body.

The analytical computation of  $\overline{W}$  for a given material is a subtle issue. Bhattacharya and Kohn [4] discuss this for shape-memory alloys and study upper and lower bounds on  $\overline{W}$  and in particular on the zero-set of  $\overline{W}$ .

An upper bound on  $\overline{W}$  is obtained by choosing a constant test field  $u = \bar{\varepsilon}x$  on  $\Omega$ . Then

$$\overline{W}(\bar{\varepsilon}) \leq \int_{\Omega} \widehat{W}(R^t \bar{\varepsilon} R) dx =: \overline{W}_T(\bar{\varepsilon}).$$

We shall call  $\overline{W}_T(\bar{\varepsilon})$  the *Taylor bound* on  $\overline{W}$ . In analogy to [4, p. 125] we next derive a lower bound on  $\overline{W}(\bar{\varepsilon})$ . To this end we recall the definition of the Legendre-Fenchel transform of a function  $f : \mathbb{R}_{\text{sym}}^{D \times D} \rightarrow \mathbb{R}$ ,

$$f^*(\sigma) = \sup_{\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}} \{\varepsilon : \sigma - f(\varepsilon)\}, \quad \sigma \in \mathbb{R}_{\text{sym}}^{D \times D}.$$

Thus for any  $R \in SO(3)$  and  $\sigma \in \mathbb{R}_{\text{sym}}^{D \times D}$ ,

$$\begin{aligned} \widehat{W}^*(R\sigma R^t) &= \sup_{\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}} \{\varepsilon : R\sigma R^t - \widehat{W}(\varepsilon)\} \\ &= \sup_{\varepsilon' \in \mathbb{R}_{\text{sym}}^{D \times D}} \{\varepsilon' : \sigma - \widehat{W}(R^t \varepsilon' R)\} \\ &\geq \varepsilon' : \sigma - \widehat{W}(R^t \varepsilon' R) \quad \text{for any } \varepsilon' \in \mathbb{R}_{\text{sym}}^{D \times D}. \end{aligned}$$

Integration yields

$$\int_{\Omega} \widehat{W}(R^t \varepsilon' R) dx \geq \int_{\Omega} \varepsilon' : \sigma - \widehat{W}^*(R\sigma R^t) dx.$$

Note that the inequality still holds true if we maximize over all  $\sigma : \Omega \rightarrow \mathbb{R}_{\text{sym}}^{D \times D}$ . Then we minimize over all  $u'$  such that  $u' = \bar{\varepsilon}x$  on  $\partial\Omega$  and obtain by (6)

$$\overline{W}(\bar{\varepsilon}) \geq \min_{u'|_{\partial\Omega} = \bar{\varepsilon}x} \max_{\sigma : \Omega \rightarrow \mathbb{R}_{\text{sym}}^{D \times D}} \int_{\Omega} \varepsilon' : \sigma - \widehat{W}^*(R\sigma R^t) dx.$$

Now note that for  $\text{div } \sigma = 0$  and  $u'$  with  $u'|_{\partial\Omega} = \bar{\varepsilon}x$ , we have  $\int_{\Omega} \varepsilon' : \sigma dx = \int_{\Omega} \bar{\varepsilon} : \sigma dx$ . Hence we finally obtain the lower bound

$$\overline{W}(\bar{\varepsilon}) \geq \max_{\text{div } \sigma = 0} \int_{\Omega} \bar{\varepsilon} : \sigma - \widehat{W}^*(R\sigma R^t) dx. \quad (7)$$

From (7) we can go even one step further and consider constant stress-fields  $\bar{\sigma}$  as test functions, which yields the *Sachs bound*  $\overline{W}_S(\bar{\varepsilon})$ . Explicitly,

$$\overline{W}(\bar{\varepsilon}) \geq \max_{\bar{\sigma} \in \mathbb{R}_{\text{sym}}^{D \times D}} \left\{ \bar{\varepsilon} : \bar{\sigma} - \int_{\Omega} \widehat{W}^*(R\bar{\sigma}R^t) dx \right\} \quad (8)$$

$$= \left( \int_{\Omega} \widehat{W}^*(R\bar{\sigma}R^t) dx \right)^* (\bar{\varepsilon}) =: \overline{W}_S(\bar{\varepsilon}). \quad (9)$$

We refer to [4] for a discussion of upper and lower bounds for special cases of elastic energies. In particular, the bounds for scalar materials are studied there, which we recall and slightly extend here.

Scalar materials reduce the dimension of the problem: instead of considering a vector-valued displacement field  $u : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ , the displacement is assumed to be a scalar-valued function on  $\mathbb{R}^2$ , i.e.,  $\eta : \mathbb{R}^2 \rightarrow \mathbb{R}$ . This corresponds to anti-plane shear. The strains  $f = f(\eta) = \nabla \eta$  are vectors in  $\mathbb{R}^2$  as are the stresses, which leads to the advantage of having a convex relaxed energy, [15]. The transformation behavior is now described by  $R^t f$  with  $R \in SO(2)$ , instead of  $R^t \varepsilon R$ ,  $R \in SO(3)$ , required above. With this change, all the above formulas can be defined and derived correspondingly for scalar materials. For instance, the effective behavior of a polycrystalline scalar material reads

$$\overline{W}(f) = \inf_{\eta|_{\partial\Omega} = \bar{f} \cdot x} \int_{\Omega} \widehat{W}(R^t(x)f(\eta(x))) dx. \quad (10)$$

In the following we consider the example of a four-variant scalar material with quadratic energy wells minimized at  $(1, 1)$ ,  $(-1, 1)$ ,  $(-1, -1)$  and  $(1, -1)$ , cf., e.g., [4]. For  $f = (f_1, f_2) \in \mathbb{R}^2$  let

$$W^{\text{four}}(f) := \frac{1}{2} \min \{ (f_1 - 1)^2 + (f_2 - 1)^2, (f_1 + 1)^2 + (f_2 - 1)^2, \\ (f_1 - 1)^2 + (f_2 + 1)^2, (f_1 + 1)^2 + (f_2 + 1)^2 \}$$

be the corresponding microscopic energy, see Figure 3. The mesoscopic energy is the convexification of  $W^{\text{four}}$  and thus reads

$$\widehat{W}^{\text{four}}(f) = \frac{1}{2} ((|f_1| - 1)_+^2 + (|f_2| - 1)_+^2),$$

where  $(a)_+ = \max\{a, 0\}$ , cf. Figure 4. Its zero-set is  $\{f \in \mathbb{R}^2 \mid |f_1| \leq 1, |f_2| \leq 1\}$ . To illustrate the effect of texture on the macroscopic energy  $\overline{W}$ , we consider the chessboard texture as well as the isotropic texture. If the material has a chessboard



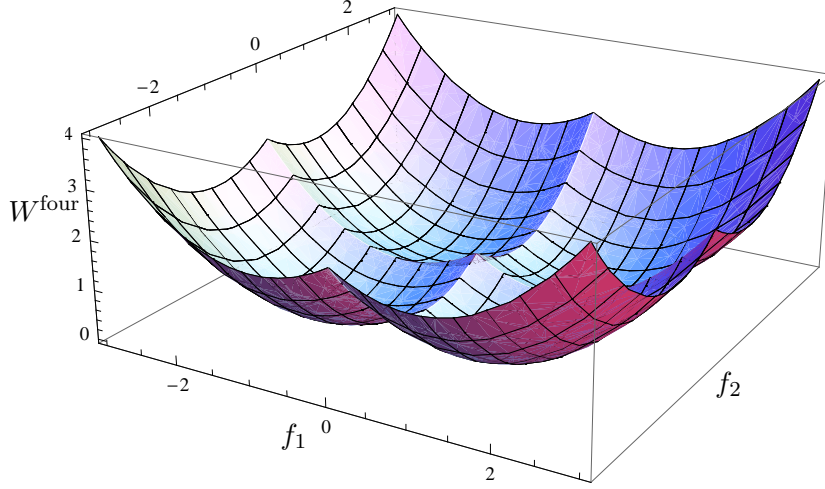


Figure 3: Plot of the microscopic energy  $W^{\text{four}}$ .

