# Existence of Lipschitz minimizers for the three-well problem in solid-solid phase transitions

January 30, 2006

Sergio Conti<sup>1</sup>, Georg Dolzmann<sup>2</sup>, and Bernd Kirchheim<sup>3</sup>

- <sup>1</sup> Fachbereich Mathematik, Universität Duisburg-Essen Lotharstr. 65, 47057 Duisburg, Germany
- <sup>2</sup> Mathematics Department, University of Maryland, College Park, MD 20742-4015, U.S.A.
  - <sup>3</sup> Mathematical Institute, 24-29 St Giles' Oxford, OX1 3LB, England

The three-well problem consists in looking for minimizers  $u:\Omega\subset\mathbb{R}^3\to\mathbb{R}^3$  of a functional  $I(u)=\int_\Omega W(\nabla u)\,\mathrm{d} x$ , where the elastic energy W models the tetragonal phase of a phase-transforming material. In particular, W attains its minimum on  $K=\bigcup_{i=1}^3\mathrm{SO}(3)U_i$ , with  $U_i$  being the three distinct diagonal matrices with eigenvalues  $(\lambda,\lambda,\widetilde{\lambda}),\,\lambda,\widetilde{\lambda}>0$  and  $\lambda\neq\widetilde{\lambda}$ . We show that, for boundary values F in a suitable relatively open subset of  $\mathbb{M}^{3\times3}\cap\{F:\det F=\det U_1\}$ , the differential inclusion

$$\begin{cases} \nabla u \in K & \text{in } \Omega \\ u(x) = Fx & \text{on } \partial\Omega \,. \end{cases}$$

has Lipschitz solutions.

#### 1 Introduction

The direct method in the calculus of variations is a powerful tool to prove the existence of minimizers for variational integrals that are lower semicontinuous in some class of admissible functions  $\mathcal{A}$ . In the context of nonlinear elasticity, the total energy of the system is typically modeled by

$$I(u) = \int_{\Omega} W(\nabla u) \, \mathrm{d}x$$

where  $\Omega \subset \mathbb{R}^3$  is the reference configuration,  $u:\Omega \to \mathbb{R}^3$  the elastic deformation, and  $W:\mathbb{M}^{3\times 3} \to \mathbb{R}$  the free energy density which depends

only on the deformation gradient  $\nabla u$ . We may assume that  $W \geq 0$  with  $K = \{X : W(X) = 0\} \neq \emptyset$  and that W satisfies a p-growth condition of the form  $c_1|X|^p - c_2 \leq W(X) \leq c_3(1+|X|^p)$  with p > 1 and  $c_1, c_3 > 0$ ; the natural space of admissible functions is then a subspace of the Sobolev space  $W^{1,p}(\Omega;\mathbb{R}^3)$  subject to suitable displacement and traction boundary conditions. In this setting, the direct method is applicable if I is weakly lower semicontinuous in  $W^{1,p}$  and Morreys [16] fundamental theorem states that I is weakly lower semicontinuous if and only if W is quasiconvex in the sense that

$$\int_{U} W(F) \, \mathrm{d}x \le \int_{U} W(F + \nabla \phi) \, \mathrm{d}x$$

for all  $F \in \mathbb{M}^{3\times 3}$ , for all  $\phi \in C_0^{\infty}(U; \mathbb{R}^3)$ , and for all open and bounded sets U.

In this note we are interested in variational models for phase transformations in solids in the spirit of [2, 3, 5] for which the energy fails to be quasiconvex in the sense of Morrey. The fact that the direct method based on quasiconvexity of W and lower semicontinuity of I cannot be applied does not imply that the variational problem does not have minimizers. In fact, several methods based on Gromov's idea of convex integration or on Baire's category theorem have been developed that allow one to establish the existence of solutions to the partial differential inclusion

$$\nabla u \in K$$
 a.e.,

which are automatically minimizers of I(u), see e.g. [7, 8, 13, 14, 18, 20, 17, 15] and the references therein. In the case of affine boundary conditions u(x) = Fx on  $\partial\Omega$ , this method works if the matrix F belongs to a certain semiconvex hull of K, the rank-one convex hull  $K^{\rm rc}$ , and  $K^{\rm rc}$  satisfies an additional geometric condition, see Section 2 for more information. This approach is very powerful in its generality, but few explicit examples are known in the literature, see in particular Problem 17 in [1]. In [18] existence of solutions for the two-well problem in two dimensions was obtained. This paper presents the first application to a multi-well problem with a discrete point group in three dimensions and with physical relevance; for a related case with continuous symmetry see [6, 9].

