RELAXATION OF A MODEL ENERGY FOR THE CUBIC TO TETRAGONAL PHASE TRANSFORMATION IN TWO DIMENSIONS

SERGIO CONTI AND GEORG DOLZMANN

Abstract. We consider a two-dimensional problem in nonlinear elasticity which corresponds to the cubic-to-tetragonal phase transformation. Our model is frame invariant and the energy density is given by the squared distance from two potential wells. We obtain the quasiconvex envelope of the energy density and therefore the relaxation of the variational problem. Our result includes the constraint of positive determinant.

1. Introduction and statement of the result

Fully nonlinear models for the description of solid to solid phase transformations within the mathematical framework of elasticity theory have attracted a lot of attention in the past twenty five years, starting with the seminal papers [2, 3, 6]. One of the questions of interest is the characterization of macroscopic models which capture the essential features of the mechanical behavior of a given system without resolving all the structures which may develop on small scales. In this context, the theory of relaxation and generalizations of the convex hulls of functions and sets play an important role. The most important notion of convexity is the notion of quasiconvexity in the sense of Morrey [26] and the related definitions of quasiconvex envelopes of functions and hulls of sets [14, 29, 27].

In this note we focus on a model for a specific solid to solid phase transformation of austenite-martensite type, namely the cubic to tetragonal phase transformation. Suppose that the energy of such a material in the martensitic or high temperature phase is characterized by an energy density \( W_{3d} \) which we may assume to be nonnegative with \( K_{3d} = W_{3d}^{-1}(0) \neq \emptyset \). It follows from the invariance under change in observer and the symmetry of the underlying point group that in the three-dimensional setting

\[
K_{3d} = \bigcup_{i=1}^{3} SO(3)U_i, \quad U_i = \frac{1}{\lambda} I_3 + (\lambda^2 - \frac{1}{\lambda}) e_i \otimes e_i,
\]

where \( \lambda \in (0, \infty) \), and where \((e_i)_{i=1,...,n}\) denotes for \( n \in \mathbb{N} \) the canonical basis in \( \mathbb{R}^n \), \( I_n \) the \( n \times n \) identity matrix, and \( SO(n) \) the group of proper rotations of \( \mathbb{R}^n \). We chose \( \det U_i = 1 \) since in most materials the phase transformation occurs without significant change of volume. A basic model energy in this situation is given by

\[
W_{3d}(F) = \text{dist}^2(F, K_{3d}) = \min_{i=1,2,3} \min_{Q \in SO(3)} |F - QU_i|^2.
\]

To the best of our knowledge, both the computation of the full relaxation \( W_{3d}^{qc} \) of the energy density and the computation of the quasiconvex hull \( K_{3d}^{qc} \) of the set of its minimizers \( K_{3d} \) are open problems. Partial results were obtained in [4, 17, 10].

Considerable progress has been achieved, however, in the case of two potential wells. The quasiconvex hull of two wells in three dimensions, i.e., of the set \( \tilde{K}_{3d} = SO(3)U_1 \cup SO(3)U_2 \),
was computed in [3], some generalizations were analyzed in [18, 25], and various proofs were
given for the characterization of the quasiconvex hull of two wells in two dimensions, even in the
more general case of two wells with different determinant, i.e., for the set $K = SO(2)I_2 \cup
SO(2)\text{diag}(\lambda, \mu)$ with $\lambda, \mu > 0$, see, e.g., [32, 27, 10]. The linear case has been analyzed, also for
more general energies, in [22, 24, 21, 28].

In this paper we provide an explicit relaxation formula for the analogue of (1.1) in the corre-
sponding two-dimensional model, namely,

\begin{equation}
W(F) = \text{dist}^2(F, K) + \theta(\det F),
\end{equation}

where $\theta : \mathbb{R} \to [0, \infty]$ is convex and lower semicontinuous and

\begin{equation}
K = SO(2)U_1 \cup SO(2)U_2,
\end{equation}

where $U_1 = \begin{pmatrix} \lambda & 0 \\ 0 & 1/\lambda \end{pmatrix}$, $U_2 = \begin{pmatrix} 1/\lambda & 0 \\ 0 & \lambda \end{pmatrix}$,

for some fixed $\lambda > 1$. The function $\theta$ permits to incorporate easily the constraint that the
determinant of the deformation gradient $F$ has to be positive in order to rule out interpenetration
of matter. Here and in the following, $\text{dist}(\cdot)$ denotes the Euclidean distance.

One important ingredient in the proof is to view the energy in the appropriate variables.
Motivated by the formula for $\overline{K}_c$ in [3] we set

\begin{equation}
v = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad w = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}
\end{equation}

and define for $F \in \mathbb{R}^{2 \times 2}$ the coordinates

\begin{equation}
x(F) = |Fv|, \quad y(F) = |Fw|, \quad d(F) = \det F.
\end{equation}

The main theorem can now be stated as follows.

