

*A sharp interface evolutionary model  
for shape memory alloys*

*H. Knüpfner, M. Kružík*

Preprint no. 2015-09



# A sharp interface evolutionary model for shape memory alloys

Hans Knüpfers<sup>1</sup> and Martin Kružík<sup>2,3</sup>

<sup>1</sup>University of Heidelberg, Institute of Applied Mathematics and IWR, Im Neuenheimer Feld 294, 69120 Heidelberg, Germany

<sup>2</sup>Institute of Information Theory and Automation, of the CAS, Pod vodárenskou věží 4, CZ-182 08 Prague 8, Czech Republic,

<sup>3</sup>Faculty of Civil Engineering, Czech Technical University, Thákurova 7, 166 29 Prague, Czech Republic

August 12, 2015

## Abstract

We show the existence of an energetic solution to a quasistatic evolutionary model of shape memory alloys. Elastic behavior of each material phase/variant is described by polyconvex energy density. Additionally, to every phase boundary, there is an interface-polyconvex energy assigned, introduced by M. Šilhavý in [44]. The model considers internal variables describing the evolving spatial arrangement of the material phases and a deformation mapping with its first-order gradients. It allows for injectivity and orientation-preservation of deformations. Moreover, the resulting material microstructures have finite length scales.

**Keywords:** polyconvexity; shape memory materials; rate-independent problems

## 1 Introduction

In elasticity theory, it is assumed that experimentally observed patterns are minimizers or stable states of some energy. Shape memory alloys in particular have a preferred high-temperature lattice structure called austenite and a preferred low-temperature lattice structure called martensite. Such shape memory alloys, as e.g. Ni-Ti, Cu-Al-Ni or In-Th, have various technological

applications, for an overview see e.g. [24]. The austenitic phase has only one phase/variant but the martensitic phase exists in many symmetry related phases/variants; the mixing of these different phases can lead to the formation of complex microstructure. In the continuum theory, the total energy of the system is described in terms of a bulk energy which describes elastic stresses and an interfacial energy, concentrated on the interfaces between the different phases. We establish existence of quasistationary solutions for a model, where it is assumed that the bulk part of the energy is polyconvex while the interfacial part of the energy satisfies a corresponding condition of interfacial polyconvexity introduced by Šilhavý [44, 45]. The model describes the evolving spatial arrangement of the material phases and the deformation of the sample. It allows for injectivity and orientation-preservation of deformations. Moreover, the resulting material microstructures have finite length scales.

To investigate the existence of a global minimizer of the energy for static variational problems from elasticity, different notions of convexity have been considered. For problems with a single material phase, a well justified notion of convexity which is sufficient to ensure the existence of a minimizer is the notion of polyconvexity due to Ball [2, 3]. It is also fairly easy to construct examples of polyconvex functions which makes it attractive for continuum mechanics of solids. On the other hand, in shape memory alloys, many different phases might coexist. If interfacial energy is not taken into account, then global minimizers of the energy in general do not exist. A way out is to use relaxation methods, searching for the so-called quasiconvex envelope of the specific stored energy [18, 41] or using Young measures [25, 26, 34, 38]. Let us point out some partial results which have been obtained in this direction: We refer to [7] for a weak\* lower semicontinuity results for sequences of bi-Lipschitz orientation-preserving maps in the plane and to [6] for an analogous result along sequences of quasiconformal maps. Then [32] found relaxation including orientation preservation for  $p < d$ , where  $d$  is a spatial dimension. Finally, [17] derived a relaxation result for orientation preserving deformations with an extra assumption on the resulting functional, namely that the quasiconvex envelope is polyconvex. There also exist various phenomenological models of shape memory alloys which are convenient for numerical computations; see e.g. [8].

On the other hand, models have been considered where interfacial energy is taken into account. Such models have been e.g. used to estimate the scaling of the minimal energy and to derive typical length scales of patterns. The minimal scaling of the energy of an austenite-martensite interface has

been studied by Kohn & Müller and Conti in [30, 31, 16] for a 2-d model problem, the three-dimensional case and more realistic models have been investigated e.g. in [47, 11, 9, 10, 27, 28], for similar analysis on related models see e.g. [12, 13, 29]. In these models, either a  $BV$ -penalization of the interfacial has been used or a penalization of some  $L^p$ -norm for the Hessian of the deformation function. In general, the specific form of the energy is, however, not clear from physical considerations. In the literature, necessary and sufficient conditions for the specific form of the interfacial energy have been investigated recently which allow for the existence of minimizers [21, 42]. Recently, Šilhavý has introduced a notion of interface polyconvexity and has proved that this notion is sufficient to ensure existence of minimizers for the corresponding static problem [44, 45]. In this note, we extend this static model to a rate-independent evolutionary model and prove existence of an energetic solution.

In shape memory allows, the stored energy density  $W : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$  is minimized on wells  $\text{SO}(3)F_i$ ,  $i = 0, \dots, M$ , defined by  $M$  positive definite and symmetric matrices  $F_0, \dots, F_M$ , each corresponding austenite and  $M$  variants of martensite, respectively. By the choice of reference configuration, we may furthermore assume  $F_0 := \text{Id}$  (the identity), i.e. the stress-free strain of austenite is described just by the special orthogonal group  $\text{SO}(3)$ . In non-linear elasticity, the energy density  $W$  is usually formulated as a function of the right Cauchy-Green strain tensor  $F^\top F$ . Note that this tensor maps the whole group  $O(3)$  of orthogonal matrices with determinant  $\pm 1$  onto the same point. Thus, for example,  $F \mapsto |F^\top F - \text{Id}|$  is minimized on two energy wells, i.e., on  $\text{SO}(3)$  and also on  $O(3) \setminus \text{SO}(3)$ . However, the latter set is not acceptable in elasticity since corresponding deformations do not preserve the orientation. Additionally, notice that, for example, considering arbitrary  $Q \in O(3) \setminus \text{SO}(3)$  and an arbitrary  $R \in \text{SO}(3)$  such that  $Q$  and  $R$  are rotations around the same axis of the Cartesian system then  $\text{rank}(Q - R) = 1$ , i.e.  $Q$  and  $R$  are rank-one connected and determinant changes its sign on the line segment  $[Q; R]$ . Convex combinations of rank-one connected matrices play a key role in relaxation approaches of the variational calculus [4, 5, 18, 33]. This shows that it is important but also not straightforward to ensure that solutions of static or evolutionary problems are physically sound, in the sense that they preserve orientation. This is, in particular, unclear on models based on quasiconvexification as described above, since usually there is no closed formula of the envelope at disposal and since physically justified conditions on deformations as orientation-preservation and injectivity are not included in these models. On the other hand, our

solutions are constructed in a way such that the obtained time dependent deformations are orientation preserving and injective and no additional regularization of variables is needed if passing from a static to an evolutionary model. Injectivity and orientation preservation is not very often considered in the theory of rate-independent processes. We refer to [37] for treatment of a model in nonlinear elastoplasticity.