texture as in Figure 2, the rotations  $R_0 = \text{Id}$  and  $R_{\frac{\pi}{4}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$  occur equally distributed. Hence

$$\overline{W}_T^{\text{four}}(\bar{f}) = \frac{1}{2} \widehat{W}^{\text{four}} \left( \begin{pmatrix} \bar{f}_1 \\ \bar{f}_2 \end{pmatrix} \right) + \frac{1}{2} \widehat{W}^{\text{four}} \left( \frac{1}{\sqrt{2}} \begin{pmatrix} \bar{f}_1 + \bar{f}_2 \\ -\bar{f}_1 + \bar{f}_2 \end{pmatrix} \right),$$

plotted in Figure 5. Its zero-set is the intersection of  $\{|f_1| \leq 1, |f_2| \leq 1\}$  with this set rotated by  $R_{\frac{\pi}{4}}$ , thus  $\{|f_1| \leq 1, |f_2| \leq 1, |f_1 \pm f_2| \leq \sqrt{2}\}$ .

In an isotropic texture all rotations in  $SO(2)$  occur equidistributed. Hence

$$\overline{W}_T(\bar{f}) = \frac{1}{2\pi} \int_0^{2\pi} \widehat{W} \left( \begin{pmatrix} \bar{f}_1 \cos \vartheta + \bar{f}_2 \sin \vartheta \\ -\bar{f}_1 \sin \vartheta + \bar{f}_2 \cos \vartheta \end{pmatrix} \right) d\vartheta,$$

which has  $\{f \in \mathbb{R}^2 \mid |f| \leq 1\}$  as zero-set and deviates from this quadratically with rotational symmetry.

So far we have assumed that the constant temperature in our system is such that the microscopic elastic energy has several global minima. For instance, for shape

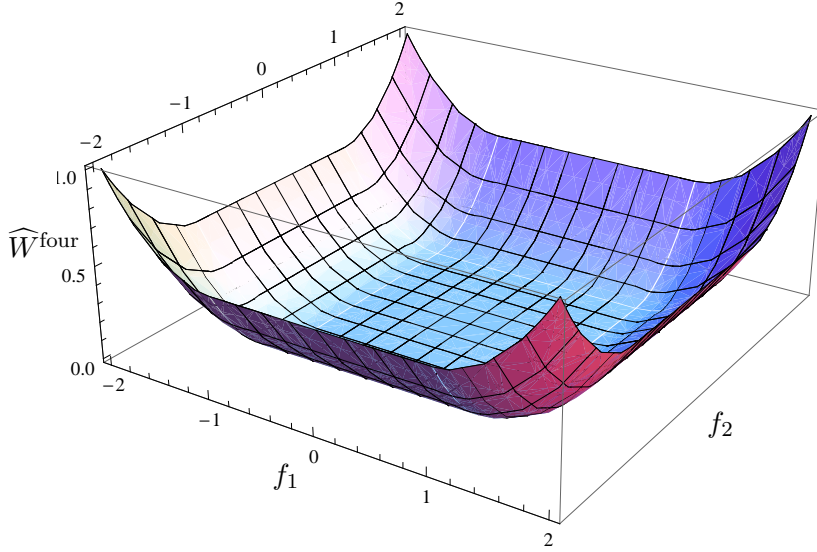


Figure 4: Plot of  $\widehat{W}^{\text{four}}$ .

memory alloys this means that we are below the transformation temperature in the martensitic phase. This is a realistic assumption for real-life segregation processes. However, here we do not want to exclude another case which is interesting in particular if external forces are applied. Having shape-memory alloys and martensitic phase transformations in other materials such as steels in mind, we discuss in the following what happens if the material is above its phase transformation temperature. Then the microscopic elastic energy has one global minimum only that corresponds to the lattice structure of the so-called austenitic phase; and it has several local minima that correspond to the lattice structures of the martensitic variants. A phase transformation from austenite to martensite can be induced by an applied load and results in pseudo-elastic behavior.

We allow the applied load to be not only uniaxial but multi-axial; for multi-axial loading experiments in shape-memory alloys see for instance [23]. For a comparison of the models cited in the following with other models related to multi-axial loading experiments in shape-memory alloys we refer to [22].

In [5, 26], Bhattacharya and Schlömerkemper discuss polycrystalline vectorial ma-

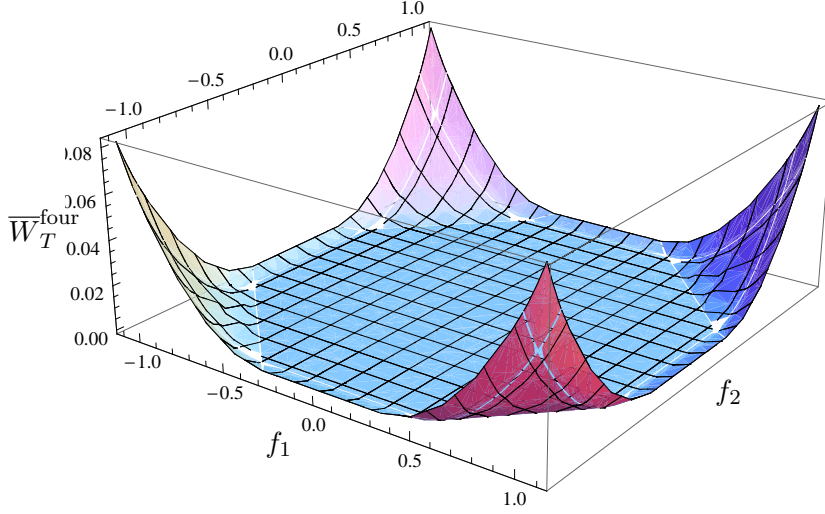


Figure 5: The Taylor bound on  $W^{\text{four}}$  with chessboard texture.

materials under an applied stress with a special focus on the yield set, which is defined as the set of all stresses such that the material is in its austenitic state. The boundary of this set gives the yield stress, i.e., the stress at which the transformation from austenite to martensite starts. For the definition of the yield set, Sachs and Taylor bounds are taken into account and the effect of texture on the yield set is studied. This is made explicit for cubic-to-orthorhombic phase transformations in shape-memory alloys there. In [6, 7], the same authors study the scalar case, to which we shall come back below.

Once again we begin by formulating the theory for the vector-valued case in the geometrically linear setting, i.e., stresses and strains are elements of  $\mathbb{R}_{\text{sym}}^{D \times D}$ . As outlined in (23), the energy due to a uniform external applied load is  $W_{\text{ext}}(\varepsilon) = -\sigma_{\text{ext}} : \varepsilon$ . Since in a single crystalline material the integrand does not depend on  $x$ , minimization of this energy corresponds to minimizing its integrand

$$W^{\sigma_{\text{ext}}}(\varepsilon) := W(\varepsilon) - \sigma_{\text{ext}} : \varepsilon$$

over all  $\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}$ . Assume that the global minimum of  $W$  is 0. Then there is no

phase transformation as long as  $\sigma_{\text{ext}}$  is such that

$$\inf_{\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}} W^{\sigma_{\text{ext}}}(\varepsilon) \geq \inf_{\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}} \{W_{\text{aust}}(\varepsilon) - \sigma_{\text{ext}} : \varepsilon\},$$

where  $W_{\text{aust}}$  denotes that part of the energy  $W$  which corresponds to austenite, i.e., it denotes the energy of the high-symmetry phase whose well is close to the global minimum. Equivalently we have

$$W^*(\sigma_{\text{ext}}) = \sup_{\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}} \{\sigma_{\text{ext}} : \varepsilon - W(\varepsilon)\} \leq \sup_{\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}} \{\sigma_{\text{ext}} : \varepsilon - W_{\text{aust}}(\varepsilon)\} = W_{\text{aust}}^*(\sigma_{\text{ext}}).$$