Assume for definiteness that the energy density W describes the tetragonal phase of a material that undergoes a cubic to tetragonal phase transformation, such as InTl or NiAl. In this case the zero set K of W is given

by

$$K = \bigcup_{i=1}^{3} SO(3) \left( \lambda^{2} e_{i} \otimes e_{i} + \frac{1}{\lambda} \left( \operatorname{Id} - e_{i} \otimes e_{i} \right) \right)$$
 (1.1)

where  $\{e_1, e_2, e_3\}$  is the standard basis in  $\mathbb{R}^3$ ,  $\lambda > 1$ , and SO(3) the group of proper rotations, i.e., of all matrices  $Q \in \mathbb{M}^{3\times 3}$  with  $Q^TQ = \mathrm{Id}$  and  $\det Q = 1$ . More generally we consider the set K given by

$$K = \bigcup_{i=1}^{6} SO(3)U_i \tag{1.2}$$

where  $U_1 = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$  with  $0 < \lambda_1 \le \lambda_2 \le \lambda_3$  and where at least one inequality is strict. The remaining matrices  $U_2, \ldots, U_6$  are given by the permutations of the three eigenvalues on the diagonal. For simplicity we assume that  $\lambda_1 \lambda_2 \lambda_3 = 1$ .

Our main result is the following existence theorem, which provides a partial answer to a question raised by Ball [1, Problem 17] and discussed in the lower part of page 40 there.

**Theorem 1.1.** Let K be as in (1.2), and let  $\Omega \subset \mathbb{R}^3$  be a bounded domain. Then there is a  $\rho > 0$  such that for all  $v \in C^{1,\alpha}(\Omega; \mathbb{R}^3)$  with

$$\nabla v \in B_{\rho}(\mathrm{Id}) \cap \{X : \det X = 1\} \quad everywhere$$
 (1.3)

there exists a Lipschitz solution to the partial differential relation

$$\begin{cases} \nabla u \in K & \text{in } \Omega, \\ u = v & \text{on } \partial \Omega. \end{cases}$$

Moreover, u can be obtained arbitrarily close to v, in the supremum norm.

It is clear that any solution u given in Theorem 1.1 is a minimizer of I. Concerning the regularity of the solutions, the rigidity results in [12] imply that  $\nabla u$  is not a function of bounded variation if K is as in (1.1). This result is a generalization of the corresponding statement in two dimensions in [11]. This implies that these ground states have necessarily infinite surface energy in the sense that the area of the phase boundaries, i.e., the perimeter of the sets  $E_i = \{x \in \Omega : \nabla u(x) \in SO(3)U_i\}$ , is infinite. Every solution with finite

surface area is necessarily locally a function of one variable, also referred to as a simple laminate, which cannot have affine boundary conditions unless  $F \in K$ .

The proof of Theorem 1.1 uses the approach by Müller and Šverák [18], who have extended Gromov's method of convex integration to the case of Lipschitz mappings with constraints on the determinant, together with constructions which are related to those in [10]. The key difficulty is that the rank-one convex hulls of the sets K in (1.1) and (1.2) are not explicitly known. In [4] it was shown that the identity belongs to  $K^{\rm rc}$ . In [10] the hull was shown to be eight-dimensional, and it was shown that a relatively open neighbourhood of the identity matrix Id, with radius scaling quadratically in  $\lambda_3 - \lambda_1$ , is contained in  $K^{\rm rc}$ . However, this does not suffice in order to construct solutions since it does not deliver an in-approximation, see Section 2. The main step in the proof of Theorem 1.1 is to show that there are matrices  $F \in K^{\rm rc}$  arbitrarily close to K for which an open neighbourhood is also contained in  $K^{\rm rc}$ . Once this statement is verified by an explicit construction, an in-approximation of K can easily be obtained. The convex integration approach of [18] provides the existence.

### 2 Preliminaries

A function  $f: \mathbb{M}^{m \times n} \to \mathbb{R}$  is said to be rank-one convex if  $t \mapsto f(F + tR)$  is convex in t for all  $F \in \mathbb{M}^{m \times n}$  and all  $R \in \mathbb{M}^{m \times n}$  with  $\operatorname{rank}(R) = 1$ . The rank-one convex hull  $K^{\operatorname{rc}}$  of a compact set  $K \subset \mathbb{M}^{m \times n}$  is the set of all matrices F that cannot be separated from K by rank-one convex functions,

$$K^{\mathrm{rc}} = \big\{ F : f(F) \leq \sup_{X \in K} f(X) \text{ for all } f \text{ rank-one convex} \big\}.$$