**Theorem 1.1.** Let $\lambda > 1$, $K \subset \mathbb{R}^{2 \times 2}$ be given by (1.3), let $O = \{ (x, y, d) \in \mathbb{R}^3, x, y > 0, xy > |d| \}$, define the functions $A, g : \overline{O} \to \mathbb{R}$ by

\begin{equation}
A(x, y, d) = (x^2 + y^2) \frac{|U_1|^2}{2} + (\lambda^2 - \frac{1}{\lambda^2}) \sqrt{x^2y^2 - d^2} + 2d,
\end{equation}

\begin{equation}
g(x, y, d) = x^2 + y^2 + |U_1|^2 - 2 \sqrt{A(x, y, d)},
\end{equation}

and, for a given convex and lower semicontinuous function $\theta : \mathbb{R} \to [0, \infty]$, the energy density $W : \mathbb{R}^{2 \times 2} \to \mathbb{R} \cup \{ \infty \}$ by (1.2).

Then $W^{qc} = W^{qc} = W^{qc}$ and the quasiconvex envelope $W^{qc}$ is given by

\begin{equation}
W^{qc}(F) = h(x(F), y(F), d(F)) + \theta(\det F),
\end{equation}

where $h : \overline{O} \to \mathbb{R}$ is defined by

\begin{equation}
h(x, y, d) = \min_{\xi \in [x, \infty), \eta \in [y, \infty)} g(\xi, \eta, d).
\end{equation}

**Remarks.**

(i) The minimum in the definition of $h$ can be computed explicitly in terms of the roots of
a polynomial equation of fourth order, see Section 3.1.

(ii) As a special case, if $\theta(t) = 0$ for $t = 1$, and $\infty$ otherwise, we obtain a result for incompressible materials.

(iii) The set $O$ is not convex.

(iv) A typical example in nonlinear elasticity is the choice of $\theta \in C^1((0, \infty))$ which satisfies
$\lim_{t \to 0} \theta(t) = \lim_{t \to \infty} \theta(t) = \infty$, for example, $\theta(t) = \log^2(t)$, in order to obtain a density
which rules out interpenetration of matter (and $\theta(t) = \infty$ for $t \leq 0$).

(v) If $\theta$ has at most linear growth, then $W$ has quadratic growth and the lower semiconvex envelope of $\int W(Du)dx$ is given by $\int W^{qc}(Du)dx$, see [13, 27]. A corresponding result incorporating constraints on the determinant of the type mentioned in (ii) and (iv) will be discussed elsewhere [9].
(vi) For \( \lambda = 1 \) our formula reduces to the well-known relaxation of the squared distance function to \( \text{SO}(2) \), as given for example in [30].

We recall that a function \( f : \mathbb{R}^{2 \times 2} \to \mathbb{R} \cup \{ \infty \} \) is said to be quasiconvex if \( f(F) \leq \int_{(0,1)^2} f(F + D\varphi) \, dx \) for all \( F \in \mathbb{R}^{2 \times 2} \) and \( \varphi \in W^{1,\infty}_0((0,1)^2; \mathbb{R}^2) \). The function \( f \) is said to be rank-one convex if for all \( F, R \in \mathbb{R}^{2 \times 2} \) with \( \text{rank}(R) = 1 \) the function \( t \to f(F + tR) \) is convex. The function \( f \) is said to be polyconvex if it can be written as \( f(F) = g(F, \det F) \) with \( g : \mathbb{R}^5 \to \mathbb{R} \cup \{ \infty \} \) convex and lower semicontinuous. The rank-one convex, quasiconvex, and polyconvex envelopes \( f^{\text{rc}} \) and \( f^{\text{pc}} \) are the largest rank-one convex, quasiconvex and polyconvex functions less than or equal to \( f \), respectively. If \( f \) is polyconvex, then it is also rank-one convex, hence \( f^{\text{pc}} \leq f^{\text{rc}} \). We refer to [14, 27] for more information on these notions of convexity and their relations. In the following we use for two vectors \( a, b \in \mathbb{R}^2 \) and two matrices \( A, B \in \mathbb{R}^{2 \times 2} \) the notation \( a \cdot b \) and \( A : B \) for the inner product in \( \mathbb{R}^2 \) and \( \mathbb{R}^{2 \times 2} \), respectively. Hence \( |A|^2 = A : A = \text{tr}(AA^T) \). Finally \( a \otimes b \in \mathbb{R}^{2 \times 2} \) is given by \((a \otimes b)_{ij} = a_i b_j \). We write \( \mathbb{R}_+ = (0, \infty) \).

2. Proof

The general strategy of the proof is to verify first that the rank-one convex and the polyconvex envelope coincide. Let \( \tilde{W} \) be the formula on the right-hand side in (1.6). In order to prove \( W^{\text{pc}} = W^{\text{rc}} = \tilde{W} \) it suffices to show that \( W^{\text{rc}} \leq \tilde{W} \leq W \) and that \( W \) is polyconvex. Then \( W^{\text{pc}} \leq W^{\text{rc}} \leq \tilde{W} \leq W^{\text{pc}} \) and therefore \( W^{\text{rc}} = W^{\text{pc}} = \tilde{W} \). The quasiconvex envelope will be discussed at the end. We divide the proof into several steps.