Hence, the yield set in a single crystal is naturally defined as

$$Y := \{\sigma_{\text{ext}} \in \mathbb{R}_{\text{sym}}^{D \times D} \mid W^*(\sigma_{\text{ext}}) \leq W_{\text{aust}}^*(\sigma_{\text{ext}})\}, \quad (11)$$

where we neglect any fatigue of the material such as hardening. When we wish to work with the relaxed energy, we consider the mesoscopic energy under an applied load, namely

$$\begin{aligned} \widehat{W}^{\sigma_{\text{ext}}}(\varepsilon) &= \min_{\tilde{u}|_{\partial\Omega}=\varepsilon x} \int_{\Omega} W(\tilde{\varepsilon}(\tilde{u})) - \sigma_{\text{ext}} : \tilde{\varepsilon}(\tilde{u}) \, dx \\ &= \min_{\tilde{u}|_{\partial\Omega}=\varepsilon x} \left\{ \int_{\Omega} W(\tilde{\varepsilon}(\tilde{u})) \, dx - \sigma_{\text{ext}} : \int_{\Omega} \tilde{\varepsilon}(\tilde{u}) \, dx \right\}. \end{aligned} \quad (12)$$

Due to (1) we obtain  $\int_{\Omega} \tilde{\varepsilon}(\tilde{u}) \, dx = \varepsilon$ . Hence

$$\begin{aligned} \widehat{W}^{\sigma_{\text{ext}}}(\varepsilon) &= \min_{\tilde{u}|_{\partial\Omega}=\varepsilon x} \int_{\Omega} W(\tilde{\varepsilon}(\tilde{u})) \, dx - \sigma_{\text{ext}} : \varepsilon \\ &= \widehat{W}(\varepsilon) - \sigma_{\text{ext}} : \varepsilon. \end{aligned} \quad (13)$$

In analogy to (11), we set

$$\widehat{Y} := \left\{ \sigma_{\text{ext}} \in \mathbb{R}_{\text{sym}}^{D \times D} \mid \widehat{W}^*(\sigma_{\text{ext}}) \leq \widehat{W}_{\text{aust}}^*(\sigma_{\text{ext}}) \right\}.$$

Finally, the macroscopic energy of a polycrystal under uniform applied load reads

$$\begin{aligned} \overline{W}^{\sigma_{\text{ext}}}(\bar{\varepsilon}) &= \min_{u|_{\partial\Omega}=\bar{\varepsilon}x} \int_{\Omega} \widehat{W}(R^t \varepsilon(u) R) - \sigma_{\text{ext}} : \varepsilon(u) \, dx \\ &= \overline{W}(\bar{\varepsilon}) - \sigma_{\text{ext}} : \bar{\varepsilon}. \end{aligned}$$

Correspondingly, we set

$$\overline{Y} := \left\{ \sigma_{\text{ext}} \in \mathbb{R}_{\text{sym}}^{D \times D} \mid \overline{W}^*(\sigma_{\text{ext}}) \leq \overline{W}_{\text{aust}}^*(\sigma_{\text{ext}}) \right\}.$$

Note that  $Y$ ,  $\widehat{Y}$  and  $\overline{Y}$  can be defined correspondingly in the scalar setting. In the following we will elaborate on this further and consider the energy  $W : \mathbb{R}^2 \rightarrow \mathbb{R}$  defined by

$$W(e) := \min_{f \in \mathbb{R}^2} \left\{ \frac{C}{2} |e - f|^2 + w(f) \right\}, \quad (14)$$

where

$$w(e) := \begin{cases} 0 & \text{if } e = 0, \\ \omega & \text{if } e = e^{(i)}, i = 1, \dots, n, \\ \infty & \text{else} \end{cases}$$

with a constant  $\omega > 0$  and  $e^{(1)}, \dots, e^{(n)}$  being the local minima of  $W$  and  $w$ . In the case of shape-memory alloys these are the stress-free variants of the martensite and  $e = 0$  corresponds to austenite. Note that here  $W_{\text{aust}}(e) = \frac{C}{2} e^2$  for  $e$  close to 0, which leads to  $W_{\text{aust}}^*(s) = \frac{s^2}{2C}$ . The applied load now yields the energy  $-s_{\text{ext}} \cdot e$ . Thus, by (11),

$$Y = \left\{ s_{\text{ext}} \in \mathbb{R}^2 \mid W^*(s_{\text{ext}}) \leq \frac{s_{\text{ext}}^2}{2C} \right\}.$$

Furthermore, by [7] or elementary calculations,  $W^*(s) = \frac{s^2}{2C} + w^*(s)$  and  $w^*(s) = \max \{0, \max_i s \cdot e^{(i)} - \omega\} \geq 0$ . Hence

$$Y = \left\{ s_{\text{ext}} \in \mathbb{R}^2 \mid \max_i s_{\text{ext}} \cdot e^{(i)} \leq \omega \right\}.$$

For the scalar case that we consider here we have  $\widehat{W} = W^{**}$  and therefore,  $\widehat{W}^*(s) = W^*(s)$ . Similarly,  $\widehat{W}_{\text{aust}}^*(s) = \widehat{W}_{\text{aust}}(s)$ , implying  $\widehat{Y} = Y$ .

In order to calculate also the yield set of a polycrystalline material  $\overline{Y}$ , we apply a result from [7] for the energy in (14), which asserts that the Sachs bound  $Y_S$  on the yield set, which is obtained under the assumption of constant stress throughout the sample, equals  $\overline{Y}$  and thus is sharp. In formulas,

$$\overline{Y} = Y_S, \quad (15)$$

where  $Y_S = \bigcup_{x \in \Omega} Y_{R(x)}$  with  $Y_{R(x)} = \{s \mid R^t s \in Y\}$ .

To give a specific example, we consider a four-variant scalar material in the constrained model, i.e., for  $C \rightarrow \infty$ . Then  $W$  in (14) reads

$$W(e) = w(e) = \begin{cases} 0 & \text{if } e = 0, \\ \omega & \text{if } e \in \{(1, 1); (-1, 1); (-1, -1); (1, -1)\}, \\ \infty & \text{else} \end{cases}$$

and

$$W^*(s) = \max\{0, |s_1 \pm s_2| - \omega\},$$

whose zero-set is the square  $\{s = (s_1, s_2) \in \mathbb{R}^2 \mid |s_1 \pm s_2| \leq \omega\} = Y$ , see Figure 6.

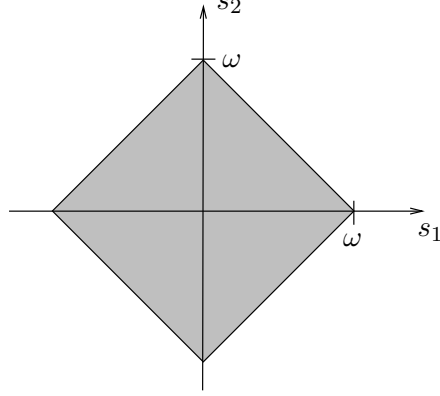


Figure 6: The yield set  $Y$  of a scalar four-variant single crystal.

By (15) we thus obtain for a polycrystalline material with a chessboard structure as in Figure 2,

$$\begin{aligned} \bar{Y}_{\text{chess}} &= \{s \mid |s_1 \pm s_2| \leq \omega\} \cap \left\{s \mid |s_1| \leq \frac{\omega}{\sqrt{2}}, |s_2| \leq \frac{\omega}{\sqrt{2}}\right\} \\ &= \left\{s \mid |s_1 \pm s_2| \leq \omega, |s_1| \leq \frac{\omega}{\sqrt{2}}, |s_2| \leq \frac{\omega}{\sqrt{2}}\right\}, \end{aligned}$$

which is an octahedron. Similarly, for a polycrystal with isotropic texture, the macroscopic yield set  $\bar{Y}$  is a disc with radius  $\frac{\omega}{\sqrt{2}}$ .