*Structure of the paper:* After introducing used notations, in Section 2, we first describe our model, the stored elastic energy, loading, and dissipation. In Section 3, we state and prove our main result, the existence of an energetic solution. As it is nowadays a standard procedure; cf. e.g., [22] we only sketch the main steps and pay more attention to injectivity of deformations which is not frequently treated in the frameworks of rate-independent evolutions. We refer, however, to [37] for numerical approaches to finite elastoplasticity including injectivity.

*Notation:* The spaces  $W^{1,p}$ ,  $1 \leq p < \infty$ , denote the standard Sobolev space of  $L^p$ -functions with weak derivative in  $L^p$ . Further,  $BV$  stands for the space of integrable maps with bounded variations, see e.g. [1, 20] for references. For a (measurable) set  $E \subset \mathbb{R}^3$ , we denote its three-dimensional Lebesgue measure by  $\mathcal{L}^3(E)$  and its two-dimensional Hausdorff measure by  $\mathcal{H}^2(E)$ . The space of vector valued Radon measures on  $\Omega$  with values in  $Y$  is denoted by  $\mathcal{M}(\Omega, Y)$ .

Let  $\tilde{\Omega} \subset \Omega \subset \mathbb{R}^3$  be Lebesgue measurable sets and let  $B(x, r) := \{a \in \mathbb{R}^3 : |x - a| < r\}$ . For  $x \in \Omega$  we denote the *density* of  $\tilde{\Omega}$  at  $x$  by  $\theta(\tilde{\Omega}, x) := \lim_{r \rightarrow 0} \mathcal{L}^3(\tilde{\Omega} \cap B(x, r)) / \mathcal{L}^3(B(x, r))$  whenever this limit exists. A point  $x \in \Omega$  is called *point of density* of  $\tilde{\Omega}$  if  $\theta(\tilde{\Omega}, x) = 1$ . If  $\theta(\tilde{\Omega}, x) = 0$  for some  $x \in \Omega$ , then  $x$  is called *point of rarefaction* of  $\tilde{\Omega}$ . The measure-theoretic boundary  $\partial^* \tilde{\Omega}$  of  $\tilde{\Omega}$  is the set of all points  $x \in \Omega$  such that either  $\theta(\tilde{\Omega}, x)$  does not exist or  $\theta(\tilde{\Omega}, x) \notin \{0, 1\}$ . We call  $\tilde{\Omega}$  a set of finite perimeter if  $\mathcal{H}^2(\partial^* \tilde{\Omega}) < +\infty$ . Let  $n \in \mathbb{R}^3$  be a unit vector and let  $H(x, n) := \{\tilde{x} \in \Omega : (\tilde{x} - x) \cdot n < 0\}$ . We say that  $n$  is the (outer) measure-theoretic normal to  $\tilde{\Omega}$  at  $x$  if  $\theta(\tilde{\Omega} \cap H(x, -n), x) = 0$  and  $\theta((\Omega \setminus \tilde{\Omega}) \cap H(x, n), x) = 0$ . The measure-theoretic normal exists for  $\mathcal{H}^2$  almost every point in  $\partial^* \tilde{\Omega}$ , see e.g. [20, 46].

For two matrices  $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{3 \times 3}$ , we define  $A : B = a_{ij} b_{ij}$  with Einstein's sum convention. By  $A \times n$  we denote the tensor defined by  $(A \times n)b = A(n \times b)$ , i.e.  $(A \times n)_{kj} = \epsilon_{\ell ij} a_{k\ell} n_i$ , where  $\epsilon_{\ell ij}$  is the Levi-Civita symbol. One can easily check that the cofactor matrix of  $A \in \mathbb{R}^{3 \times 3}$  in terms of the Levi-Civita can be expressed as  $\text{cof } A = \frac{1}{2}(\epsilon_{ik\ell} \epsilon_{jppq} a_{kp} a_{\ell q})_{ij}$ . In

particular, we get  $\partial_{a_{k\ell}}(\text{cof } A)_{ij} = \frac{1}{2}\partial_{a_{k\ell}}(\epsilon_{ik\ell}\epsilon_{jpp}a_{kp}a_{\ell q})_{ij} = \epsilon_{ikq}\epsilon_{jlp}a_{qp}$ . We refer e.g. to [23] for a definition of the surface gradients  $\nabla_S$ . If  $n \in \mathbb{R}^3$  is an outer unit normal to the surface  $S$ , then  $\nabla_S := \nabla(\text{Id} - n \otimes n)$ , where we recall that  $\text{Id}$  denotes the unit matrix in  $\mathbb{R}^{3 \times 3}$ .

## 2 Model description

### 2.1 Elastic energy

*Admissible States:* We assume that the specimen in its reference configuration is represented by a bounded Lipschitz domain  $\Omega \subset \mathbb{R}^3$ . We consider a shape memory alloy which allows for  $M$  different variants of martensite. The region occupied by the  $i$ -th variant of martensite is described by the set  $\Omega_i \subset \Omega$  for  $1 \leq i \leq M$ , while the region occupied by austenite is given by  $\Omega_0 \subset \Omega$ . We assume that the sets  $\Omega_i$  are open and have finite perimeter. Furthermore, the sets  $\Omega_i$  are pairwise disjoint for  $0 \leq i \leq M$  and  $N := \Omega \setminus \bigcup_i \Omega_i$  is a set of zero Lebesgue measure. The case  $\Omega_i = \emptyset$  for some  $0 \leq i \leq M$  is not excluded. The partition of  $\Omega$  into  $\{\Omega_i\}_{i=0}^M$  can be then identified with a mapping  $z : \Omega \rightarrow \mathbb{R}^{M+1}$  such that  $z_i(x) = 1$  if  $x \in \Omega_i$  and  $z_i(x) = 0$  else. We call  $z$  the *partition map* corresponding to  $\{\Omega_i\}_{i=0}^M$ . Clearly, with the sets  $\Omega_i$  chosen as before, we have  $\sum_{i=0}^M z_i(x) = 1$  for almost every  $x \in \Omega$  and the function  $z$  is of bounded variation. We hence consider  $z \in \mathcal{Z}$ , where

$$\mathcal{Z} := \left\{ z \in \text{BV}(\Omega, \{0, 1\}^{M+1}) : z_i z_j = 0 \text{ for } i \neq j, \sum_{i=0}^M z_i = 1 \text{ a.e. in } \Omega \right\}.$$