It follows from the definition that for  $A, B \in K$  with rank(A - B) = 1 the entire segment

$$[A, B] = \{\lambda A + (1 - \lambda)B, \lambda \in [0, 1]\}$$

is contained in  $K^{\text{rc}}$ . To iterate this construction, we define  $K^{(0)}=K$  and

$$K^{(i+1)} = K^{(i)} \cup \{ [A, B] : A, B \in K^{(i)}, \operatorname{rank}(A - B) = 1 \}.$$

Matrices in  $K^{(i)}$  are also referred to as averages of *i*th order laminates. The lamination convex hull  $K^{lc}$  is the infinite union

$$K^{\mathrm{lc}} = \bigcup_{i=1}^{\infty} K^{(i)}.$$

The proof of Theorem 1.1 is based on the construction of a large subset of  $K^{\rm lc}$  using this iterated construction. However, in general the rank-one convex hull of a set K cannot be obtained through this process and the inclusion  $K^{\rm lc} \subset K^{\rm rc}$  may be strict. It is an open problem to find the rank-one convex hulls for the sets (1.1) and (1.2) and to decide whether they can be determined by taking finitely many convex combinations of matrices along rank-one lines.

Following [18] we define  $\Sigma = \{X \in \mathbb{M}^{n \times n} : \det X = 1\}$ . Suppose that  $K \subset \Sigma$ . Then a sequence  $\mathcal{U}_i \subset \Sigma$  is an in-approximation of K in  $\Sigma$  if the sets  $\mathcal{U}_i$  are open in  $\Sigma$  and if the following three conditions are satisfied:

- i) the  $\mathcal{U}_i$  are uniformly bounded;
- ii)  $\mathcal{U}_i \subset (\mathcal{U}_{i+1})^{\mathrm{rc}};$
- iii)  $\mathcal{U}_i \to K$  in the following sense: if  $F_i \in \mathcal{U}_i$  and  $F_i \to F$ , then  $F \in K$ .

In this situation the following existence result holds.

**Theorem 2.1** (Theorem 1.3 in [18]). Suppose that  $\mathcal{U}_i$  is an in-approximation for the compact set  $K \subset \Sigma$ , and that  $v \in C^{1,\alpha}(\Omega; \mathbb{R}^n)$  with  $\nabla v \in \mathcal{U}_1$  in  $\Omega$ . Then there exists a Lipschitz map  $u \in W^{1,\infty}(\Omega; \mathbb{R}^n)$  with

$$\nabla u \in K$$
 a.e. in  $\Omega$ ,  
 $u = v$  on  $\partial \Omega$ .

In view of this result the key step in the proof of Theorem 1.1 is the construction of an in-approximation. This is accomplished in the next section.

## 3 Construction of an in-approximation

We start by recalling a result on the two-well problem in two dimensions.

**Lemma 3.1.** *Let* s, t > 0,

$$V_1 = \begin{pmatrix} s & 0 \\ 0 & t \end{pmatrix}$$
,  $V_2 = \begin{pmatrix} t & 0 \\ 0 & s \end{pmatrix}$ .

Then matrices X of the form X = QF, for  $Q \in SO(2)$ ,

$$F = \begin{pmatrix} s' & a \\ 0 & t' \end{pmatrix} \,,$$

are in the lamination convex hull of  $SO(2)V_1 \cup SO(2)V_2$  if and only if

$$s't' = st$$
,  $2|s'||a| + a^2 \le |s - t|^2 - |s' - t'|^2$ .

*Proof.* This follows from the characterization of the semiconvex hulls for the two-well problem in two dimensions,

$$(SO(2)V_1 \cup SO(2)V_2)^{lc} = \{F : \det F = \det V_1, |F(e_1 \pm e_2)| \le |V_1(e_1 \pm e_2)| \}$$
  
see [3, 19].

**Lemma 3.2.** Let  $\alpha > 0$  and  $\lambda_i \in [1/\alpha, \alpha]$ ,  $1 \leq i \leq n$ . Then, for any  $F \in \mathbb{M}^{n \times n}$  there is  $Q \in SO(n)$  such that QF is upper triangular, and

$$|Q - \operatorname{Id}| \le C|F - \operatorname{diag}(\{\lambda_i\})|$$
.

Here C depends only on  $\alpha$  and n.

Proof. It suffices to prove the statement if the right-hand side is small, in particular we can suppose F to have full rank with "nearly" orthogonal columns. For simplicity we write  $F_i = Fe_i$  for the ith column in F. There is nothing to prove for n = 1. Assume the statement holds for some  $n - 1 \ge 0$ . Then it suffices to show that we can find Q close to the identity, which rotates  $F_1$  onto  $e_1$ . To do this, apply the Gram-Schmidt orthogonalization algorithm to  $(F_1, \ldots, F_n)$ , to generate an orthonormal set  $f_1, \ldots, f_n$ , with  $f_1$  parallel to  $F_1$ . It is clear that  $|F_i - \lambda_i f_i| \le C_n |F - \text{diag}(\{\lambda_i\})|$ , and the same holds for  $|e_i - f_i|$ . Set  $Q = \sum e_i \otimes f_i$ . This concludes the proof.