Step 1: \( \tilde{W} \leq W \). This follows immediately once we have shown that

\[
W(F) = g(x(F), y(F), d(F)) + \theta(\det F).
\]

In order to establish (2.1), we denote the signed singular values of a matrix \( F \in \mathbb{R}^{2 \times 2} \) by \( \lambda_i = \lambda_i(F) \) and use the convention that \( \lambda_2 \geq |\lambda_1| \geq 0 \), \( \lambda_1 \lambda_2 = \det F \). Since \( |U_1| = |U_2| \) we obtain

\[
dist^2(F, SO(2)U_1 \cup SO(2)U_2) = \min_{i=1,2} \min_{Q \in SO(2)} \|F - QU_i\|^2 \\
= |F|^2 + |U_1|^2 - 2 \max_{i=1,2} \max_{Q \in SO(2)} \langle FU_i, Q \rangle \\
= |F|^2 + |U_1|^2 - 2 \max_{i=1,2} (\lambda_2 + \lambda_1)(FU_i) \\
= |F|^2 + |U_1|^2 - 2 \max_{i=1,2} \sqrt{\|FU_i\|^2 + 2 \det F}.
\]

Moreover,

\[
|FU_1|^2 = \lambda^2 |Fe_1|^2 + \frac{1}{\lambda^2} |Fe_2|^2 = (\lambda^2 + \frac{1}{\lambda^2}) \left( |Fv|^2 + \frac{|Fw|^2}{2} \right) + (\lambda^2 - \frac{1}{\lambda^2}) Fv \cdot Fw.
\]

Since replacing \( U_1 \) by \( U_2 \) corresponds to interchanging \( \lambda \) and \( 1/\lambda \), the maximum over \( i \) is given by

\[
\max_{i=1,2} |FU_i|^2 = (\lambda^2 + \frac{1}{\lambda^2}) \frac{x^2(F) + y^2(F)}{2} + (\lambda^2 - \frac{1}{\lambda^2}) |Fv \cdot Fw|,
\]

where we used the coordinates defined in (1.4). From \( \sin^2 \phi + \cos^2 \phi = 1 \) we obtain

\[
|Fv \cdot Fw| = \sqrt{x^2(F) y^2(F) - \det^2(F)}
\]

and therefore

\[
W(F) = x^2(F) + y^2(F) + |U_1|^2 - 2 \sqrt{A(x(F), y(F), d)} + \theta(\det F),
\]

where \( A \) is given by (1.5). This establishes (2.1).
**Step 2: The upper bound** $W^{rc} \leq \tilde{W}$. This bound follows from standard arguments based on a minimization along rank-one lines which has been used in most examples for explicit relaxation results in nonlinear elasticity and plasticity, see, e.g., [1, 5, 11, 12, 13, 15, 30, 31] and the references therein.

In the following we use for $(x, y, d) \in \bar{O}$ the notation $z(x, y, d) = \sqrt{x^2y^2 - d^2}$. Note that $A$ and $g$ are continuous and nonnegative functions on $\bar{O}$. Fix a matrix $F$ and define the rank-one line $t \mapsto F_t$ by

$$F_t = F(Id + tv \otimes w).$$

Since the vectors $v$ and $w$ are orthogonal we obtain

$$d(F_t) = d(F), \quad x(F_t) = x(F) \quad \text{and} \quad y(F_t) = |Fw + tFv|.$$

If $Fv \neq 0$ then $y(F_t)$ tends to infinity for $t \to \pm \infty$ and by continuity for every $y' > y(F)$ there exist $t_- < 0 < t_+$ such that $y(F_{t_\pm}) = y'$. Then there is $\mu \in (0, 1)$ such that $F = \mu F_{t_+} + (1-\mu) F_{t_-}$, and from the convexity of $W^{rc}$ along the rank-one line $t \mapsto F_t$ and (2.1) we infer

$$(2.3) \quad W^{rc}(F) \leq g(x(F), y(F), d(F)) + \theta(\det F) \quad \text{for all} \quad y' \geq y(F).$$

If $Fv = 0$ we take instead $F_t = F + tw \otimes w$. Then $d(F_t) = d(F) = 0$, $x(F_t) = x(F) = 0$, $y(F_t) = |Fw + tw|$ tends to infinity for $t \to \pm \infty$ and (2.3) follows as above.

If one interchanges $v$ and $w$ one obtains

$$W^{rc}(F) \leq h(x(F), y(F), d(F)) + \theta(\det F)$$

where $h$ is defined in (1.7). Note that by continuity and growth the infimum in (1.7) is attained.

**Step 3: The lower bound** $W \leq W^{rc}$. The general idea is to show that $h$ is the restriction to $O$ of a convex function $f$, nondecreasing in the first two arguments, which will be constructed below. Since $h$ is continuous on $\bar{O}$ the result will follow.