In order to describe the state of the elastic material, we also need to introduce the deformation function  $y \in W^{1,p}(\Omega, \mathbb{R}^3)$ ,  $p > 3$ , which describes the deformation of the elastic body with respect to the reference configuration  $\Omega$ . We hence consider deformations  $y \in \mathcal{Y}$ , where

$$\mathcal{Y} = \left\{ y \in W^{1,p}(\Omega, \mathbb{R}^3) : \det \nabla y > 0 \text{ a.e.}, \int_{\Omega} \det \nabla y(x) \, dx \leq \mathcal{L}^3(y(\Omega)) \right\},$$

where we will always use the assumption  $p > 3$ . The integral inequality together with the orientation-preservation is the so-called Ciarlet-Nečas condition which ensures invertibility of  $y$  almost everywhere in  $\Omega$  [14, 15]. In the following, we will assign to each state of the material  $(y, z) \in \mathcal{Y} \times \mathcal{Z}$  an elastic energy  $\mathcal{E}$ . In our model, the energy consists of a bulk part  $E_b$ , penalizing deformation within the single phases, an interfacial energy  $E_{\text{int}}$ , measuring

deformation of the interfaces between the phases and a contribution  $L(t, \cdot)$  which measures work of external loads, i.e.

$$\mathcal{E}(t, y, z) := E_b(y, z) + E_{\text{int}}(y, z) - L(t, y). \quad (1)$$

Here  $t$  denotes time to indicate that we will deal with time-dependent problems. We will specify these three parts of the energy in the following.

*Bulk energy:* The total bulk energy of the specimen has the form

$$E_b(y, z) := \int_{\Omega} W(z(x), \nabla y(x)) \, dx, \quad (2)$$

where we assume that the specific energy  $W : \mathbb{R}^{M+1} \times \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R} \cup \{+\infty\}$  of the specimen can be written as

$$W(z, F) := \sum_{i=0}^M z_i \hat{W}_i(F) =: z \cdot \hat{W}(F), \quad (3)$$

where  $\hat{W}_i$ ,  $0 \leq i \leq M$ , is the specific energy related to the  $i$ -th phase of the material and  $\hat{W} := (\hat{W}_0, \dots, \hat{W}_M)$ . We will work in the framework of hyperelasticity, where the first Piola-Kirchhoff stress tensors of austenite and martensite have polyconvex potentials denoted by  $\hat{W}_0$  (austenite) and  $\hat{W}_i$ ,  $i = 1, \dots, M$  for each variant of martensite, see e.g. [44] and the references therein. For  $0 \leq i \leq M$ , we therefore assume

$$\hat{W}_i(F) := \begin{cases} h_i(F, \text{cof } F, \det F) & \text{if } \det F > 0, \\ +\infty & \text{otherwise} \end{cases} \quad (4)$$

for some convex functions  $h_i : \mathbb{R}^{19} \rightarrow \mathbb{R}$ . We use the following additional standard assumptions on the specific bulk energies  $\hat{W}_i$ . For  $0 \leq i \leq M$  and  $F \in \mathbb{R}^{3 \times 3}$ , we assume that for some  $C > 0$  and  $p > 3$

$$\hat{W}_i(F) \geq C(-1 + |F|^p) \quad \forall F \in \mathbb{R}^{3 \times 3}, \quad (5)$$

$$\hat{W}_i(RF) = \hat{W}_i(F) \quad \forall R \in \text{SO}(3), F \in \mathbb{R}^{3 \times 3}, \quad (6)$$

$$\lim_{\det F \rightarrow 0_+} \hat{W}_i(F) = +\infty. \quad (7)$$

*Interfacial energy:* We consider the interfacial energy in the form introduced by Šilhavý in [44, 45]: We hence assume that the specific interfacial energy

$f_{ij}$  between the two different phases  $i, j \in \{0, \dots, M\}$  can be written in the form

$$\frac{1}{2}f_{ij}(F, n) = g_i(F, n) + g_j(F, n), \quad (8)$$

where  $F \in \mathbb{R}^{3 \times 3}$  and  $n \in \mathbb{R}^3$  is a unit vector such that  $Fn = 0$ . We assume

$$g_i(F, n) := \Psi_i(n, F \times n, \text{cof } F n), \quad (9)$$

where the functions  $\Psi_i : \mathbb{R}^{15} \rightarrow \mathbb{R}$  are nonnegative convex and positively one-homogeneous for  $i = 0, \dots, M$ . Here,  $F \times n : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  is for any  $F \in \mathbb{R}^{3 \times 3}$  and any  $n, a \in \mathbb{R}^3$  defined as  $(F \times n)a := F(n \times a)$ . As in [44], we assume for  $0 \leq i \leq M$ ,  $\forall F \in \mathbb{R}^{3 \times 3}$ ,  $\forall n \in S^2$

$$g_i(RF, n) = g_i(F, n) \quad \forall R \in \text{SO}(3), \quad (10)$$

$$g_i(F, n) = g_i(F, -n), \quad (11)$$

As in [44], we assume that there is some  $c > 0$  such that

$$\Psi_i(A) \geq c|A| \quad . \quad (12)$$

for all  $0 \leq i \leq M$  and all  $A \in \mathbb{R}^{15}$ . We introduce a subspace  $\mathcal{Q} \subset \mathcal{Y} \times \mathcal{Z}$  of functions with ‘‘finite interfacial energy’’, using a slightly modified version of [44, Def. 3.1]. It is given as follows:

**Definition 2.1** (Interfacial energy). *For any pair  $(y, z) \in \mathcal{Y} \times \mathcal{Z}$  let  $S_i = \partial^* \Omega_i \cap \Omega$  where  $\Omega_i := \text{supp } z_i$  and  $\partial^* \Omega_i$  is the measure-theoretic boundary of  $\Omega_i$  with outer (measure-theoretic) normal  $n_i$ . We denote by  $\mathcal{Q} \subset \mathcal{Y} \times \mathcal{Z}$  the set of all pairs  $(y, z) \in \mathcal{Y} \times \mathcal{Z}$  such that for every  $0 \leq i \leq M$  there exists a measure  $J_i := (a_i, H_i, c_i) \in \mathcal{M}(\Omega; \mathbb{R}^{15})$  with*

$$a_i := n_i \mathcal{H}_{|S_i}^2, \quad H_i := \nabla_{S_i} y \times n_i \mathcal{H}_{|S_i}^2 \quad \text{and} \quad c_i := (\text{cof } \nabla_{S_i} y) n_i|_{S_i} \quad . \quad (13)$$

The interfacial energy is then defined as

$$E_{\text{int}}(y, z) := \begin{cases} \sum_{i=0}^M \int_{\Omega} \Psi_i \left( \frac{dJ_i}{d|J_i|} \right) d|J_i| & \text{for } (y, z) \in \mathcal{Q}, \\ \infty & \text{else.} \end{cases} \quad (14)$$

Here  $|J_i|$  denotes the total variation of the measure  $J_i$ .



We recall that the function  $f_{ij}$  is called interface quasiconvex if

$$\int_{\mathcal{S}} f(\nabla_{\mathcal{S}} y, n) d\mathcal{H}^2 \geq \mathcal{H}^2(\mathcal{T}) f(G, m) \quad (15)$$

for every surface deformation gradient  $G$ , every unit vector  $m$  with  $Gm = 0$ , every planar two-dimensional region  $\mathcal{T}$  with normal  $m$ , every (curved) surface  $\mathcal{S}$  with normal  $n$  and every smooth map  $y : \mathcal{S} \rightarrow \mathbb{R}^3$  with  $\text{bd} \mathcal{S} = \text{bd} \mathcal{T}$  (where  $\text{bd} \mathcal{S} = \text{bd} \mathcal{T}$  denote the relative boundaries of the two two-dimensional surfaces) and such that  $y = Gx$  for  $x \in \text{bd} \mathcal{T}$ , see [44, 45]. A surface energy is called Null-Lagrangian if (15) is satisfied with equality. Furthermore, it has been shown in [43] that  $f$  is an interface Null-Lagrangian if and only if  $f$  is a linear function of  $n$ ,  $F \times n$  and  $\text{cof } Fn$ . This motivates the definition of interface polyconvexity (8)–(9), in the analogy to the definition of the standard notion of polyconvexity. The set of configurations  $\mathcal{Q}$  in Definition 2.1 is the natural space where an energy of type (8)–(9) can be defined. Let us remark that the measures  $H_i$  and  $c_i$  can be expressed as

$$\int_{\Omega} v \, dH_i = \int_{\Omega_i} \nabla y (\nabla \times v) \, dx, \quad \int_{\Omega} v \cdot dc_i = \int_{\Omega_i} (\text{cof } \nabla y) : \nabla v \, dx \quad (16)$$

for all  $v \in C_0^\infty(\Omega; \mathbb{R}^3)$ . Indeed, for  $k \in \{1, 2, 3\}$  and  $0 \leq i \leq M$ , we have

$$\begin{aligned} \int_{\Omega_i} [\nabla y (\nabla \times v)]_k &= \int_{\Omega_i} [\partial_j y_k \epsilon_{j\ell m} \partial_\ell v_m] dx = \int_{\partial\Omega_i} [n_\ell \partial_j y_k \epsilon_{j\ell m} v_m] dx \\ &= \int_{\partial\Omega_i} [\nabla v]_{kj} [n \times v]_j dx = \int_{\partial\Omega_i} [(\nabla y \times n)v]_k dx, \end{aligned}$$

since  $\nabla \times \nabla y = 0$ . With the notation  $(\text{cof } \nabla y)_{ij} = b_{ij}$ , we also have

$$\begin{aligned} \int_{\Omega_i} (\text{cof } \nabla y) : (\nabla v) dx &= \int_{\Omega_i} [b_{kj} \partial_j v_k] dx = - \int_{\Omega_i} [\partial_j b_{kj} v_k] dx + \int_{\partial\Omega_i} [n_j b_{kj} v_k] dx \\ &= \int_{\partial\Omega_i} [(\text{cof } \nabla y)n]_k v_k dx = \int_{\partial\Omega_i} (\text{cof } \nabla y)n \cdot v dx, \end{aligned}$$

where we used the Piola identity  $\nabla \cdot (\text{cof } \nabla y) = 0$ .

We also note that by the assumption (12), we have the bound

$$\|Dz\|_{\mathcal{M}(\Omega; \mathbb{R}^{(M+1) \times 3})} \leq CE_{\text{int}}(y, z). \quad (17)$$

for some constant  $C < \infty$ . Consequently, the norm  $\|z\|_{\text{BV}(\Omega; \mathbb{R}^{M+1})}$  is controlled in terms of the interfacial energy in our setting. On the other hand,

the norm  $\|Dz\|_{\mathcal{M}(\Omega; \mathbb{R}^{(M+1) \times 3})}$  satisfies the conditions in Definition 2.1. Indeed, this follows from the choice  $g_i(F, n) = \alpha|F| = \alpha|F \times n|$  for  $\alpha > 0$ . Another example of an interfacial energy which is included in the Definition (2.1) is given by the choice  $g_i(F, n) = \alpha|\operatorname{cof} Fn|$ , see [45] for more details. Notice that the first example penalizes surface gradients which are nonconstant along interfaces while the latter one increases with the area of the interface.