**Proposition 3.3.** Let  $\alpha > 0$ ,  $0 < 1/\alpha < \lambda_1 \le \lambda_2 \le \lambda_3 < \alpha$ , and let  $U_1, \ldots, U_6$  be the six diagonal matrices with the six permutations of  $\lambda_1, \lambda_2, \lambda_3$ 

on the diagonal, not necessarily distinct. Let  $\varepsilon > 0$ , and suppose that  $\mu_i$ , i = 1, 2, 3, satisfy

$$\mu_1\mu_2\mu_3 = \lambda_1\lambda_2\lambda_3$$
,  $\lambda_1 \le \mu_1 \le \mu_2 \le \mu_3 \le \lambda_3$ 

with

$$\lambda_1 + \varepsilon \le \mu_i \le \lambda_3 - \varepsilon$$
,  $i = 1, 2, 3$ ,

and

$$|\mu_i - \lambda_i| \le \alpha \varepsilon, \quad i = 1, 2, 3,$$

Then there exists a constant C which depends only on  $\alpha$ , such that

$$B_{\eta}(\operatorname{diag}(\mu_1, \mu_2, \mu_3)) \cap \{F : \det F = \lambda_1 \lambda_2 \lambda_3\} \subset \left(\bigcup_{i=1}^6 \operatorname{SO}(3)U_i\right)^{\operatorname{lc}}$$

for all  $\eta \leq C\varepsilon^2$ . If additionally

$$\min\left(\lambda_3 - \lambda_2, \lambda_2 - \lambda_1\right) \ge \frac{1}{\alpha} \tag{3.1}$$

then the same holds for all  $\eta \leq C\varepsilon$ .

Proof. In this proof  $\alpha$  denotes the (fixed) constant entering the statement, C a generic constant which might change from line to line and depends only on  $\alpha$ . Let  $V_0 = \operatorname{diag}(\mu_1, \mu_2, \mu_3)$ ,  $F \in B_{\eta}(V_0) \cap \{X : \det X = \lambda_1 \lambda_2 \lambda_3\}$ , and  $K = \bigcup_{i=1}^6 \operatorname{SO}(3)U_i$ . By Lemma 3.2, there exists a  $Q \in \operatorname{SO}(3)$  such that F' = QF is upper triangular and  $|F' - V_0| \leq C\eta$ . By invariance of  $K^{\operatorname{lc}}$  under rotations it suffices to show that  $F' \in K^{\operatorname{lc}}$ .

We follow [10] and write

$$F' = \begin{pmatrix} X & u \\ \hline 0 & 0 & \delta \end{pmatrix}, \qquad X \in \mathbb{M}^{2 \times 2}, \ u \in \mathbb{R}^2, \ \delta \in \mathbb{R}.$$

The goal of the next few steps is to write F' as an average along rank-one lines of matrices which have a special structure and for which one can show by an explicity construction that they are contained in  $K^{lc}$ .

**Step 1.** Let 
$$u_1 = X_2 = Xe_2$$
,  $u_2 = X_1 = Xe_1$ , and

$$Y^i = X - t_i u_i \otimes e_i$$

for  $t_i \in \mathbb{R}$  to be chosen below. We observe that, for all values of  $t_i$ ,

$$\det Y^i = \det X \,, \qquad i = 1, 2 \,.$$

Indeed,  $\det(X - tu_1 \otimes e_1) = (\det X) \det(\operatorname{Id} - te_2 \otimes e_1) = \det X$ . We choose  $t_i \in \mathbb{R}$  so that  $Y^i = QD$ , with  $Q \in SO(2)$  and D diagonal. This corresponds to the requirement that the two columns of  $Y^i$  be orthogonal, i.e.

$$0 = Y_1^1 \cdot Y_2^1 = (X_1 - t_1 u_1) \cdot X_2 = (X_1 - t_1 X_2) \cdot X_2,$$

and analogously for  $Y^2$ . Therefore we choose

$$t_1 = \frac{X_1 \cdot X_2}{|X_2|^2}, \qquad t_2 = \frac{X_1 \cdot X_2}{|X_1|^2}.$$