Our next goal is to generalize the above notions of energies for polycrystalline materials to energies that take into account also prescribed volume fractions of the phases. For this we return to the general case of vector-valued deformations. This generalization then allows us to develop an extension of the Cahn-Hilliard model for nonlinear elastic energies that takes into account effects of polycrystalline structures of the systems under consideration.

To this end we recall the definition of the mesoscopic energy  $\widehat{W}(d, \varepsilon)$  in the geometrically linear theory of elasticity which takes phase fractions into account, see Section 2.1. Let  $e^{(i)} \in \mathbb{R}_{\text{sym}}^{D \times D}$ ,  $i = 1, 2$ , be two stress-free strains and  $\tilde{d}_1 \equiv \tilde{d}$ ,  $\tilde{d}_2 = 1 - \tilde{d}$  their corresponding phase fractions such that  $\tilde{d}_i \in BV(\Omega; \{0, 1\})$  and

$\tilde{d}_1 + \tilde{d}_2 = 1$  a.e. in  $\Omega$ . Then

$$\widehat{W}(d, \varepsilon) = \inf_{\langle \tilde{d} \rangle = d} \inf_{\tilde{u}|_{\partial\Omega} = \varepsilon x} \int_{\Omega} \tilde{d} W_1(\tilde{\varepsilon}(\tilde{u})) + (1 - \tilde{d}) W_2(\tilde{\varepsilon}(\tilde{u})) dx,$$

where  $W_i$ ,  $i = 1, 2$  are defined as in (3).

Now let again  $\Omega$  be the reference configuration of a polycrystalline material whose texture is described by some piecewise-constant map  $R : \Omega \rightarrow SO(3)$ . For prescribed phase fractions we proceed with the mesoscopic energy  $\widehat{W}_d(\varepsilon)$  as in (5) and set in analogy to (6) for the macroscopic energy

$$\overline{W}_d(\bar{\varepsilon}) := \inf_{u|_{\partial\Omega} = \bar{\varepsilon} x} \int_{\Omega} \widehat{W}_d(\varepsilon(u)) dx.$$

If the phase fractions are not prescribed, there is another step of homogenization to be done. Combining the earlier definitions, it is natural to define the macroscopic energy which takes volume fractions into account by

$$\overline{W}(\bar{d}, \bar{\varepsilon}) := \inf_{\langle \bar{d} \rangle = \bar{d}} \inf_{u|_{\partial\Omega} = \bar{\varepsilon} x} \int_{\Omega} \widehat{W}(d, \varepsilon(u)) dx. \quad (16)$$

In Subsection 3.3 we outline how this energy leads to an extension of the Allen-Cahn/Cahn-Hilliard model to polycrystalline materials.

### 3 THE AC-CH MODEL AND EXTENSIONS

Let as above  $\Omega \subset \mathbb{R}^D$ ,  $D \geq 1$ , be a bounded domain with Lipschitz boundary. For a stop time  $T > 0$ , let  $\Omega_T := \Omega \times (0, T)$  denote the space-time cylinder. To the Allen-Cahn/Cahn-Hilliard system, first derived in [13], we add elasticity, possibly respecting the lamination microstructure of the material, and introduce the system

$$\partial_t a = \lambda \operatorname{div} \left( M(a, b) \nabla \frac{\partial F}{\partial a} \right), \quad (17)$$

$$\partial_t b = -M(a, b) \frac{\partial F}{\partial b}, \quad (18)$$

$$0 = \operatorname{div} \left( \partial_{\varepsilon} \widehat{W}(a + b, \varepsilon(u)) \right), \quad (19)$$

which has to be solved in  $\Omega_T$  subject to the initial conditions

$$a(t = 0) = a_0, \quad b(t = 0) = b_0 \quad \text{in } \Omega$$

for given functions  $a_0, b_0 : \Omega \rightarrow \mathbb{R}$  subject to the Neumann boundary conditions for  $a$ , the no-flux boundary conditions, and the equilibrium condition for applied forces

$$\nabla a \cdot \vec{n} = 0, \quad J(a, b, u) = 0, \quad \sigma \cdot \vec{n} = \sigma_{\text{ext}} \cdot \vec{n} \quad \text{on } \partial\Omega, \quad t > 0. \quad (20)$$

See also (17')–(19') below for an explicit formulation.

In (17)–(19), the function  $a : \Omega_T \rightarrow \mathbb{R}_0^+$  is a *conserved* order parameter, typically a concentration,  $b : \Omega_T \rightarrow \mathbb{R}_0^+$  is an *unconserved* order-parameter, specifying the reordering of the underlying lattice,  $M(a, b) \geq 0$  denotes the mobility tensor,  $u : \Omega \rightarrow \mathbb{R}^D$  describes as before the displacement field,  $\varepsilon(u)$  is the (linearized) strain tensor defined in (1), and  $\lambda > 0$  is a small constant determining the interfacial thickness. Finally,  $\widehat{W}(a + b, \varepsilon(u))$  is the stored elastic energy density as defined in (4) for composites.

In (20),  $\vec{n}$  is the unit outer normal to  $\partial\Omega$ . For simplicity, body forces are neglected and it is assumed that the boundary tractions are dead loads given by a constant symmetric tensor  $\sigma_{\text{ext}}$  as in Section 2. By  $J$  we denote the mass flux, given by

$$J(a, b, u) := -M(a, b)\nabla\mu = -M(a, b)\nabla\frac{\partial F}{\partial a}(a, b, u),$$

with  $\mu := \frac{\partial F}{\partial a}$  the chemical potential.

The system (17)–(19) is completed with the definition of the free energy

$$F(a, b, u) := \int_{\Omega} \psi(a, b) + \frac{\lambda}{2} (|\nabla a|^2 + |\nabla b|^2) + \widehat{W}(a + b, \varepsilon(u)) + W_{\text{ext}}(\varepsilon(u)) \, dx, \quad (21)$$

where  $\psi(a, b)$  is the free energy density

$$\begin{aligned} \psi(a, b) &:= \frac{\vartheta}{2} (g(a + b) + g(a - b)) + \kappa_1 a(1 - a) - \kappa_2 b^2, \\ g(s) &:= s \ln s + (1 - s) \ln(1 - s) \end{aligned} \quad (22)$$

for scalars  $\kappa_1, \kappa_2 > 0$ . The term  $\frac{1}{2}[g(a + b) + g(a - b)]$  in (22) defines the entropic part of the free energy, given in the canonical Bernoulli form for perfect mixing, and  $\vartheta > 0$  is the constant temperature.

The functional  $W_{\text{ext}}(\varepsilon)$  in (21) represents energy effects due to applied forces. In the absence of body forces, the work necessary to transform the undeformed body  $\Omega$  into a state with displacement  $u$  is then

$$-\int_{\partial\Omega} u \cdot \sigma_{\text{ext}} \vec{n} = -\int_{\Omega} \nabla u : \sigma_{\text{ext}} = -\int_{\Omega} \varepsilon(u) : \sigma_{\text{ext}},$$

where we use the symmetry of  $\sigma_{\text{ext}}$ . Consequently,

$$W_{\text{ext}}(\varepsilon) = -\sigma_{\text{ext}} : \varepsilon \quad (23)$$

is the energy density of the applied outer forces.



The valid parameter range for  $a$  and  $b$  is, see Theorem 1,

$$0 \leq a + b \leq 1, \quad 0 \leq a - b \leq 1. \quad (24)$$

The inequalities are strict unless  $(a, b) = (0, 0)$  or  $(a, b) = (1, 0)$ . The system (17)–(19) includes as special cases the elastic Cahn-Hilliard system (setting  $b \equiv 0$ , [19]) and the elastic Allen-Cahn equations (setting  $a \equiv \frac{1}{2}$ , [10]). The system studied here is exemplary for an isothermal model that exhibits simultaneously ordering and phase transitions.