*Body and surface loads:* We assume that the body is exposed to possible body and surface loads, and that it is elastically supported on a part  $\Gamma_0$  of its boundary. The part of the energy related to this loading is given by a functional  $L \in C^1([0, T]; W^{1,p}(\Omega; \mathbb{R}^3))$  in the form

$$L(t, y) := \int_{\Omega} b(t) \cdot y \, dx + \int_{\Gamma_1} s(t) \cdot y \, d\mathcal{H}^2(x) + \frac{K}{2} \int_{\Gamma_0} |y - y_D(t)|^2 \, d\mathcal{H}^2(x). \quad (18)$$

Here,  $b(t, \cdot) : \Omega \rightarrow \mathbb{R}^3$  represents the volume density of some given external body forces and  $s(t, \cdot) : \Gamma_1 \subset \partial\Omega \rightarrow \mathbb{R}^3$  describes the density of surface forces applied on a part  $\Gamma_1$  of the boundary. The last term in (18) with  $y_D(t, \cdot) \in W^{1,p}(\Omega; \mathbb{R}^3)$  represents energy of a spring with a spring stiffness constant  $K > 0$ . Thus our specimen is elastically supported on  $\Gamma_0$  in such a way, that for  $K \rightarrow \infty$   $y$  is forced to be close to  $y_D$  on  $\Gamma_0$  in the sense of the  $L^2(\Gamma_0; \mathbb{R}^3)$  norm. A term of this type already appeared in [35] and its static version also in [38]. Namely, prescribing a boundary condition from  $W^{1-1/p,p}(\partial\Omega; \mathbb{R}^3)$  [36], it is generally not known whether it can be extended to the whole  $\Omega$  in such a way that the extension lives in  $\mathcal{Y}$ . It is, to our best knowledge, an unsolved problem in three dimensions and therefore it is generically assumed in nonlinear elasticity that such an extension exists; cf. [14], for instance. The last term in (18) overcomes this drawback. Namely, if  $y_D$  cannot be extended from the boundary as an orientation-preserving map the term in question will never be zero regardless values of  $K > 0$ .

## 2.2 Dissipation

Evolution is typically connected with dissipation of energy. Experimental evidence shows that it is a reasonable approximation in a wide range of rates of external loads to anticipate a rate-independent dissipation mechanism. In order to set up such a process, we need to define a suitable dissipation function. Since we consider rate-independent processes, this dissipation will be positively one-homogeneous. We associate the dissipation to the magnitude

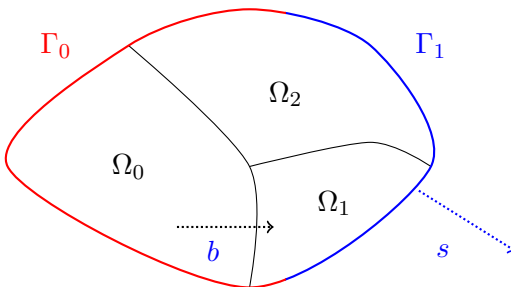


Figure 1: The domain is decomposed into subdomains according to the variants of austenite and martensite. At  $\Gamma_0$ , an elastic Dirichlet-type condition is imposed, while it is assumed that a force  $s$  acts on the interface  $\Gamma_1$ . Furthermore, a bulk force  $b$  acts on  $\Omega$ .

of the time derivative of  $z$ , i.e., to  $|\dot{z}|_{M+1}$ , where  $|\cdot|_{M+1}$  is a norm on  $\mathbb{R}^{M+1}$ . Therefore, the specific dissipated energy associated to a change of the variant distribution from  $z^1$  to  $z^2$  is postulated as in [19]

$$D(z^1, z^2) := |z^1 - z^2|_{M+1}. \quad (19)$$

Then the total dissipation reads

$$\mathcal{D}(z^1, z^2) := \int_{\Omega} D(z^1(x), z^2(x)) \, dx .$$

The  $\mathcal{D}$ -dissipation of a curve  $z : [0, T] \rightarrow BV(\Omega, \{0, 1\})$  with  $[s, t] \subset [0, T]$  is correspondingly given by (see e.g. [22])

$$\text{Diss}_{\mathcal{D}}(z, [s, t]) := \sup \left\{ \sum_{j=1}^N \mathcal{D}(z(t_{j-1}), z(t_j)) : N \in \mathbb{N}, s = t_0 \leq \dots \leq t_N = t \right\}.$$

### 2.3 Energetic solution

Suppose, that we look for the time evolution of  $t \mapsto y(t) \in \mathcal{Y}$  and  $t \mapsto z(t) \in \mathcal{Z}$  during a process time interval  $[0, T]$  where  $T > 0$  is the time horizon. We use the following notion of solution from [22], see also [39, 40]: For every admissible configuration, we ask the following conditions to be satisfied for all  $t \in [0, T]$ .

**Definition 2.2** (Energetic solution). *We say that  $(y, z) \in \mathcal{Y} \times \mathcal{Z}$  is an energetic solution to  $(\mathcal{E}, \mathcal{D})$  on the time interval  $[0, T]$  if  $t \mapsto \partial_t E(y(t), z(t)) \in L^1((0, T))$  and if for all  $t \in [0, T]$ , the stability condition*

$$\mathcal{E}(t, y(t), z(t)) \leq \mathcal{E}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}) \quad \forall (\tilde{y}, \tilde{z}) \in \mathcal{Q}. \quad (20)$$

and the condition of energy balance

$$\mathcal{E}(t, y(t), z(t)) + \text{Diss}_{\mathcal{D}}(z; [0, t]) = \mathcal{E}_0 + \int_0^t \frac{\partial \mathcal{E}}{\partial t}(s, y(s), z(s)) ds \quad (21)$$

where  $\mathcal{E}_0 = \mathcal{E}(0, y(0), z(0))$ , are satisfied.

An important role in the theory of rate-independent solutions is played by the so-called stable states defined for each  $t \in [0, T]$ . We set

$$\mathcal{S}(t) := \{(y, z) \in \mathcal{Y} \times \mathcal{Z} : \mathcal{E}(t, y, z) \leq \mathcal{E}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z, \tilde{z}) \forall (\tilde{y}, \tilde{z}) \in \mathcal{Q}\}.$$

Note that by (20), any energetic solution  $(y, z)$  is stable for any fixed time.

### 3 Existence of the energetic solution

A standard way how to prove the existence of an energetic solution is to construct time-discrete minimization problems and then to pass to the limit. Before we give the existence proof we need some auxiliary results. For given  $N \in \mathbb{N}$  and for  $0 \leq k \leq N$ , we define the time increments  $t_k := kT/N$ . Furthermore, we use the abbreviation  $q := (y, z) \in \mathcal{Q}$ . Assume that at  $t = 0$  there is given an initial distribution of phases  $z^0 \in \mathcal{Z}$  and  $y^0 \in \mathcal{Y}$  such that  $q^0 = (y^0, z^0) \in \mathcal{S}(0)$ . For  $k = 1, \dots, N$ , we define a sequence of minimization problems

$$\text{minimize } \mathcal{E}(t_k, y, z) + \mathcal{D}(z, z^{k-1}), \quad (y, z) \in \mathcal{Q}. \quad (22)$$

We denote a minimizer of (22) for a given  $k$  as  $(y^k, z^k) \in \mathcal{Q}$ . The following proposition shows that a minimizer always exists if the elastic energy is not identically infinite on  $\mathcal{Q}$ .