Since  $|X - \operatorname{diag}(\mu_1, \mu_2)| \leq C\eta$ , we have  $|t_1| + |t_2| \leq C\eta$ . This implies that the angle between  $u_1$  and  $u_2$  is larger than 1/C, hence we can write the vector u in the form

$$u = \gamma_1 u_1 + \gamma_2 u_2$$

with  $|\gamma_1| + |\gamma_2| \leq C\eta$ . We further define

$$s_i = \operatorname{sgn}(\gamma_i)(|\gamma_1| + |\gamma_2|),$$

so that

$$u = \frac{|\gamma_1|}{|\gamma_1| + |\gamma_2|} s_1 u_1 + \frac{|\gamma_2|}{|\gamma_1| + |\gamma_2|} s_2 u_2.$$

Therefore the matrix F' is the average of a laminate supported on

$$F^{1} = \begin{pmatrix} X & s_{1}u_{1} \\ \hline 0 & 0 & \delta \end{pmatrix}, \qquad F^{2} = \begin{pmatrix} X & s_{2}u_{2} \\ \hline 0 & 0 & \delta \end{pmatrix}.$$

Using the rank-one direction  $u_i \otimes (t_i e_i - s_i e_3)$  we see that  $F^i$  is the average of a laminate supported on

$$P^{i} = \begin{pmatrix} X - t_{i}u_{i} \otimes e_{i} & 2s_{i}u_{i} \\ \hline 0 & 0 & \delta \end{pmatrix}, \qquad \widetilde{P}^{i} = \begin{pmatrix} X + t_{i}u_{i} \otimes e_{i} & 0 \\ \hline 0 & 0 & \delta \end{pmatrix},$$

which obey  $|P^i - V_0| + |\widetilde{P}^i - V_0| \leq C\eta$ . Notice that the first two columns of each of the matrices  $P^i$  are orthogonal, and that the  $\widetilde{P}^i$ 's are block-diagonal. These two matrices are dealt with in the following two steps.

**Step 2.** We next consider the matrices  $P^i$ , and we write P for simplicity in the sequel. Let  $Q \in SO(3)$  be such that QP is upper triangular. By Lemma 3.2 we have  $|QP - V_0| \leq C\eta$ . Since the first two columns of P are orthogonal,

$$QP = \begin{pmatrix} \mu_1' & 0 & a \\ 0 & \mu_2' & b \\ 0 & 0 & \mu_3' \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \mu_1' & 0 & 2a \\ 0 & \mu_2' & 0 \\ 0 & 0 & \mu_3' \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \mu_1' & 0 & 0 \\ 0 & \mu_2' & 2b \\ 0 & 0 & \mu_3' \end{pmatrix} .$$

Here,  $|\mu'_i - \mu_i| + |a| + |b| \le C\eta$ . Consider the second of the two matrices on the right-hand side, call it  $R^2$ . We apply Lemma 3.1 to the  $(2,3) \times (2,3)$  block. Let s,t>0 be such that

$$st = \mu_2' \mu_3', \qquad \lambda_1 \le s \le t \le \lambda_3,$$

and |s-t| is maximal. This implies that either  $s=\lambda_1$ , or  $t=\lambda_3$ , or both. We observe that, for i=2,3,

$$\mu_i' - \lambda_1 \ge \mu_i - \lambda_1 - |\mu_i' - \mu_i| \ge \varepsilon - C\eta$$

and

$$\lambda_3 - \mu_i' \ge \lambda_3 - \mu_i - |\mu_i' - \mu_i| \ge \varepsilon - C\eta$$
.

Choose  $\eta$  so small, that both terms are larger than  $\varepsilon/2$ . Then, it follows that

$$|s-t| \ge |\mu_2' - \mu_3'| + \frac{1}{2}\varepsilon.$$

By Lemma 3.1 the matrix  $R^2$  is in the lamination convex hull of

$$SO(3)\operatorname{diag}(\mu'_1, s, t) \cup SO(3)\operatorname{diag}(\mu'_1, t, s) \tag{3.2}$$

provided that

$$C|a| \le (s-t)^2 - (\mu_2' - \mu_3')^2$$
. (3.3)

In turn,

$$(s-t)^2 - (\mu_2' - \mu_3')^2 \ge \varepsilon |\mu_2' - \mu_3'| + \frac{1}{4}\varepsilon^2.$$

Since  $|a| \leq C\eta$ , condition (3.3) is always verified if  $\eta \leq \varepsilon^2/C$ . If (3.1) additionally holds, then also  $|\mu_2' - \mu_3'| \geq 1/C$ , and it suffices to take  $\eta \leq \varepsilon/C$ .