Equation (17) is a diffusion law for  $a$  governed by the flux  $J$  and states the conservation of mass in  $\Omega$ . Equation (18) is a simple gradient flow in the direction  $\frac{\partial F}{\partial b}$ . Equation (19) is a consequence of Newton's second law under the additional assumption that the acceleration  $\partial_{tt}u$  originally appearing on the left hand side can be neglected (this can be proved formally by a scaling argument and formally matched asymptotics). The term  $\sigma := \partial_\varepsilon \widehat{W}(a + b, \varepsilon(u))$  defines the stress. Equation (19) serves to determine the unknown displacement  $u$ .

**Remark 1.** *Equations (17)–(19) can be generalized to vector-valued mappings  $a$  and  $b$ . This allows to study situations with more than two phases present. To fix ideas and for the sake of a clear presentation, we restrict ourselves throughout this paper to scalar quantities  $a$  and  $b$ .*

**Remark 2.** *Equations (17)–(19) with boundary conditions (20) comply with the second law of thermodynamics, which in case of isothermal conditions reads for a closed system*

$$\partial_t F(a(t), b(t), u(t)) \leq 0.$$

*This inequality can be verified by direct inspection similar to the calculations in [8].*

Next we discuss existence and uniqueness results for the Allen-Cahn/Cahn-Hilliard model extended to linear elasticity and geometrically linear elasticity, respectively. In Section 3.3 we show how the above model can be extended to polycrystalline materials exhibiting ordering and phase transition simultaneously.

### 3.1 EXISTENCE AND UNIQUENESS RESULTS OF THE AC-CH MODEL WITH LINEAR ELASTICITY

The existence of solutions to the Allen-Cahn/Cahn-Hilliard equation without elasticity was studied in [11] with the help of a semigroup calculus. Existence and uniqueness of weak solutions to the Cahn-Hilliard equation with linear elasticity is proved in [19], with geometrically linear elasticity in [8]. Existence and uniqueness of weak solutions to the Allen-Cahn equation with linear elasticity is shown in [10].

Subsequently we provide existence and uniqueness results for (17)–(19). First we require some mathematical tools. We introduce the operator  $\mathcal{M}$  associated to  $w \mapsto -M\Delta w$  as a mapping from  $H^1(\Omega)$  to its dual by

$$\mathcal{M}(w)\eta := \int_{\Omega} M\nabla w \cdot \nabla \eta, \quad (25)$$

where  $M$  is the mobility tensor which we assume in the following to be positive definite. From the Poincaré inequality and the Lax-Milgram theorem (which can be applied now thanks to the assumption that  $M$  is positive definite) we know that  $\mathcal{M}$  is invertible and we denote its inverse by  $\mathcal{G}$ , the Green function. We have

$$(M\nabla \mathcal{G}f, \nabla \eta)_{L^2} = \langle \eta, f \rangle \quad \text{for all } \eta \in H^1(\Omega), f \in (H^1(\Omega))'.$$

For  $f_1, f_2 \in (H^1(\Omega))'$ , we define the inner product

$$(f_1, f_2)_M := (M\nabla \mathcal{G}f_1, \nabla \mathcal{G}f_2)_{L^2}$$

with the corresponding norm

$$\|f\|_M := \sqrt{(f, f)_M} \quad \text{for } f \in (H^1(\Omega))'$$

which is applied in (27) in the proof of Theorem 1.

For  $M \equiv 1$ , the explicit formulation of (17)–(19), used in the proofs below, is

$$\partial_t a = \lambda \Delta \left[ \frac{\vartheta}{2} (g'(a+b) + g'(a-b)) + \kappa_1(1-2a) + \frac{\partial \widehat{W}}{\partial d}(a+b, \varepsilon(u)) - \Delta a \right], \quad (17')$$

$$\partial_t b = \lambda \Delta b + \frac{\vartheta}{2} [g'(a-b) - g'(a+b)] + 2\kappa_2 b - \frac{\partial \widehat{W}}{\partial d}(a+b, \varepsilon(u)), \quad (18')$$

$$0 = \operatorname{div} \left( \partial_\varepsilon \widehat{W}(a+b, \varepsilon(u)) \right). \quad (19')$$

Now we prove the existence of solutions to (17)–(19) with  $\widehat{W}$  being the linear energy  $W_{\text{lin}}$  as given by (2). For the existence proof below, the energy does not have to have exactly the form of  $W_{\text{lin}}$ . We highlight the required conditions by introducing the general class of elastic energies which satisfy the following assumption (A1). The functional  $\widehat{W} = W_{\text{lin}}$  is then one particular example.

(A1) The elastic energy density  $\widehat{W} \in C^1(\mathbb{R} \times \mathbb{R}^D; \mathbb{R})$  satisfies:

(A1.1)  $\widehat{W}(d, \varepsilon)$  only depends on the symmetric part of  $\varepsilon \in \mathbb{R}^{D \times D}$ , i.e.,

$$\widehat{W}(d, \varepsilon) = \widehat{W}(d, \varepsilon^t) \quad \text{for all } d \in \mathbb{R} \text{ and all } \varepsilon \in \mathbb{R}^{D \times D}.$$

(A1.2)  $\partial_\varepsilon \widehat{W}(d, \cdot)$  is strongly monotone uniformly in  $d$ , i.e., there exists a constant  $c_1 > 0$  such that for all  $\varepsilon_1, \varepsilon_2 \in \mathbb{R}_{\text{sym}}^{D \times D}$

$$\left( \partial_\varepsilon \widehat{W}(d, \varepsilon_2) - \partial_\varepsilon \widehat{W}(d, \varepsilon_1) \right) : (\varepsilon_2 - \varepsilon_1) \geq c_1 |\varepsilon_2 - \varepsilon_1|^2.$$

(A1.3) There exists a constant  $C_1 > 0$  such that for all  $d \in \mathbb{R}$  and all  $\varepsilon \in \mathbb{R}_{\text{sym}}^{D \times D}$

$$\begin{aligned} |\widehat{W}(d, \varepsilon)| &\leq C_1(|\varepsilon|^2 + |d|^2 + 1), \\ |\partial_d \widehat{W}(d, \varepsilon)| &\leq C_1(|\varepsilon|^2 + |d|^2 + 1), \\ |\partial_\varepsilon \widehat{W}(d, \varepsilon)| &\leq C_1(|\varepsilon| + |d| + 1). \end{aligned} \tag{26}$$

**Theorem 1** (Existence of solutions for linear elasticity). *Let the mobility tensor  $M$  in (25) be positive definite, let  $\widehat{W}$  fulfill (A1) and let  $\psi$  be given by (22). In addition, let the initial data satisfy*

$$\psi(a_0, b_0) < \infty.$$

*Then, there exists a solution  $(a, b, u)$  to (17)–(19) that satisfies*

- (i)  $a, b \in C^{0, \frac{1}{4}}([0, T]; L^2(\Omega))$ .
- (ii)  $\partial_t a, \partial_t b \in L^2(\Omega_T)$ .
- (iii)  $u \in L^\infty(0, T; H^1(\Omega; \mathbb{R}^D))$ .
- (iv) *The feasible parameter range for  $(a, b)$  is given by (24).*

In particular, Theorem 1 confirms the existence of solutions to (17)–(19) with linear elasticity as defined in (2).

**Proof:** The statements of the theorem can be proved with the methods developed in [10]. Here we only sketch the main steps.