We compute for $(x, y, d) \in O$ the gradient

$$Dg(x, y, d) = D(x^2 + y^2) - \frac{DA}{\sqrt{A}}(x, y, d)$$

and the matrix of second derivatives,

$$D^2 g = 2(e_1 \otimes e_1 + e_2 \otimes e_2) - \frac{D^2 A}{\sqrt{A}} + \frac{DA \otimes DA}{2A^{3/2}}.$$

From the explicit form of $A$ we obtain with $z = \sqrt{x^2y^2 - d^2}$

$$\partial_x A(x, y, d) = x|U_1|^2 + (\lambda^2 - \frac{1}{\lambda^2}) \frac{xy^2}{\sqrt{x^2y^2 - d^2}} = x|U_1|^2 + (\lambda^2 - \frac{1}{\lambda^2}) \frac{xy^2}{z}$$

and since $\partial_x A$ is linear in $x$, except from the dependence of $z$ on $x$,

$$\partial_x \partial_x A(x, y, d) = \frac{\partial_x^2 A(x, y, d)}{x} - (\lambda^2 - \frac{1}{\lambda^2}) \frac{x^2y^4}{z^3}.$$

The analogous formulas for the other derivatives imply that

$$D^2 A(x, y, d) = \begin{pmatrix}
\frac{\partial_x A(x, y, d)}{x} & 0 & 0 \\
0 & \frac{\partial_y A(x, y, d)}{y} & 0 \\
0 & 0 & 0
\end{pmatrix}
- (\lambda^2 - \frac{1}{\lambda^2}) \frac{1}{z^3} \begin{pmatrix}
x^2y^4 & 2d^2xy - x^3y^3 & -dx^2y \\
x^4y^2 & x^4y^2 & -dx^2y \\
-dxy^2 & -dx^2y & x^2y^2
\end{pmatrix}.$$
Note that
\[
\partial_x g(x, y, d) = 2x - \frac{\partial_x A}{\sqrt{A}}(x, y, d) \geq 0 \iff \frac{\partial_x g(x, y, d)}{x} = 2 - \frac{\partial_x A(x, y, d)}{x\sqrt{A(x, y, d)}} \geq 0.
\]
Therefore
\[
D^2 g(x, y, d) = \begin{pmatrix}
\partial_{x\partial_x y} g(x, y, d) & 0 & 0 \\
0 & \partial_{x\partial_y y} g(x, y, d) & 0 \\
0 & 0 & 0
\end{pmatrix} + \frac{DA \otimes DA}{2A^{1/2}}(x, y, d)
\]
\[
+ \left(\lambda^2 - \frac{1}{\lambda^2}\right) \frac{1}{z^3} \frac{y^2}{A(x, y, d)} \begin{pmatrix}
x^2y^4 & 2d^2xy - x^3y^3 & -dxy^2 \\
x^3y^3 & x^4 - d^2y^2 & dxy^2 \\
dx^2y & -dx^2 & -dy^2
\end{pmatrix}.
\]

The last matrix in this expression is positive semidefinite. To see this, note that the determinant of the matrix is equal to zero and that the determinant of the first 2 × 2 block is equal to 4d^2x^2y^2(x^2y^2 - d^2) and thus positive on O. The assertion follows now by continuity of the determinant if one adds ε > 0 to the (3,3) element, computes the determinant, and considers the limit as ε tends to zero. Therefore each of the three terms is positive semidefinite in the region
\[
\text{(2.5)} \quad V = \{ (x, y, d) \in O, \partial_x g \geq 0 \text{ and } \partial_y g \geq 0 \}.
\]

We conclude that \(D^2 g \geq 0\) in \(V\). To identify \(V\), we study for fixed \(y\) and \(d\) the sign of the function
\[
x \mapsto \partial_x g(x, y, d),
\]
defined on \(x \in (|d|/y, \infty)\). As \(x \to |d|/y\), we have \(z \to 0\), hence \(\partial_z A \to \infty\) and \(\partial_x g \to -\infty\) (if \(d = 0\), then still \(\partial_x g/x \to -\infty\)). Similarly, for \(x \to \infty\) we have \(\partial_x g(x, y, d) \sim 2x + O(1) > 0\). Therefore there is at least one zero in \(x \in (|d|/y, \infty)\). The condition \(\partial_x g = 0\) is equivalent to
\[
\frac{\partial_x A(x, y, d)}{x} = 2\sqrt{A(x, y, d)},
\]
which, in view of the foregoing definitions, is equivalent to
\[
\text{(2.6)} \quad |U| = \frac{y^2}{\sqrt{x^2y^2 - d^2}} = 2 \sqrt{(x^2 + y^2) \frac{|U|^2}{2} + (\lambda^2 - \frac{1}{\lambda^2}) \sqrt{x^2y^2 - d^2} + 2d}.
\]

The left-hand side is strictly monotone decreasing in \(x\), the right-hand side strictly monotone increasing. Therefore there is at most one solution and since we have already shown that there exists at least one solution, we conclude that for every pair \(y > 0, d \in \mathbb{R}\) there is a unique value \(x = \varphi(y, d) \in (|d|/y, \infty)\) such that
\[
\partial_x g(\varphi(y, d), y, d) = 0.
\]

The above discussion then shows that
\[
\partial_x g(\xi, y, d) \geq 0 \text{ for all } \xi \geq \varphi(y, d).
\]