Finally, the matrices in (3.2) are in the lamination convex hull of  $\bigcup_{i=1}^6 \mathrm{SO}(3)U_i$ . Indeed, assume  $s = \lambda_1$  (the case  $t = \lambda_3$  is analogous). Then,  $\mu'_1 t = \lambda_2 \lambda_3$ , and since  $t \leq \lambda_3$ , we have  $\mu'_1 \geq \lambda_2$ . Another application of Lemma 3.1 (with a = 0) concludes the proof of Step 2.

**Step 3.** We consider  $\widetilde{P}^i$ , and call it  $\widetilde{P}$  for simplicity. Let  $Q \in SO(3)$  be such that  $Q\widetilde{P}$  is upper triangular, and  $|Q - \operatorname{Id}| \leq C\eta$ . Then,

$$Q\widetilde{P} = \begin{pmatrix} \mu_1' & a & 0\\ 0 & \mu_2' & 0\\ 0 & 0 & \mu_3' \end{pmatrix}$$

and we can treat it as  $R^2$  above.

Proof of Theorem 1.1. If  $\lambda_2 \leq (\lambda_1 + \lambda_3)/2$  we set, for  $k \in \mathbb{N}$ ,

$$\mu_1^k = \lambda_1 (1 + 2^{-k}), \qquad \mu_2^k = \lambda_2 (1 + 2^{-k}), \qquad \mu_3^k = \lambda_3 (1 + 2^{-k})^{-2};$$

if instead  $\lambda_2 > (\lambda_1 + \lambda_3)/2$  we take

$$\mu_1^k = \lambda_1 (1 + 2^{-k}), \qquad \mu_2^k = \lambda_2 (1 + 2^{-k})^{-1/2}, \qquad \mu_3^k = \lambda_3 (1 + 2^{-k})^{-1/2}.$$

In both cases, for large enough k (say,  $k \ge k_0$ ), we have

$$\lambda_1 + c_1 2^{-k} \le \mu_1^k \le \mu_2^k \le \mu_3^k \le \lambda_3 - c_1 2^{-k}$$

where  $c_1$  is constant depending on the  $\lambda_i$ , but not on k.

We define

$$K^k = \bigcup_{\sigma} SO(3) \operatorname{diag}(\mu_{\sigma(1)}^k, \mu_{\sigma(2)}^k, \mu_{\sigma(3)}^k)$$

where  $\sigma$  runs over the six permutations of the indices  $\{1,2,3\}$  and, for some  $c_* > 0$  to be chosen below,

$$\mathcal{U}^k = \{ F : \operatorname{dist}(F, K^k) \le c_* 2^{-2k} \,, \, \det F = 1 \} \qquad k \ge k_0 \,,$$

and

$$\mathcal{U}^k = (\mathcal{U}^{k_0})^{\mathrm{rc}}, \qquad 0 \le k < k_0.$$

Proposition 3.3, applied with  $\varepsilon = c_1 2^{-k}$ , guarantees that the set  $\mathcal{U}^k$  is contained in the lamination convex hull of  $K^{k+1} \subset \mathcal{U}^{k+1}$  if  $c_*$  is chosen small enough. Moreover,  $F_k \in \mathcal{U}^k$  and  $F_k \to F$  imply  $F \in K$ . Therefore the family  $\mathcal{U}^k$  is an in-approximation of K. At the same time, by Proposition 3.3 there is  $\rho > 0$  such that

$$B_{\rho}(\mathrm{Id}) \cap \{X : \det X = 1\} \subset \mathcal{U}^1 = (\mathcal{U}^{k_0})^{\mathrm{rc}}.$$

The result follows from Theorem 2.1.

We finally show that if (3.1) holds then there exists an r > 0 such that  $K^{lc}$  contains the intersection of a full-dimensional half cone centered in  $U_1$  with the set  $\{X : \det X = 1\} \cap B(U_1, r)$ . In general, we only obtain a quadratic cusp.

Corollary 3.4. Let  $0 < \lambda_1 \le \lambda_2 \le \lambda_3$ , with  $\lambda_1 \ne \lambda_3$ ,  $\lambda_1 \lambda_2 \lambda_3 = 1$ , and let  $U_1 = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$ , and  $U_2, \ldots, U_6$  be obtained via permutation as above. For  $t \in [0, 1]$ , let  $V(t) = \operatorname{diag}(e^{\sigma_1 t}, e^{\sigma_2 t}, e^{\sigma_3 t})$ , where  $\sigma_i = \ln \lambda_i$ . Then there is a constant C such that

$$B_{r(t)}(V(t)) \cap \{F : \det F = 1\} \subset \left(\bigcup_{i=1}^{6} \operatorname{SO}(3)U_{i}\right)^{\operatorname{lc}},$$

where  $r(t) = |V(t) - U_1|^2/C$ . If additionally

$$\min\left(\lambda_3 - \lambda_2, \lambda_2 - \lambda_1\right) \ge \frac{1}{\alpha_*} \tag{3.4}$$

holds, then the same is true with  $r(t) = |V(t) - U_1|/C$ . The constants depend on  $\{\lambda_i\}$  and  $\alpha_*$  (in the second case).