**Lemma 3.1.** *Assume that  $p > 3$ , (4)-(7), (9), (11)-(12) hold and let  $L \in C^1([0, T]; W^{1,p}(\Omega; \mathbb{R}^3))$ . Let  $q_0^N := (y_0, z_0) \in \mathcal{Q}$  satisfy  $\mathcal{E}(0, y, z) < +\infty$ . Then there exists a solution  $q_k^N := (y_k, z_k)$  to (22) for each  $1 \leq k \leq N$ . Moreover,  $q_k^N \in \mathcal{S}(t_k)$  for all  $1 \leq k \leq N$ .*

*Proof.* The proof follows the same lines as the proof of [44, Thm. 3.3]. We apply the direct method of the calculus of variations. We denote the elements of the minimizing sequence by a lower index in brackets in order to distinguish it from the components of  $z = (z_0, \dots, z_M)$ . Fix  $k$ , so that  $z^{k-1} \in \mathcal{Z}$  is given. Let  $\{(y_{(j)}, z_{(j)})\}_{j \in \mathbb{N}} \subset \mathcal{Q}$  be a minimizing sequence for  $\mathcal{E}(t_k, \cdot, \cdot) + \mathcal{D}(\cdot, z^{k-1})$ . Using the growth conditions (5), (10), and in view of the form of  $L$ , it follows that there is  $C > 0$  such that  $\|y_{(j)}\|_{W^{1,p}(\Omega; \mathbb{R}^3)} + \|z_{(j)}\|_{\text{BV}(\Omega; \mathbb{R}^{M+1})} \leq C$  for all  $j \in \mathbb{N}$ . Furthermore,

$$\sup_j (\|\text{cof } \nabla y_{(j)}\|_{L^{p/2}(\Omega; \mathbb{R}^{3 \times 3})} + \|\det \nabla y_{(j)}\|_{L^{p/3}(\Omega)}) < +\infty,$$

where  $p/3 > 1$  by our assumption  $p > 3$ . Consequently, after taking a subsequence, we may assume that  $y_{(j)} \rightharpoonup y$  in  $W^{1,p}(\Omega; \mathbb{R}^3)$ ,  $\det \nabla y_{(j)} \rightharpoonup \det \nabla y$  in  $L^{p/3}(\Omega)$ ,  $\text{cof } \nabla y_{(j)} \rightharpoonup \text{cof } \nabla y$  in  $L^{p/2}(\Omega; \mathbb{R}^{3 \times 3})$ , and  $z_{(j)} \overset{*}{\rightharpoonup} z$  in  $\text{BV}(\Omega; \mathbb{R}^{M+1})$ . In particular, we have  $z_{(j)} \rightarrow z$  in  $L^1(\Omega; \{0, 1\}^{M+1})$  and  $z \in \mathcal{Z}$ . Moreover, in view of (16),  $(J_i)_{(j)}$  converges weakly\* in measures to  $J_i$  as  $j \rightarrow \infty$  for all  $0 \leq i \leq M$ . Standard results for polyconvex materials [2, 14, 44] show  $\liminf_{j \rightarrow \infty} E_b(y_{(j)}, z_{(j)}) \geq E_b(y, z)$ . Similarly,  $\liminf_{j \rightarrow \infty} L(t_k, y_{(j)}) \geq L(t_k, y)$  and  $\lim_{j \rightarrow \infty} \mathcal{D}(z_{(j)}, z^{k-1}) = \mathcal{D}(z, z^{k-1})$  due to the strong convergence of  $z_{(j)} \rightarrow z$  in  $L^1(\Omega; \mathbb{R}^{M+1})$ . Finally,

$$\liminf_{j \rightarrow \infty} E_{\text{int}}(y_{(j)}, z_{(j)}) \geq E_{\text{int}}(y, z)$$

due to [1, Thm. 2.38]. Thus,  $(y, z) \in \mathcal{Y} \times \mathcal{Z}$ . Using weak sequential continuity of  $y \mapsto \text{cof } \nabla y$  and  $y \mapsto \nabla y$  we see that the limiting measures  $J_i$  have the form of (13). This together with a limit passage in the Ciarlet-Nečas condition (see [15, Thm. 5]) shows that  $(y, z) \in \mathcal{Q}$ . Namely,  $y$  is injective almost everywhere in  $\Omega$  and  $\det \nabla y > 0$  almost everywhere in  $\Omega$ . From (22), one furthermore easily sees that  $q_k^N \in \mathcal{S}(t_k)$  for all  $1 \leq k \leq N$ .  $\square$

Denoting by  $B([0, T]; \mathcal{Y})$  the set of bounded maps  $t \mapsto y(t) \in \mathcal{Y}$  for all  $t \in [0, T]$ , we have the following result showing the existence of an energetic solution.

**Theorem 3.2.** *Let  $T > 0$ ,  $p > 3$ ,  $y_D \in C^1([0, T]; W^{1,p}(\Omega; \mathbb{R}^3))$ , (4)-(7), (9), (11)-(12). Let  $(y(0), z(0)) \in S(0)$  and let there be  $(y, z) \in \mathcal{Q}$  such that  $\mathcal{E}(0, y, z) < +\infty$ . Then there is an energetic solution to the problem  $(\mathcal{E}, \mathcal{D})$  such that  $y \in B([0, T]; \mathcal{Y})$ ,  $z \in \text{BV}([0, T]; L^1(\Omega; \mathbb{R}^{M+1}) \cap L^\infty(0, T; \mathcal{Z}))$ .*

*Proof.* Let  $q_k^N := (y^k, z^k)$  be the solution of (22) which exists by Lemma 3.1 and let  $q^N : [0, T] \rightarrow \mathcal{Q}$  be given by

$$q^N(t) := \begin{cases} q_k^N & \text{if } t \in [t_k, t_{k+1}) \text{ if } k = 0, \dots, N-1, \\ q_N^N & \text{if } t = T. \end{cases} \quad (23)$$

