

An investigation of non-planar austenite–martensite interfaces

Article (Accepted Version)

Ball, J M and Koumatos, K (2014) An investigation of non-planar austenite–martensite interfaces. *Mathematical Models and Methods in Applied Sciences*, 24 (10). pp. 1937-1956. ISSN 0218-2025

This version is available from Sussex Research Online: <http://sro.sussex.ac.uk/id/eprint/66421/>

This document is made available in accordance with publisher policies and may differ from the published version or from the version of record. If you wish to cite this item you are advised to consult the publisher's version. Please see the URL above for details on accessing the published version.

Copyright and reuse:

Sussex Research Online is a digital repository of the research output of the University.

Copyright and all moral rights to the version of the paper presented here belong to the individual author(s) and/or other copyright owners. To the extent reasonable and practicable, the material made available in SRO has been checked for eligibility before being made available.

Copies of full text items generally can be reproduced, displayed or performed and given to third parties in any format or medium for personal research or study, educational, or not-for-profit purposes without prior permission or charge, provided that the authors, title and full bibliographic details are credited, a hyperlink and/or URL is given for the original metadata page and the content is not changed in any way.

AN INVESTIGATION OF NON-PLANAR AUSTENITE-MARTENSITE INTERFACES

KONSTANTINOS KOUMATOS AND JOHN M. BALL

ABSTRACT. Motivated by experimental observations on CuAlNi single crystals, we present a theoretical investigation of non-planar austenite-martensite interfaces. Our analysis is based on the nonlinear elasticity model for martensitic transformations and we show that, under suitable assumptions on the lattice parameters, non-planar interfaces are possible, in particular for transitions with cubic austenite.

KEYWORDS: austenite-martensite interfaces; non-classical; non-planar.

MSC (2010): 74B20, 74N15.

1. INTRODUCTION

A classical austenite-martensite interface is a plane - the habit plane - separating undistorted austenite from a simple laminate of martensite, i.e. a region where the deformation gradient jumps between two constant matrices, say A and B , on alternating bands of width λ and $1 - \lambda$, respectively, where $\lambda \in (0, 1)$. These interfaces have been broadly studied and are well understood. On the other hand, the nonlinear elasticity model for martensitic transformations (see e.g. [4, 5]) allows for interfaces separating undistorted austenite from more complicated microstructures of martensite; such interfaces are broadly referred to as non-classical.

Seiner and Landa [18], observed such non-classical interfaces in a CuAlNi shape-memory alloy, in which the martensite consists of two laminates - a compound and a Type-II twin¹ - crossing each other; this morphology is usually referred to as parallelogram or twin-crossing microstructure. More strikingly, the volume fraction, say Λ , of the compound twin varied as a function of position, resulting in a non-planar habit surface.

In [6], an analysis was provided for the macroscopically homogeneous case, i.e. when the volume fractions of the two crossing laminates remain constant. It was shown that the observed non-classical austenite-martensite interface is compatible in the sense that, under restrictions on the lattice parameters, given any compound volume fraction $\Lambda \in (0, 1)$, there exist precisely two Type-II volume fractions λ ensuring continuity of the overall deformation across a planar interface; see Fig. 1.

Equivalently, the continuity of the overall deformation across the planar interface can be expressed in terms of Hadamard's jump condition, i.e. that there exist vectors b , m and a rotation R - all being functions of the volume fractions λ , Λ - such that

$$R(\lambda, \Lambda)M(\lambda, \Lambda) = \mathbf{1} + b(\lambda, \Lambda) \otimes m(\lambda, \Lambda), \quad (1.1)$$

where $M(\lambda, \Lambda)$ denotes the macroscopic deformation gradient corresponding to the parallelogram microstructure with volume fractions λ , Λ . In particular, $m(\lambda, \Lambda)$ is the normal to the habit plane and varying the volume fraction Λ (as in the experimental observations) forces the habit plane normal to vary accordingly, giving some insight into the inhomogeneous case; see Fig. 2. However, explicit attempts to treat the inhomogeneous microstructure analytically proved to

¹The terminology is not important for our purposes and the reader is referred to e.g. [18]

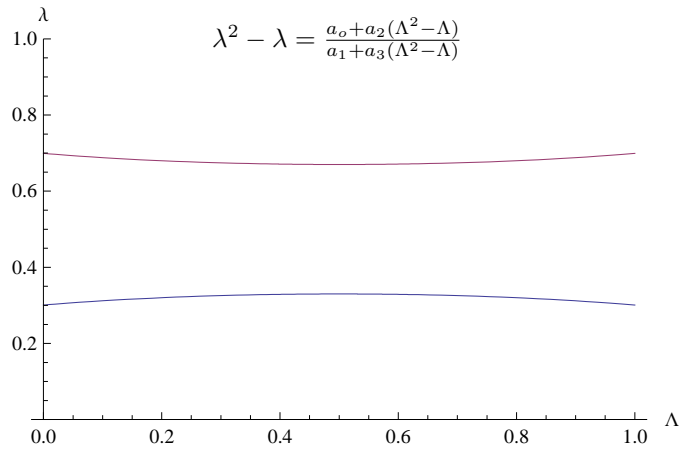


FIGURE 1. Type-II volume fractions λ that make the interface compatible plotted against the compound volume fraction $\Lambda \in [0, 1]$; a_i , $i = 0, \dots, 3$ are functions of the lattice parameters.

be either intractable, due to the algebraic complexity of the cubic-to-orthorhombic transition of CuAlNi, or in some cases seemingly impossible.