*Proof.* Let  $\mu_i(t) = e^{\sigma_i t}$ . By Proposition 3.3 there is a ball  $B_{1/C}(\mathrm{Id})$  contained in the hull. Therefore it suffices to prove the statement for  $t \geq 1/C$ . Then, if (3.4) holds, then it holds uniformly in t, in the sense that

$$\min (\mu_3 - \mu_2, \mu_2 - \mu_1)(t) \ge \frac{1}{\alpha'_{+}}, \qquad \frac{1}{C} \le t \le 1$$

for some  $\alpha'_* > 0$ . Let

$$\varepsilon(t) = \min(|\mu_1(t) - \lambda_1|, |\mu_3(t) - \lambda_3|).$$

Clearly  $(1-t)/C \le \varepsilon(t) \le C(1-t)$  on [0,1]. We define

$$c_0 = \max \left\{ \frac{|\mu_i(t) - \lambda_i|}{\varepsilon(t)} : i \in \{1, 2, 3\}, t \in [0, 1] \right\}.$$

It is easy to see that  $c_0$  is finite. For each t, we apply Proposition 3.3 with  $\varepsilon = \varepsilon(t)$ , and  $\mu_i = \mu(t)$ , and  $\alpha = \max(c_0, \lambda_3, 1/\lambda_1)$  in the first case,  $\alpha = \max(c_0, \lambda_3, 1/\lambda_1, \alpha'_*)$  if (3.4) holds. The constant  $\alpha$ , and hence C, does not depend on t.

We obtain that, for each t,

$$B_{\eta(t)}(V(t)) \cap \{F : \det F = 1\} \subset \left(\bigcup_{i=1}^{6} \operatorname{SO}(3)U_{i}\right)^{\operatorname{lc}},$$

for  $\eta(t) = \varepsilon^2(t)/C$ , and for  $\eta(t)\varepsilon(t)/C$  if (3.4) holds. The conclusion follows, since  $|V(t) - U_1| \le C\varepsilon(t)$ .

Using a compactness argument and constructing an in-approximation with a suitably large  $\mathcal{U}^0$  one easily establishes the following generalization.

**Corollary 3.5.** The result of Theorem 1.1 holds also if (1.3) is replaced by

$$\nabla v \in \bigcup_{t \in [0,1)} \bigcup_{j=1}^{6} B_{r(t)}(V_j(t)) \cap \{F : \det F = 1\} \quad on \ \bar{\Omega},$$

where  $V_j$  is obtained from V (defined as in Corollary 3.4) by permutation of the entries on the diagonal, and  $r(t) = (1-t)^2/C$ . If additionally (3.1) holds, then the same is true with r(t) = (1-t)/C.

We finally observe that the quadratic estimate given in [10] for the size of the neighborhood of the identity contained in the rank-one hull of K is optimal. Even more, we show that a quadratic inner radius is optimal also for the convex hull.

**Lemma 3.6.** Let  $\lambda_1, \lambda_2, \lambda_3 > 0$ ,  $\lambda_1 \lambda_2 \lambda_3 = 1$ , and K be as in (1.2). Then for any  $|t| \geq c \max_{ij} |\lambda_i - \lambda_j|^2$  the matrix

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & t \\ 0 & 0 & 1 \end{pmatrix} \tag{3.5}$$

is not in the convex hull of K. Here c is a universal constant.

*Proof.* Let  $\varepsilon = \max_{ij} |\lambda_i - \lambda_j|$ . The result is trivial for large  $\varepsilon$ , hence it suffices to focus on small  $\varepsilon$ . In this regime, the lemma follows by testing the matrix with the vectors  $v_{\pm} = (1, \pm 1, 1)$ . Precisely, for any matrix  $F \in K$  we have

$$|Fv_{+}|^{2} = |Fv_{-}|^{2} = \sum_{i=1}^{3} \lambda_{i}^{2} = \sum_{i=1}^{3} \left[ 1 + 2(\lambda_{i} - 1) + (\lambda_{i} - 1)^{2} \right]$$

$$\leq 3 + 2 \sum_{i=1}^{3} (\lambda_{i} - 1) + 3\varepsilon^{2}.$$

An analogous expansion of the determinant gives

$$1 = \lambda_1 \lambda_2 \lambda_3 = 1 + \sum_{i=1}^{3} (\lambda_i - 1) + O(\varepsilon^2).$$

Therefore the linear term cancels, and the foregoing inequality simplifies to

$$|Fv_+|^2 \le 3 + c\varepsilon^2$$
,  $\forall F \in K$ .