Following [22], we get for some  $C > 0$  and for all  $N \in \mathbb{N}$  the estimates

$$\|z^N\|_{BV(0,T;L^1(\Omega;\mathbb{R}^{M+1}))} \leq C, \quad \|z^N\|_{L^\infty(0,T;BV(\Omega;\mathbb{R}^{M+1}))} \leq C, \quad (24a)$$

$$\|y^N\|_{L^\infty(0,T;W^{1,p}(\Omega;\mathbb{R}^3))} \leq C, \quad (24b)$$

as well as the following two-sided energy inequality

$$\begin{aligned} \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(\theta, q_k^N) \, d\theta &\leq \mathcal{E}(t_k, q_k^N) + \mathcal{D}(z^k, z^{k-1}) - \mathcal{E}(t_{k-1}, q_{k-1}^N) \\ &\leq \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(\theta, q_{k-1}^N) \, d\theta. \end{aligned} \quad (25)$$

The second inequality in (25) follows since  $q_k^N$  is a minimizer of (22) and by comparison of its energy with  $q := q_{k-1}^N$ . The lower estimate is implied by the stability of  $q_{k-1}^N \in \mathbb{S}(t_{k-1})$  when compared with  $\tilde{q} := q_k^N$ . Having this inequality, the a-priori estimates and a generalized Helly's selection principle [40, Cor. 2.8] we get that there is indeed an energetic solution obtained as a limit for  $N \rightarrow \infty$ . In particular, the fact that  $\det \nabla y > 0$  a.e. in  $\Omega$  follows from the fact that if  $t_j \rightarrow t$ ,  $(y_{(j)}, z_{(j)}) \in \mathbb{S}(t_j)$  and  $(y_{(j)}, z_{(j)}) \rightarrow (y, z)$  in  $W^{1,p}(\Omega; \mathbb{R}^3) \times BV(\Omega; \mathbb{R}^{M+1})$ , then  $(y, z) \in \mathbb{S}(t)$ . Indeed, in particular we have  $z_{(j)} \rightarrow z$  in  $L^1(\Omega; \mathbb{R}^{M+1})$  and hence for all  $(\tilde{y}, \tilde{z}) \in \mathcal{Q}$ , we get

$$\begin{aligned} \mathcal{E}(t, y, z) &\leq \liminf_{j \rightarrow \infty} \mathcal{E}(t_j, y_{(j)}, z_{(j)}) \leq \liminf_{j \rightarrow \infty} \mathcal{E}(t_j, \tilde{y}, \tilde{z}) + \liminf_{j \rightarrow \infty} \mathcal{D}(z_{(j)}, \tilde{z}) \\ &= \mathcal{E}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z, \tilde{z}). \end{aligned}$$

In particular, as  $\mathcal{E}(t_j, \tilde{y}, \tilde{z})$  is finite for some  $(\tilde{y}, \tilde{z}) \in \mathcal{Q}$  we get  $\mathcal{E}(t, y, z) < +\infty$  and thus  $\det \nabla y > 0$  a.e. in  $\Omega$  in view of (4).  $\square$

**Remark 3.3.** Adding a term of the form  $F \mapsto |\operatorname{cof} F|^p / (\det F)^{p-1}$ , which is polyconvex, to the bulk stored energy density we can even show injectivity of deformations everywhere in  $\Omega$  for all time instants. See e.g. [7, Rem. 1.2] and also [3] where such term already appeared.

**Acknowledgment.** This work was initiated during a visit of MK in the Institute of Applied Mathematics at the University of Heidelberg and further conducted during a visit of HK in the Institute of Information Theory and Automation at Prague. The hospitality and support of both institutions is gratefully acknowledged. MK was further supported by GAČR through the project 14-15264S.

## References

- [1] L. Ambrosio, N. Fusco, and D. Pallara. Functions of bounded variation and free discontinuity problems. Oxford Mathematical Monographs. The Clarendon Press, New York, 2000.
- [2] J. M. Ball. Convexity conditions and existence theorems in nonlinear elasticity. Arch. Rat. Mech. Anal., 63:337–403, 1977.
- [3] J. M. Ball. Global invertibility of Sobolev functions and the interpenetration of matter. Proc. Roy. Soc. Edinburgh, Series A, 88:315–328, 1981.
- [4] J. M. Ball and R. D. James. Fine phase mixtures as minimizers of energy. Arch. Rational Mech. Anal., 100(1):13–52, 1987.
- [5] J. M. Ball and R. D. James. Proposed experimental tests of a theory of fine microstructure and the two-well problem. Phil. Trans. Roy. Soc. London Ser. A, 338:389–450, 1992.
- [6] B. Benešová and M. Kampschulte. Gradient Young measures generated by quasiconformal maps the plane. Preprint at RWTH Aachen, 2014.
- [7] B. Benešová and M. Kružík. Characterization of gradient Young measures generated by homeomorphisms in the plane. ESAIM Control Optim. Calc. Var., <http://dx.doi.org/10.1051/cocv/2015003>.
- [8] A.-L. Bessoud, M. Kružík, and U. Stefanelli. A macroscopic model for magnetic shape-memory single crystals. ZAMM Z. Angew. Math. Phys., 64(2):343–359, 2013.
- [9] A. Capella and F. Otto. A rigidity result for a perturbation of the geometrically linear three-well problem. Comm. Pure Appl. Math., 62(12):1632–1669, 2009.