For a small discrete step size  $h > 0$ , chosen such that  $Th^{-1} \in \mathbb{N}$ , for time steps  $m \in \mathbb{N}$  with  $0 < m < Th^{m-1}$ , and given values  $a^{m-1}, b^{m-1} \in \mathbb{R}$ , we introduce the discrete free energy functional

$$F^{m,h}(a, b, u) := F(a, b, u) + \frac{1}{2h} \|a - a^{m-1}\|_M^2 + \frac{1}{2h} \|b - b^{m-1}\|_{L^2}^2, \tag{27}$$

where (in case of  $m = 1$ ) it holds  $a^0 = a_0, b^0 = b_0$ , the initial values for  $a$  and  $b$ . By the direct method in the calculus of variations and Assumption (A.1), it is possible to show that for  $h$  sufficiently small,  $F^{m,h}$  possesses a minimizer  $(a^m, b^m, u^m) \in H^1(\Omega) \times H^1(\Omega) \times H^1(\Omega; \mathbb{R}^D)$ . This minimizer solves the fully implicit time discretisation of (17')–(19'). Next the discrete solution is extended affine linearly to  $(\bar{a}, \bar{b}, \bar{u})$  by setting for  $t = (\tau m + (1 - \tau)(m - 1))h$  with suitable  $\tau \in [0, 1]$

$$(\bar{a}, \bar{b}, \bar{u})(t) := \tau(a^m, b^m, u^m) + (1 - \tau)(a^{m-1}, b^{m-1}, u^{m-1}).$$

The validity of the second law of thermodynamics (cf. Remark 2) implies that  $F$  is non-increasing in time. This allows to derive uniform estimates for  $(\bar{a}, \bar{b}, \bar{u})$ . Compactness arguments then allow to pass to the limit  $h \searrow 0$  and the limit solves (17)–(19).  $\square$

**Theorem 2** (Uniqueness of solutions for linear elasticity). *Let  $\widehat{W} = W_{\text{lin}}$  be given by (2), let the material be homogeneous, that is the elasticity tensor  $C$  is independent of  $d$ , and let  $M \equiv 1$ . Then the solution  $(a, b, u)$  of Theorem 1 is unique in the spaces stated in the theorem.*

**Proof:** Fix  $t_0 \in (0, T)$ . Let  $(a_i, b_i, u_i)$ ,  $i = 1, 2$  be two pairs of solutions to (17')–(19') and (2). The differences  $a := a_1 - a_2$ ,  $b := b_1 - b_2$ ,  $u := u_1 - u_2$  with corresponding difference of the chemical potentials  $\mu := \mu_1 - \mu_2 := \frac{\partial F}{\partial a}(a_1, b_1) - \frac{\partial F}{\partial a}(a_2, b_2)$  solve the weak equations

$$\int_{\Omega_T} [-a \partial_t \xi + \lambda \nabla \mu \cdot \nabla \xi] = 0, \quad (28)$$

$$\begin{aligned} & \int_{\Omega_T} [\partial_t b \eta + \lambda \nabla b \cdot \nabla \eta - \underline{\varepsilon} : C(\varepsilon(u) - \underline{\varepsilon}(a + b)) \eta] \\ &= \int_{\Omega_T} \left[ \frac{\vartheta}{2} (g'(a_2 + b_2) - g'(a_1 + b_1) + g'(a_1 - b_1) - g'(a_2 - b_2)) \eta + 2\kappa_2 b \eta \right], \end{aligned} \quad (29)$$

$$\int_{\Omega_{t_0}} C(\varepsilon(u) - \underline{\varepsilon}(a + b)) : \varepsilon(u) = 0 \quad (30)$$

for every  $\xi, \eta \in L^2(0, T; H_0^1(\Omega)) \cap L^\infty(\Omega_T)$  with  $\partial_t \xi, \partial_t \eta \in L^2(\Omega_T)$ ,  $\xi(T) = 0$ , where in order to get (30) we plugged in  $(u_2 - u_1)\mathcal{X}_{(0, t_0)}$  as a test function and integrated by parts. As a test function in (28) we pick

$$\xi(x, t) := \begin{cases} \int_t^{t_0} \mu(x, s) ds, & \text{if } t \leq t_0, \\ 0, & \text{if } t > t_0. \end{cases}$$

This shows

$$\int_{\Omega_{t_0}} a \mu + \lambda \nabla(\mathcal{G}a) \cdot \nabla(\partial_t \mathcal{G}a) = 0. \quad (31)$$

The difference of the chemical potentials fulfills, with the help of (21),

$$\begin{aligned} \int_{\Omega_T} \mu \zeta &= \int_{\Omega_T} \left[ \frac{\vartheta}{2} (g'(a_1 + b_1) - g'(a_2 + b_2) + g'(a_2 - b_2) - g'(a_1 - b_1)) \zeta \right. \\ &\quad \left. - 2\kappa_1 a \zeta + \lambda \nabla a \cdot \nabla \zeta - \underline{\varepsilon} : C(\varepsilon(u) - \underline{\varepsilon}(a + b)) \zeta \right]. \end{aligned}$$

We pick  $\zeta := (a_1 - a_2)\mathcal{X}_{(0,t_0)}$ . With (31) we obtain

$$\begin{aligned} \frac{\lambda}{2} \|a\|_M^2(t_0) + \int_{\Omega_{t_0}} \lambda |\nabla a|^2 - a\varepsilon : C(\varepsilon(u) - \varepsilon(a+b)) \leq \\ \int_{\Omega_{t_0}} 2\kappa_1 a^2 + \frac{\vartheta}{2} \left[ |g'(a_1+b_1) - g'(a_2+b_2)| + |g'(a_1-b_1) - g'(a_2-b_2)| \right] |a|. \end{aligned} \quad (32)$$

In (29) we choose  $\eta := (b_2 - b_1)\mathcal{X}_{(0,t_0)}$  as a test function and add the resulting equation to (32) and use (30). We end up with

$$\begin{aligned} \frac{\lambda}{2} \|a\|_M^2(t_0) + \frac{1}{2} \|b(t_0)\|_{L^2}^2 + \int_{\Omega_{t_0}} \left[ \lambda (|\nabla a|^2 + |\nabla b|^2) + \widehat{W}(a+b, \varepsilon(u)) \right] \\ \leq \int_{\Omega_{t_0}} 2(\kappa_1 |a|^2 + \kappa_2 |b|^2) \\ + \int_{\Omega_{t_0}} \frac{\vartheta}{2} \left[ |g'(a_1+b_1) - g'(a_2+b_2)| + |g'(a_1-b_1) - g'(a_2-b_2)| \right] (|a| + |b|). \end{aligned}$$

From Theorem 1 we know that the terms  $g'(a_i \pm b_i)$ ,  $i = 1, 2$  are finite, and  $g'$  is Lipschitz continuous (even real analytic). Applying first Young's inequality, then Gronwall's inequality, as  $t_0 \in (0, T)$  was arbitrary, we find  $a = b = 0$  in  $\Omega_T$ . This finally yields

$$\int_{\Omega_T} \varepsilon(u) : C\varepsilon(u) = 0.$$

With Korn's inequality this proves  $u = 0$  in  $\Omega_T$ .  $\square$

### 3.2 EXISTENCE AND UNIQUENESS OF THE AC-CH MODEL WITH GEOMETRICALLY LINEAR ELASTICITY

For the existence theory in the case of the Allen-Cahn/Cahn-Hilliard model extended to geometrically linear elasticity, the above definition (4) of  $\widehat{W}$  is not practical since it is based on a local minimization. To this end we collect here explicit analytic formulas for the relaxed energy  $\widehat{W}$  and its derivatives which are valid for  $D = 2$ .

$$\widehat{W}(d, \varepsilon) := d_1 W_1(\varepsilon_1^*) + d_2 W_2(\varepsilon_2^*) + \beta^* d_1 d_2 \det(\varepsilon_2^* - \varepsilon_1^*). \quad (33)$$

Formula (33) is derived in [14], where also a corresponding formula in three dimensions can be found. To complete the definition, we have to introduce the quantities  $\beta^*$ ,  $\varepsilon_1^*$  and  $\varepsilon_2^*$ . First we need some notations.