Let now G be the matrix given in the statement. A simple calculation shows that

$$|Gv_{\pm}|^2 = 2 + (1 \pm t)^2 = 3 \pm 2t + t^2$$
.

We conclude that  $|t| \leq c\varepsilon^2$ .

## Acknowledgements

The work of SC was supported by the Deutsche Forschungsgemeinschaft through the Schwerpunktprogramm 1095 Analysis, Modeling and Simulation of Multiscale Problems. The work of GD was supported by the NSF through grants DMS0405853 and DMS0104118. The work of BK was supported by the EU programme MRTN-CT-2004-505226.

#### References

- [1] J. M. Ball, *Some open problems in elasticity*, Geometry, mechanics, and dynamics (P. Newton, P. Holmes, and A. Weinstein, eds.), Springer, New York, 2002, pp. 3–59.
- [2] J. M. Ball and R. D. James, Fine phase mixtures as minimizers of the energy, Arch. Ration. Mech. Analysis **100** (1987), 13–52.
- [3] \_\_\_\_\_, Proposed experimental tests of a theory of fine microstructure and the two-well problem, Phil. Trans. R. Soc. Lond. A **338** (1992), 389–450.
- [4] K. Bhattacharya, Self-accommodation in martensite, Arch. Rat. Mech. Anal. 120 (1992), 201–244.

- [5] M. Chipot and D. Kinderlehrer, *Equilibrium configurations of crystals*, Arch. Rational Mech. Anal. **103** (1988), 237–277.
- [6] S. Conti, A. DeSimone, G. Dolzmann, S. Müller, and F. Otto, *Multiscale modeling of materials the role of analysis*, Trends in Nonlinear Analysis (Heidelberg) (M. Kirkilionis, S. Krömker, R. Rannacher, and F. Tomi, eds.), Springer, 2002, pp. 375–408.
- [7] B. Dacorogna and P. Marcellini, General existence theorems for Hamilton-Jacobi equations in the scalar and vectorial cases, Acta Math. 178 (1997), 1–37.
- [8] B. Dacorogna and P. Marcellini, *Implicit partial differential equations*, Progress in Nonlinear Differential Equations and their Applications, 37, Birkhäuser, 1999.
- [9] A. DeSimone and G. Dolzmann, Macroscopic response of nematic elastomers via relaxation of a class of SO(3)-invariant energies, Arch. Rat. Mech. Anal. **161** (2002), 181–204.
- [10] G. Dolzmann and B. Kirchheim, Liquid-like behavior of shape memory alloys, C. R. Math. Acad. Sci. Paris 336 (2003), 441–446.
- [11] G. Dolzmann and S. Müller, *Microstructures with finite surface energy:* the two-well problem, Arch. Rational Mech. Anal. **132** (1995), 101–141.
- [12] B. Kirchheim, Lipschitz minimizers of the 3-well problem having gradients of bounded variation, Preprint 12, Max Planck Institute for Mathematics in the Sciences, Leipzig, 1998.
- [13] \_\_\_\_\_, Deformations with finitely many gradients and stability of quasiconvex hulls, C. R. Acad. Sci. Paris Sér. I Math. **332** (2001), 289–294.
- [14] \_\_\_\_\_\_, Rigidity and geometry of microstructures, MPI-MIS Lecture notes 16, 2002.
- [15] B. Kirchheim, S. Müller, and V. Šverák, Studying nonlinear pde by geometry in matrix space, Geometric analysis and nonlinear partial differential equations (S. Hildebrandt and H. Karcher, eds.), Springer-Verlag, 2003, pp. 347–395.

- [16] C. B. Morrey, Quasi-convexity and the lower semicontinuity of multiple integrals, Pacific J. Math. 2 (1952), 25–53.
- [17] S. Müller and M. A. Sychev, Optimal existence theorems for nonhomogeneous differential inclusions, J. Funct. Anal. 181 (2001), no. 2, 447–475.
- [18] S. Müller and V. Šverák, Convex integration with constraints and applications to phase transitions and partial differential equations, J. Eur. Math. Soc. (JEMS) 1 (1999), 393–442.
- [19] V. Šverák, On the problem of two wells, Microstructure and phase transition, IMA Vol. Math. Appl., vol. 54, Springer, New York, 1993, pp. 183–189.
- [20] M. A. Sychev, Comparing two methods of resolving homogeneous differential inclusions, Calc. Var. Part. Diff. Eq. 13 (2001), 213–229.