By the implicit function theorem, the function \(\varphi : (0, \infty) \times \mathbb{R} \to (0, \infty)\) is smooth. By construction, \(\varphi(y, d) > |d|/y\) and in particular \(\varphi(y, d)\) tends to infinity as \(y\) tends to zero. We show in Section 3.4 below that \(y \mapsto \varphi(y, d)\) is monotonically decreasing. Therefore \(\varphi(y, d)\) has a finite limit as \(y\) tends to infinity. In particular, for all \(d \in \mathbb{R}\) the graph of \(\varphi(\cdot, d)\) intersects the line \(x = y\) and hence there exists a unique \(y\) such that \(\varphi(y, d) = y\), i.e.,
\[
\text{(2.7)} \quad \text{for all } d \text{ there exists a unique } p > 0 \text{ with } p = \varphi(p, d).
\]

Interchanging \(x\) and \(y\) similar results, with the same function \(\varphi\), hold for \(\partial_y g\) and in particular
\[
\partial_y g(x, \varphi(x, d), d) = 0.
\]
Therefore
\[
V = \{ (x, y, d) : xy - |d| > 0, x \geq \varphi(y, d), y \geq \varphi(x, d) \}.
\]
To see how the two latter conditions interact, consider for definiteness the region $\phi(y,d) \leq x \leq y$. Then $\partial_x g \geq 0$ or equivalently $\partial_x A/x \leq 2\sqrt{A}$. Since $x \leq y$, from the explicit expression for $\partial_x A$ we obtain $\partial_y A \leq \partial_x A/x \leq 2\sqrt{A}$, and therefore $\partial_y g \geq 0$ (all quantities are evaluated at $(x,y,d)$). We conclude that

\begin{equation}
\text{if } \phi(y, d) \leq x \leq y \text{ then } \phi(x, d) \leq y .
\end{equation}

To show that $h(x(F), y(F), d(F))$ is polyconvex to show that $h$ is the restriction to $\overline{O}$ of a function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ which is convex on $\mathbb{R}^3$ and monotone increasing in its first two arguments. Recall the definition of $p = p(d)$ in \eqref{2.7}. We define $f$ by

$$f(x, y, d) = \begin{cases} g(\varphi(y, d), y, d) & \text{if } p \leq y \text{ and } x \leq \varphi(y, d) , \\ g(p, p, d) & \text{if } x \leq p \text{ and } y \leq p , \\ g(x, \varphi(x, d), d) & \text{if } p \leq x \text{ and } y \leq \varphi(x, d) , \\ g(x, y, d) & \text{otherwise}, \\ \end{cases}$$

see Figure 1 for an illustration. We remark that $f$ is defined on all of $\mathbb{R}^3$, with the first three regions covering the part outside of $\overline{O}$. The monotonicity of $\varphi$ and \eqref{2.7} imply that $\varphi(y, d) \leq p$ for $y \geq p$, therefore the first region is contained in $\{x \leq y\}$ and the third in $\{y \leq x\}$. We now show that the fourth region coincides with the set $V$. Let $(x, y, d)$ be in the fourth region, assume for definiteness $y \geq x$. Since the point is not in the second region, $y > p$. Since it is not in the first one, $x > \varphi(y, d) > |d|/y$. With \eqref{2.8} we conclude $(x, y, d) \in V$. 

Figure 1. Sketch of the phase diagram for $\lambda = 1.5$, for various values of the determinant $d$. The region below the hyperbola $xy = |d|$ is not accessible. The inner boundaries represent the curves $x = \varphi(y, d)$ and $y = \varphi(x, d)$, which cross at $(p, p)$ as defined in \eqref{2.7}. For $x < p$ and $y < p$ (red region) the energy is constant (for each $d$), in the stripes close to the hyperbola ($|d|/y < x < \varphi(y, d)$ and the symmetric one, blue) the energy depends only on one of the two variables, in the region above the curves (region $V$) it coincides with the unrelaxed energy.
The function $f$ is continuous by definition. We show that $f \in C^1(\mathbb{R}^3)$. In each of the four regions which are introduced in the definition of $f$, the function $f$ is smooth, and we only have to consider the partial derivatives along the boundaries. In the first region we compute

$$
\partial_y f = \partial_x g \partial_y \varphi + \partial_y g,
$$

but since $\partial_x g(\varphi(y,d),y,d) = 0$ by definition of $\varphi$ this equals $\partial_y g(\varphi(y,d),y,d)$. Hence $\partial_y f$ is continuous on the set $x = \varphi(y,d)$ which defined the boundary between the first and the fourth region. The same holds for $\partial_d f$. The derivative $\partial_x f$ vanishes in the first region, as well as on the boundary between the first and the fourth region. The analogous arguments show the continuity of $Df$.

The same computation shows that $\partial_y f, \partial_x f \geq 0$ everywhere. Therefore $f = h$ on $O$.