Let  $\gamma^* > 0$  be given by

$$\gamma^* := \min\{\gamma_1, \gamma_2\}, \quad (34)$$

where  $\gamma_i$  is the reciprocal of the largest eigenvalue of  $\alpha_i^{-1/2} Q \alpha_i^{-1/2}$ ,  $\alpha_i$  is the elastic modulus of laminate  $i$ , and the operator  $Q : \mathbb{R}_{\text{sym}}^{2 \times 2} \rightarrow \mathbb{R}_{\text{sym}}^{2 \times 2}$  is given by

$$Q\varepsilon = \varepsilon - \text{tr}(\varepsilon)\text{Id}.$$

In [8] a recipe is given for the practical computation of  $\gamma^*$ . Here, we only remark that if the space groups of the two existing laminates are cubic, it holds

$$\gamma^* = \min\{C_{1,11} - C_{1,12}, C_{2,11} - C_{2,12}, 2C_{1,44}, 2C_{2,44}\}.$$

The first subscript of  $C$  denotes here the phase, the other two indices are the coefficients of the reduced elasticity tensor in Voigt notation, [24].

As shown in [14], the scalar  $\beta^* \in [0, \gamma^*]$  determines the amount of translation of the laminates and is given by

$$\beta^* = \beta^*(d, \varepsilon) := \begin{cases} 0 & \text{if } \varphi \equiv 0 & \text{(Regime 0),} \\ 0 & \text{if } \varphi(0) > 0 & \text{(Regime I),} \\ \beta_{II} & \text{if } \varphi(0) \leq 0 \text{ and } \varphi(\gamma^*) \geq 0 & \text{(Regime II),} \\ \gamma^* & \text{if } \varphi(\gamma^*) < 0 & \text{(Regime III).} \end{cases} \quad (35)$$

In this definition,  $\beta_{II} = \beta_{II}(d, \varepsilon)$  is the unique solution of  $\varphi(\cdot, d, \varepsilon) = 0$  with  $\varphi$  defined by

$$\begin{aligned} \varphi(\beta^*, d, \varepsilon) &= -\det(\Delta\varepsilon^*(\beta^*, d, \varepsilon)) = -\det\left[\alpha(\beta^*, d)^{-1}e(\varepsilon)\right], \\ \Delta\varepsilon^* &= \Delta\varepsilon^*(\beta^*, d, \varepsilon) := \varepsilon_2^*(\beta^*, d, \varepsilon) - \varepsilon_1^*(\beta^*, d, \varepsilon), \end{aligned} \quad (36)$$

where the so-far undefined functions are specified below.

The four regimes have the following crystallographic interpretation.

**Regime 0:** The material is homogeneous and the energy does not depend on the microstructure.

**Regime I:** There exist two optimal rank-I laminates.

**Regime II:** The unique optimal microstructure is a rank-I laminate.

**Regime III:** There exist two optimal rank-II laminates.

For illustration, we visualize prototypes of rank-I and rank-II laminates.

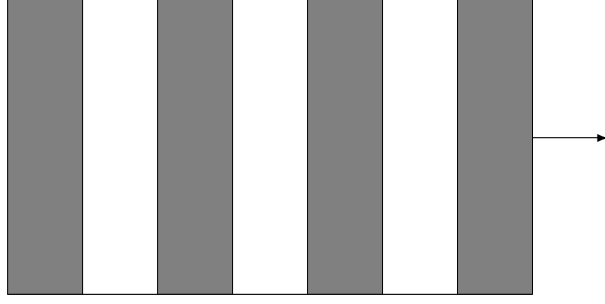


Figure 7: A two-phase rank-I laminate in two space dimensions with corresponding normal vector. The strains are constant in the shaded and in the unshaded regions. The volume fraction of both phases, 0.5 in the picture, is prescribed by the macroscopic parameter  $d$ .

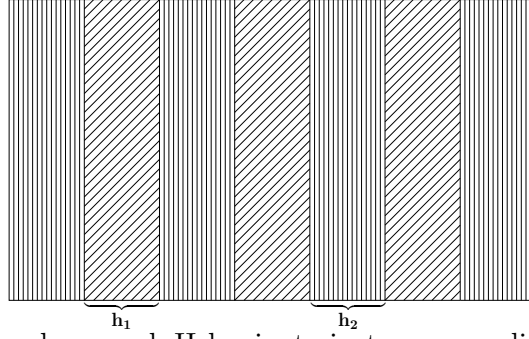


Figure 8: A two-phase rank-II laminate in two space dimensions. The widths  $h_1$  and  $h_2$  of the slabs should be much larger than the thickness of the layers between the slab.

To complete the definition (36) and for later use, set

$$\begin{aligned}
 \alpha(\beta^*, d) &:= d_2 \alpha_1 + d_1 \alpha_2 - \beta^* Q, \\
 e(\varepsilon) &:= \alpha_2 (\varepsilon_2^T - \varepsilon) - \alpha_1 (\varepsilon_1^T - \varepsilon), \\
 \varepsilon_i^* \equiv \varepsilon_i^*(\beta^*, d, \varepsilon) &:= \alpha^{-1}(\beta^*, d) e_i(\beta^*, d, \varepsilon), \\
 e_1(\beta^*, d, \varepsilon) &:= (\alpha_2 - \beta^* Q) \varepsilon - d_2 (\alpha_2 \varepsilon_2^T - \alpha_1 \varepsilon_1^T), \\
 e_2(\beta^*, d, \varepsilon) &:= (\alpha_1 - \beta^* Q) \varepsilon + d_1 (\alpha_2 \varepsilon_2^T - \alpha_1 \varepsilon_1^T).
 \end{aligned}$$

Hence  $\varepsilon_2^* - \varepsilon_1^* = [\alpha(\beta^*, d)]^{-1} e(\varepsilon)$ .

We end this section by two explicit formulas, (37) and (38), for the first partial derivatives of  $\widehat{W}$ . Their derivation is lengthy and can be found in [8].

$$\frac{\partial \widehat{W}}{\partial d}(d, \varepsilon) = (d_1 \alpha_1 (\varepsilon_1^* - \varepsilon_1^T) + d_2 \alpha_2 (\varepsilon_2^* - \varepsilon_2^T)) : \Delta \varepsilon^* + W_1(\varepsilon_1^*) - W_2(\varepsilon_2^*) + V, \quad (37)$$

where  $V$  depending on the different regimes is given by

$$V = \begin{cases} 0 & \text{in Regimes 0, I,} \\ \beta^* d(1-d) \frac{\partial \beta^*}{\partial d} \|Q \Delta \varepsilon^*\|^2 & \text{in Regime II,} \\ (2d-1) \gamma^* \varphi(\Delta \varepsilon^*) & \text{in Regime III} \end{cases}$$

and

$$\frac{\partial \beta^*}{\partial d} = \begin{cases} \frac{(Q(d_2 \alpha_1 + d_1 \alpha_2 - \beta Q)^{-1}(\alpha_2 - \alpha_1) \Delta \varepsilon^*) : \Delta \varepsilon^*}{((d_2 \alpha_1 + d_1 \alpha_2 - \beta Q)^{-1}(Q \Delta \varepsilon^*)) : (Q \Delta \varepsilon^*)} & \text{in Regime II,} \\ 0 & \text{otherwise.} \end{cases}$$

The computation of the partial derivative of  $\widehat{W}$  with respect to the second variable yields

$$\begin{aligned} \frac{\partial \widehat{W}}{\partial \varepsilon}(d, \varepsilon) &= \frac{\partial}{\partial \varepsilon} \left[ d_1 W_1(\varepsilon_1^*) + d_2 W_2(\varepsilon_2^*) + \beta^* d_1 d_2 \det(\varepsilon_2^* - \varepsilon_1^*) \right] \\ &= d_1 d_2 \left[ (\alpha_2(\varepsilon_2^* - \varepsilon_2^T) - \alpha_1(\varepsilon_1^* - \varepsilon_1^T)) : (\alpha^{-1} Q \Delta \varepsilon^*) + \det(\Delta \varepsilon^*) \right] \frac{\partial \beta^*}{\partial \varepsilon} \\ &\quad + d_1(\alpha_2 - \beta^* Q) \alpha^{-1} \alpha_1(\varepsilon_1^* - \varepsilon_1^T) \\ &\quad + d_2(\alpha_1 - \beta^* Q) \alpha^{-1} \alpha_2(\varepsilon_2^* - \varepsilon_2^T), \end{aligned} \tag{38}$$

completed with

$$\frac{\partial \beta^*}{\partial \varepsilon} = - \frac{1}{(\alpha^{-1} \Delta \varepsilon^*) : \Delta \varepsilon^*} Q \alpha^{-1} (\alpha_1 - \alpha_2) \Delta \varepsilon^*.$$

With this result the collection of analytic formulas of  $\widehat{W}$  and its partial derivatives is now complete. The given representations are essential for a numerical implementation and are required for the existence proof in Theorem 3.