- [10] A. Capella and F. Otto. A quantitative rigidity result for the cubic-to-tetragonal phase transition in the geometrically linear theory with interfacial energy. Proc. Roy. Soc. Edinburgh Sect. A, 142(2):273–327, 2012.
- [11] A. Chan and S. Conti. Energy scaling and branched microstructures in a model for shape-memory alloys with  $SO(2)$  invariance. Math. Models Methods Appl. Sci., 25(6):1091–1124, 2015.
- [12] R. Choksi and R. Kohn. Bounds on the micromagnetic energy of a uniaxial ferromagnet. Comm. Pure Appl. Math., 51(3):259–289, 1998.
- [13] R. Choksi, R. Kohn, and F. Otto. Domain branching in uniaxial ferromagnets: a scaling law for the minimum energy. Comm. Math. Phys., 201(1):61–79, 1999.
- [14] P. G. Ciarlet. Lectures on three-dimensional elasticity. Published for the Tata Institute of Fundamental Research, Bombay; by Springer-Verlag, Berlin, 1983. Notes by S. Kesavan.
- [15] P. G. Ciarlet and J. Nečas. Injectivity and self-contact in nonlinear elasticity. Arch. Rational Mech. Anal., 97(3):171–188, 1987.
- [16] S. Conti. A lower bound for a variational model for pattern formation in shape-memory alloys. Contin. Mech. Thermodyn., 17(6):469–476, 2006.
- [17] S. Conti and G. Dolzmann. On the theory of relaxation in nonlinear elasticity with constraints on the determinant. Arch. Rat. Mech. Anal., <http://dx.doi.org/10.1007/s00205-014-0835-9>.
- [18] B. Dacorogna. Direct methods in the calculus of variations, volume 78 of Applied Mathematical Sciences. Springer, New York, second edition, 2008.
- [19] A. DeSimone and M. Kružík. Domain patterns and hysteresis in phase-transforming solids: Analysis and numerical simulations of a sharp interface dissipative model via phase-field approximation. Networks Heterog. Media, 8(2):481–499, 2013.
- [20] L. Evans and R. Gariepy. Measure Theory and Fine Properties of Functions. CRC, Boca Raton, 1992.



- [21] I. Fonseca. Interfacial energy and the Maxwell rule. Arch. Rational Mech. Anal., 106(1):63–95, 1989.
- [22] G. Francfort and A. Mielke. Existence results for a class of rate-independent material models with nonconvex elastic energies. J. Reine Angew. Math., 595:55–91, 2006.
- [23] M. Gurtin and A. Struthers. Multiphase thermomechanics with interfacial structure 3. evolving phase boundaries in the presence of bulk deformation. Arch. Rat. Mech. Anal., 112:97–160, 1990.
- [24] J. Jani, M. Leary, A. Subic, and M. Gibson. A review of shape memory alloy research, applications and opportunities. Materials & Design, 56:1078–1113, APR 2014.
- [25] D. Kinderlehrer and P. Pedregal. Characterization of Young measures generated by gradients. Arch. Rat. Mech. Anal., 115:329–365, 1991.
- [26] D. Kinderlehrer and P. Pedregal. Gradient Young measures generated by sequences in Sobolev spaces. J. Geom. Anal., pages 59–90, 1994.
- [27] H. Knüpfer and R. Kohn. Minimal energy for elastic inclusions. Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci., 467(2127):695–717, 2011.
- [28] H. Knüpfer, R. Kohn, and F. Otto. Nucleation barriers for the cubic-to-tetragonal phase transformation. Comm. Pure Appl. Math., 66(6):867–904, 2013.
- [29] H. Knüpfer and C. Muratov. Domain structure of bulk ferromagnetic crystals in applied fields near saturation. Journal of Nonlinear Science, pages 1–42, 2011. 10.1007/s00332-011-9105-2.
- [30] R. Kohn and S. Müller. Branching of twins near an austenite/twinned-martensite interface. Philosophical Magazine A, 66(5):697–715, 1992.
- [31] R. Kohn and S. Müller. Surface energy and microstructure in coherent phase transitions. Comm. Pure Appl. Math., 47(4):405–435, 1994.
- [32] K. Koumatos, F. Rindler, and E. Wiedemann. Orientation-preserving Young measures. Preprint arXiv 1307.1007.v1, 2013.
- [33] M. Kružík and M. Luskin. The computation of martensitic microstructures with piecewise laminates. J. Sci. Comput., 19(1-3):293–308, 2003.

- [34] M. Kružík, A. Mielke, and T. Roubíček. Modelling of microstructure and its evolution in shape-memory-alloy single-crystals, in particular in copper. *Meccanica*, 40(4-6):389–418, 2005.
- [35] M. Kružík and F. Otto. A phenomenological model for hysteresis in polycrystalline shape memory alloys. *ZAMM Z. Angew. Math. Mech.*, 84(12):835–842, 2004.
- [36] J. Marschall. The trace of Sobolev-Slobodeckij spaces on Lipschitz domains. *Manuscr. Math.*, pages 47–65, 1987.
- [37] A. Mielke and T. Roubíček. Rate-independent elastoplasticity and its numerical approximation. In preparation, 2015.
- [38] A. Mielke and T. Roubíček. A rate-independent model for inelastic behavior of shape-memory alloys. *Multiscale Model. Simul.*, 1(4):571–597 (electronic), 2003.
- [39] A. Mielke and F. Theil. On rate-independent hysteresis models. *NoDEA Nonlinear Differential Equations Appl.*, 11(2):151–189, 2004.
- [40] A. Mielke, F. Theil, and V. I. Levitas. A variational formulation of rate-independent phase transformations using an extremum principle. *Arch. Ration. Mech. Anal.*, 162(2):137–177, 2002.
- [41] S. Müller. Variational models for microstructure and phase transitions. *Lecture Notes in Mathematics* **1713**, Springer Berlin, 1999 pp. 85–210, 1999.
- [42] G. Parry. On shear bands in unloaded crystals. *Journal of the Mechanics and Physics of Solids*, 35(3):367 – 382, 1987.
- [43] M. Šilhavý. Phase transitions with interfacial energy: convexity conditions and the existence of minimizers. In J. Schröder and P. Neff, editors, *Poly-, Quasi- and Rank-One Convexity in Applied Mechanics*, volume 516 of *CISM International Centre for Mechanical Sciences*, pages 177–239. Springer Vienna, 2010.
- [44] M. Šilhavý. Phase transitions with interfacial energy: Interface null lagrangians, polyconvexity, and existence. In K. Hackl, editor, *IUTAM Symposium on Variational Concepts with Applications to the Mechanics of Materials*, volume 21 of *IUTAM Bookseries*, pages 233–244. Springer Netherlands, 2010.

- [45] M. Šilhavý. Equilibrium of phases with interfacial energy: a variational approach. J. Elasticity, 105(1-2):271–303, 2011.
- [46] M. Šilhavý. The Mechanics and Thermodynamics of Continuous Media. Springer, Heidelberg, 1997.
- [47] B. Zwicknagl. Microstructures in low-hysteresis shape memory alloys: scaling regimes and optimal needle shapes. Arch. Ration. Mech. Anal., 213(2):355–421, 2014.