To verify the convexity of $f$ we finally compute the second derivatives. Let $\psi = (\varphi(y,d),y,d)$, so that $f = g \circ \psi$ in the first region. Then

$$
Df = Dg \circ \psi D\psi
$$

and

$$
D^2 f = D^2 g \circ \psi D\psi \otimes D\psi + Dg \circ \psi D^2 \psi.
$$

From the definition of $\psi$, $D^2 \psi = D^2 \psi_3 = 0$. From the definition of $\varphi$, $\partial_x g \circ \psi = 0$. Therefore the second term vanishes.

The first term is positive definite because $D^2 g \geq 0$ on the set $V$ where $\partial_x g, \partial_y g \geq 0$ (see 2.5). Therefore $D^2 f \geq 0$ in the first region and by symmetry in the third. In the second region $D^2 f = 0$, and in the fourth $D^2 f = D^2 g \geq 0$. Therefore $f$ is convex.

**Step 4:** $W^{qc} = W^{rc}$. From general theory we know that extended-valued polyconvex functions are quasiconvex, hence $W^{qc} \leq W^{rc}$. The inequality $W^{qc} \leq W^{rc}$ holds, however, only under additional assumptions; we prove it here for the case of interest. In particular, it was shown in [7] that any quasiconvex function which is finite on the set of matrices with determinant $t$, for some $t \neq 0$, is rank-one convex on the same set. Let $t \neq 0$. If $\theta(t) < \infty$, then $W$ is finite on $\Sigma_t = \{F : \det F = t\}$. Therefore $W^{qc}$ is also finite on $\Sigma_t$, and rank-one convex. The argument of Step 2 only involves laminates within $\Sigma_t$, therefore we obtain $W^{qc} \leq W$ on $\Sigma_t$. If $\theta(t) = \infty$ there is nothing to prove.

The case $t = 0$ requires a separate treatment. We fix a singular matrix $F$ and write $F = a \otimes b$, with $a \neq 0$. The constructions performed in Step 2 are, in this case, scalar, in the sense that the laminates involve matrices of the form $F_\pm = a \otimes b_\pm$, for some other vectors $b_\pm$ and the same $a$ (if $Fv = 0$ then one takes $F_\pm = F + ta \otimes w$ instead of $w \otimes w$). One can then construct a scalar test function $\varphi : (0,1)^2 \to \mathbb{R}$ with $D\varphi \in \{b_-, b_+\}$ on large parts of the domain and $\varphi(x) = b \cdot x$ on the boundary, and use $a \varphi$ in the definition of quasiconvexity (notice that $\det(Da \varphi) = \det(a \otimes D\varphi) = 0$) to conclude. The proof is now complete.

3. **Discussion**

3.1. **A formula for the phase boundary.** The function $(y,d) \mapsto x = \varphi(y,d)$ can be given explicitly in terms of the solutions of a fourth-order polynomial equation in $x^2$. To see this, set $L = \lambda^2 + \lambda^{-2}, M = \lambda^2 - \lambda^{-2}$. The equation (2.6) reduces to

$$
L + M \frac{y^2}{\sqrt{x^2 y^2 - d^2}} = \sqrt{2L(x^2 + y^2) + 4M \sqrt{x^2 y^2 - d^2} + 8d}.
$$

Multiplication by $z = \sqrt{x^2 y^2 - d^2}$ leads to

$$
Lz + My^2 = \sqrt{Gz^2 + 4M z^3},
$$

where $G = 2L(x^2 + y^2) + 8d$. We take the square in this identity, find

$$
Lz^2 + M^2 y^2 + 2LM y^2 = Gz^2 + 4M z^3.
$$
Figure 2. Example of a numerical computation for the relaxed energy using the algorithm from [8] for $d = 1$, $\lambda = 1.5$, with variables as specified in (3.1). The curves are the phase boundaries obtained from the analytical relaxation, the dots represent numerical results, color-coded to distinguish the order of lamination. The central region is $K^{qc}$ and is delimited by the two curves $(x \pm y)^2 + \frac{z^2}{\lambda^2} = \lambda^2 + \frac{1}{\lambda}$ and corresponds to second-order laminates. The top and bottom regions correspond to first-order laminates, in the left and right regions the relaxation coincides with the original energy.

and collect terms linear in $z$ on the right-hand side,

$$L^2 z^2 + M^2 y^4 - G z^2 = (4M z^2 - 2LM y^2)z.$$  

We square again

$$(L^2 z^2 + M^2 y^4 - G z^2)^2 = (4M z^2 - 2LM y^2)^2 z^2$$

and obtain a rational expression. The terms $G$ and $z^2$ are linear in $x^2$, the other terms do not depend on $x$. Therefore we have a fourth-order polynomial equation in $x^2$ for which a solution formula exists.

The plot in Figure 2 contains for $d = 1$ the zero set of the energy density which corresponds to the quasiconvex hull of the two martensitic wells which is given by

$$K^{qc} = \left\{ F \in \mathbb{R}^{2 \times 2}, \det F = 1, \ |F(e_1 \pm e_2)|^2 \leq \lambda^2 + \frac{1}{\lambda^2} \right\}$$

or, equivalently, in the coordinates introduced before,

$$K^{qc} = \left\{ F \in \mathbb{R}^{2 \times 2}, \det F = 1, \ x, y \leq \sqrt{\frac{1}{2} \left( \lambda^2 + \frac{1}{\lambda^2} \right)} = \sqrt{L/2} \right\}.$$ 

A short calculation shows that $x = y = \sqrt{L/2}, d = 1$, is a solution of (2.6). This is in agreement with the results in [3] that the relative interior of $K^{qc}$ is obtained from second order laminates.