**Theorem 3** (Existence of solutions for geometrically linear elasticity). *Let  $D = 2$  and  $\widehat{W}$  the energy defined in (33). Moreover, let the mobility tensor  $M$  be positive definite, let  $\psi$  be given by (22) and let the initial data satisfy*

$$\psi(a_0, b_0) < \infty.$$

*Then, there exists a solution  $(a, b, u)$  to (17)–(19) that satisfies:*

- (i)  $a, b \in C^{0, \frac{1}{4}}([0, T]; L^2(\Omega))$ .
- (ii)  $\partial_t a, \partial_t b \in L^2(\Omega_T)$ .
- (iii)  $u \in L^\infty(0, T; H^1(\Omega; \mathbb{R}^D))$ .
- (iv) *The feasible parameter range for  $(a, b)$  is given by (24).*



**Proof:** We can adapt the proof of Theorem 1. We can check with the formulas given above that  $\widehat{W}$  given by (33) satisfies (A1) except for (26) which needs to be modified to

$$|\partial_\varepsilon \widehat{W}(d, \varepsilon)| \leq C_1(|\varepsilon| + |d|^2 + 1), \quad (39)$$

see the explicit computation in (38).

Condition (26) enters in the proof of the lower semicontinuity estimates and weak convergence estimates like

$$\int_{\Omega} \widehat{W}(a + b, \varepsilon(u)) \leq \liminf_{k \rightarrow \infty} \int_{\Omega} \widehat{W}(a_k + b_k, \varepsilon(u_k))$$

for sequences  $(a_k)_{k \in \mathbb{N}}$ ,  $(b_k)_{k \in \mathbb{N}}$  that converge to  $a$  and  $b$ , respectively, weakly in  $H^1(\Omega)$  and strongly in  $L^2(\Omega)$  and for a sequence  $(u_k)_{k \in \mathbb{N}}$  that converges weakly to  $u$  in  $H^1(\Omega; \mathbb{R}^D)$ . Since  $a_k$ ,  $b_k$  converge strongly in  $L^2(\Omega)$ , the altered power  $|d|^2$  instead of  $|d|$  in (39) does not change the estimates. The proof now follows as in Theorem 1.  $\square$

**Theorem 4.** *Let  $D = 2$  and  $\widehat{W}$  be the energy defined in (33). Assume further that the elastic moduli of the two phases are equal, i.e.,  $\alpha_1 = \alpha_2$ . Then the solution  $(a, b, u)$  in Theorem 3 is unique in the spaces stated in the theorem.*

**Proof:** Let again  $(a_i, b_i, u_i)$ ,  $i = 1, 2$  be two solutions to (17)–(19). Under the assumption  $\alpha_1 = \alpha_2$  the function  $\varphi$ , cf. (36), only depends on its first argument  $\beta$ , which implies that  $\beta^*$  is identical for any solution. Thus  $\alpha$  is a constant matrix and we find that  $\varepsilon_i$  is identical for any solution. From this we learn that

$$\partial_d \widehat{W}(d_1, \varepsilon_1) = \partial_d \widehat{W}(d_2, \varepsilon_2).$$

The theorem now follows from the Lipschitz continuity of  $g'$  analogous to Theorem 2.  $\square$

**Remark 3.** *For  $\alpha_1 \neq \alpha_2$ , the given proof fails. The critical term is  $\partial_d \widehat{W}(d_1, \varepsilon_1) - \partial_d \widehat{W}(d_1, \varepsilon_2)$ . Even though  $\partial_d \widehat{W}$  can be proved to be analytic, it is not possible to absorb powers of  $\varepsilon := \varepsilon(u_1) - \varepsilon(u_2)$  on the left.*

### 3.3 THE EXTENSION OF THE AC-CH MODEL TO POLYCRYSTALLINE ELASTIC MATERIALS

In this section we outline how the Allen-Cahn/Cahn-Hilliard model can be extended to polycrystalline materials with laminates based on geometrically linear elasticity

and homogenization. To this end we consider the first two equations of the system, (17) and (18), as before, where  $a$  and  $b$  now denote the corresponding macroscopic physical quantities of the polycrystalline material. Instead of the continuity equation (19), we now choose

$$0 = \operatorname{div}(\partial_{\bar{\varepsilon}} \bar{W}(a + b, \bar{\varepsilon})). \quad (40)$$

The boundary conditions are as in (20), while in the definition of the free energy (21),  $\widehat{W}$  is replaced by  $\bar{W}$  and  $\varepsilon$  is replaced by  $\bar{\varepsilon}$ , i.e.,

$$F(a, b, u) := \int_{\Omega} \psi(a, b) + \frac{\lambda}{2}(|\nabla a|^2 + |\nabla b|^2) + \bar{W}(a + b, \bar{\varepsilon}) + W_{\text{ext}}(\bar{\varepsilon}) \, dx,$$

where  $W_{\text{ext}}$  is defined as in (23). This completes our extension of the Allen-Cahn/Cahn-Hilliard model to polycrystalline elastic materials with prescribed volume fractions.

To complete the theory, it remains to settle the existence of weak solutions also for this extended model. This question is currently open and a topic of ongoing research.

## 4 CONCLUSION

In this article we derived extensions of the Allen-Cahn/Cahn-Hilliard system to elastic materials showing laminational structures. In particular we included (i) the linear elastic energy derived by Eshelby, (ii) a geometrically linear theory of elasticity for single crystals that takes phase fractions on the microscale into account, and (iii) a polycrystalline theory based on geometrically linear elasticity taking laminational structures into account, respectively. All generalized AC-CH models contain as special cases both the Allen-Cahn [10] and the Cahn-Hilliard equation [19], which are the two most-frequently used models in practical simulations and applications, e.g., in materials science, engineering, and biology.

As a particular property, the considered elastic energy functionals incorporate the contributions of laminates on the microscale, which opens the floor for more advanced studies of segregation and precipitation phenomena in composite materials. We underline that we always assume that the temperature is kept constant. For non-isothermal settings, the thermodynamic analysis implies certain modifications to the model, which are especially challenging for the theory on the microscale. These extensions have to be done in such a way that the second law of thermodynamics continues to hold. It is currently open how this can be achieved.

Besides the limiting assumption of constant temperature, the most important pending restriction is the postulation of small strain, included in (1). The technical

problems of a large strain theory are striking and unsolved, and we refer to [3, 21] for further discussions and open questions.

Next we come back to case (ii) and in particular to the specific energy  $\hat{W}$  considered in Section 3.2. We point out that the formulas collected in Section 3.2 are essential for any numerics on the AC-CH model extended to microstructure. For further investigations and numerical studies we refer the interested reader to [8] and [9].

For the cases (i) and (ii) we showed in a mathematically rigorous way the existence and (in certain cases) the uniqueness of weak solutions, asserting the correctness of our approach. Analogous existence and uniqueness results for case (iii), i.e., for polycrystalline materials with laminational structures, remain open and are a topic of current research.

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