3.2. Comparison with the Ericksen-James energy in two dimensions. The following energy density originates in [19, 20] and is usually referred to as the two-dimensional version of the Ericksen-James energy. It is given by

$$\phi(F) = \kappa_1 (\text{tr} C - 2)^2 + \kappa_2 C_{12}^2 + \kappa_3 \left( \frac{(C_{11} - C_{22})^2}{4} - \varepsilon^2 \right)^2$$

where $C = (C_{ij})_{ij} = F^T F$ and $\varepsilon > 0, \kappa_i > 0, i = 1, 2, 3$ are parameters. Note that $\phi$ is invariant under the full orthogonal group O(2) and not only under SO(2), so that the zero set of $\phi$ is
given by
\[
K = O(2) \left( \begin{array}{cc}
\sqrt{1 - \varepsilon} & 0 \\
0 & \sqrt{1 + \varepsilon}
\end{array} \right) \cup O(2) \left( \begin{array}{cc}
\sqrt{1 + \varepsilon} & 0 \\
0 & \sqrt{1 - \varepsilon}
\end{array} \right).
\]
As a consequence, the zero set of the relaxation is much larger than SO(2). The relaxation is only known in the special case \(\kappa_3 = 0\) which leads to an energy which is convex in the right Cauchy-Green tensor \[^{23}\]. We believe that the relaxation result presented in Theorem 1.1 will be useful in the design of numerical schemes since it provides the full relaxation of a frame-indifferent energy which can serve as a model energy for a cubic to tetragonal phase transformation in two dimensions.

3.3. **Benchmark example for numerical simulations.** The relaxed energy in Theorem 1.1 can serve as a benchmark example for numerical schemes for the computation of relaxed energies and quasiconvex hulls of sets. In fact, the simulation in Figure 2 was obtained with the algorithm proposed in \[^{8}\]. The relaxation is illustrated for matrices of the form
\[
F = \begin{pmatrix}
a & b \\
0 & 1/a
\end{pmatrix}
\]
with \(a \in [0.4, 2]\), \(b \in [-1, 1]\). (3.1)
The figure shows that the numerically determined phase diagram is in excellent agreement with the present analytical results. This includes in particular the zero-set of the relaxed energy which is given by
\[
K^{qc} = \{ F \in \mathbb{R}^{2 \times 2}, |F(e_1 \pm e_2)|^2 \leq \lambda^2 + \frac{1}{\lambda^2} \text{, det } F = 1 \}.
\]
Indeed, the derivation of the analytical result in Theorem 1.1 was guided by the numerical results in \[^{8}\].

3.4. **Monotonicity of \(\varphi\).** We show here that \(\varphi(\cdot, d)\) is decreasing. From the equation \(\partial_x g(\varphi(y, d), y, d) = 0\) and the implicit function theorem we obtain
\[
\partial_x^2 g \varphi + \partial_x \partial_y g = 0.
\]
Since \(\partial_x^2 g > 0\) where \(\partial_x g = 0\), it suffices to show that \(\partial_x \partial_y g > 0\).

From the expressions in Step 3 above we write, using as before \(L = \lambda^2 + \lambda^{-2}\) and \(M = \lambda^2 - \lambda^{-2}\),
\[
\partial_x \partial_y g = \frac{\partial_x A \partial_y A}{2A^{3/2}} + \frac{Mxy}{z^3 A^{1/2}} (2d^2 - x^2 y^2).
\]
Dropping the positive factor \(xy/2A^{3/2}\), it suffices to show that
\[
\Xi = \frac{\partial_x A \partial_y A}{x} + 2AM \frac{2d^2 - x^2 y^2}{z^3}
\]
is nonnegative. Inserting the expressions above and estimating \(2d^2 - x^2 y^2 = d^2 - z^2 \geq -z^2\) we obtain
\[
\Xi \geq (L + M \frac{y^2}{z})(L + M \frac{x^2}{z}) - (LM(x^2 + y^2) + 2M^2 z + 4Md) \frac{1}{z}
\]
\[
= L^2 + LM \frac{x^2 + y^2}{z} + M^2 \frac{x^2 y^2}{z^2} - LM \frac{x^2 + y^2}{z} - 2M^2 - 4Md \frac{d}{z}
\]
\[
= L^2 + M^2 \frac{d^2 - z^2}{z^2} - 4Md \frac{d}{z}
\]
where we used \(x^2 y^2 - 2z^2 = d^2 - z^2\). Since \(L^2 = M^2 + 4\) this gives
\[
\Xi \geq 4 + M^2 \frac{d^2}{z^2} - 4M \frac{d}{z} \geq 0
\]
and concludes the proof.
REFERENCES

[1] ALBIN, N., CONTI, S., AND DOLZMANN, G. Infinite-order laminates in a model in crystal plasticity. Proc. Roy. Soc. Edinburgh A 139 (2009), 685–708.

[2] BALL, J. M., AND JAMES, R. D. Fine phase mixtures as minimizers of the energy. Arch. Ration. Mech. Analysis 100 (1987), 13–52.

[3] BALL, J. M., AND JAMES, R. D. 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] BHATTACHARYA, K. Self-accommodation in martensite. Arch. Rational Mech. Anal. 120 (1992), 201–244.

[5] CARSTENSEN, C., AND PLECHÁČ, P. Numerical solution of the scalar double-well problem allowing microstructure. Math. Comp. 66 (1997), 997–1026.

[6] CHIPOT, M., AND KINDERLEHRER, D. Equilibrium configurations of crystals. Arch. Rational Mech. Anal. (1988).

[7] CONTI, S. Quasiconvex functions incorporating volumetric constraints are rank-one convex. J. Math. Pures Appl. 90 (2008), 15–30.

[8] CONTI, S., AND DOLZMANN, G. An adaptive relaxation algorithm. In preparation.

[9] CONTI, S., AND DOLZMANN, G. On the theory of relaxation in nonlinear elasticity with constraints on the determinant. Preprint, 2014.

[10] CONTI, S., DOLZMANN, G., AND KIRCHHEIM, B. Existence of Lipschitz minimizers for the three-well problem in solid-solid phase transitions. Ann. Inst. H. Poincaré Anal. Non Linéaire 24 (2007), 953–962.

[11] CONTI, S., DOLZMANN, G., AND KREISBECK, C. Asymptotic behavior of crystal plasticity with one slip system in the limit of rigid elasticity. SIAM J. Math. Anal. 43 (2011), 2337–2353.

[12] CONTI, S., DOLZMANN, G., AND KREISBECK, C. Relaxation of a model in finite plasticity with two slip systems. Math. Models Methods Appl. Sci. 23 (2013), 2111–2128.

[13] CONTI, S., AND THEIL, F. Single-slip elastoplastic microstructures. Arch. Ration. Mech. Anal. 178 (2005), 125–148.

[14] DACOROGNA, B. Direct methods in the calculus of variations, vol. 78 of Applied Mathematical Sciences. Springer-Verlag, Berlin, 1989.

[15] DESIMONE, A., AND DOLZMANN, G. Macroscopic response of nematic elastomers via relaxation of a class of SO(3)-invariant energies. Arch. Ration. Mech. Anal. 161 (2002), 181–204.

[16] DOLZMANN, G. Variational Methods for Crystalline Microstructure - Analysis and Computation. No. 1803 in Lecture Notes in Mathematics. Springer-Verlag, 2003.

[17] DOLZMANN, G., AND KIRCHHEIM, B. Liquid-like behaviour of shape-memory alloys. C.R. Acad. Sci. Paris, Ser. I 336 (2003), 441–446.

[18] DOLZMANN, G., KIRCHHEIM, B., MÜLLER, S., AND ŠVERÁK, V. The two-well problem in three dimensions. Calc. Var. Partial Differential Equations 10 (2000), 21–40.

[19] ERICKSEN, J. Constitutive theory for some constrained elastic crystals. Int. J. Solids Struct. 22 (1986), 951–964.

[20] ERICKSEN, J. L. Some constrained elastic crystals. In Material instabilities in continuum mechanics (Edinburgh, 1985–1986), Oxford Sci. Publ. Oxford Univ. Press, New York, 1988, pp. 119–135.

[21] KOHN, R. V. The relaxation of a double-well energy. Contin. Mech. Thermodyn. 3 (1991), 193–236.

[22] KOHN, R. V., AND STRANG, G. Optimal design and relaxation of variational problems. II. Comm. Pure Appl. Math. 39 (1986), 139–182.

[23] LEĐRET, H., AND RAOULT, A. Quasiconvex envelopes of stored energy densities that are convex with respect to the strain tensor. In Calculus of variations, applications and computations (Pont-à-Mousson, 1994) (1995), vol. 326 of Pitman Res. Notes Math. Ser., Longman Sci. Tech., Harlow, pp. 138–146.

[24] LURIE, K. A., AND CHERKAEV, A. V. On a certain variational problem of phase equilibrium. In Proceedings of Partial Differential Equations and Applications (Olomouc, 1999) (2001), vol. 126, pp. 521–529.
[31] Šilhavý, M. Ideally soft nematic elastomers. *Netw. Heterog. Media* 2 (2007), 279–311.
[32] Šverák, V. On the problem of two wells. In *Microstructure and phase transition*, vol. 54 of *IMA Vol. Math. Appl.* Springer, New York, 1993, pp. 183–189.

**Institut für Angewandte Mathematik, Universität Bonn, Endenicher Allee 60, 53115 Bonn, Germany.**
E-mail address: sergio.conti@uni-bonn.de

**Fakultät für Mathematik, Universität Regensburg, 93040 Regensburg, Germany.**
E-mail address: georg.dolzmann@mathematik.uni-r.de