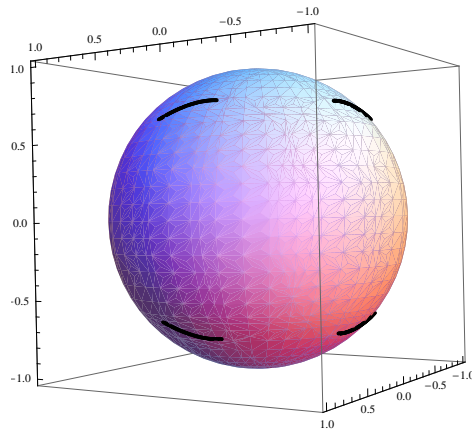


FIGURE 2. Plot of the unit normals $m(\lambda, \Lambda)$ in the compatibility equation (1.1) for (λ, Λ) as in Fig. 1.

In this paper, a theoretical approach is followed in order to investigate the possibility of non-planar austenite-martensite interfaces. It is shown that such interfaces are possible within the nonlinear elasticity model for all martensitic transformations with cubic austenite. In Section 2, the nonlinear elasticity model is briefly introduced and non-classical interfaces are explained in

greater depth. Our results are presented in Section 3. In particular, Theorem 3.2 provides a modification of Hadamard's jump condition allowing for non-planar interfaces and, in Lemma 3.3, we present a general construction of non-planar interfaces. This construction is only possible under the assumption that the austenitic well is rank-one connected to the interior of the quasiconvex hull of the martensitic wells relative to a determinant constraint; see Section 2 for the terminology. In Corollary 3.8 we show that this non-trivial assumption is satisfied in particular whenever the austenite is cubic, under appropriate restrictions on the lattice parameters.

2. NONLINEAR ELASTICITY MODEL

In the nonlinear elasticity model microstructures are identified with weak* limits of minimizing sequences (assumed bounded in $W^{1,\infty}(\Omega, \mathbb{R}^3)$) for a total free energy of the form:

$$I_\theta(y) = \int_{\Omega} \varphi(Dy(x), \theta) dx.$$

We note that interfacial energy contributions are ignored, resulting in the prediction of infinitely fine microstructure. Above, Ω represents the reference configuration of undistorted austenite at the transformation temperature θ_c and $y(x)$ denotes the deformed position of the particle $x \in \Omega$. The free-energy function $\varphi(F, \theta)$ depends on the deformation gradient $F \in \mathbb{R}^{3 \times 3}$ and the temperature θ , where $\mathbb{R}^{3 \times 3}$ denotes the space of real 3×3 matrices. By frame indifference, $\varphi(RF, \theta) = \varphi(F, \theta)$ for all F, θ and for all rotations R ; that is for all 3×3 matrices in

$$\text{SO}(3) = \{R : R^T R = \mathbf{1}, \det R = 1\}.$$

Also, by material symmetry $\varphi(FQ, \theta) = \varphi(F, \theta)$ for all $Q \in \mathcal{P}^\alpha$, where $\mathcal{P}^\alpha \subset \text{SO}(3)$ denotes the symmetry group of the austenite, e.g for cubic austenite $\mathcal{P}^\alpha = \mathcal{P}^{24}$ consists of the 24 rotations mapping the cube back to itself. Without loss of generality we assume that $\min_F \varphi(F, \theta) = 0$ and we denote by

$$K_\theta = \{F : \varphi(F, \theta) = 0\}$$

the zero set of $\varphi(\cdot, \theta)$. Assuming a transformation strain $U_1(\theta)$ and using frame indifference and material symmetry, we suppose that

$$K_\theta = \begin{cases} \alpha(\theta) \text{SO}(3) & \theta > \theta_c \text{ (austenite)} \\ \text{SO}(3) \cup \bigcup_{i=1}^N \text{SO}(3) U_i(\theta_c) & \theta = \theta_c \\ \bigcup_{i=1}^N \text{SO}(3) U_i(\theta) & \theta < \theta_c \text{ (martensite)}, \end{cases}$$

where the positive definite, symmetric matrices $U_i(\theta) \in \{R^T U_1(\theta) R : R \in \mathcal{P}^\alpha\}$ correspond to the N distinct variants of martensite and $\alpha(\theta)$ is the thermal expansion coefficient of the austenite with $\alpha(\theta_c) = 1$.

As a simple illustration of non-classical interfaces, let us restrict attention to planar ones. Then, a non-classical planar austenite-martensite interface $\{x \cdot m = k\}$ at the critical temperature θ_c corresponds to a choice of habit-plane normal m for which there exists an energy-minimizing sequence of deformations y^j such that, as $j \rightarrow \infty$,

$$Dy^j \rightarrow \text{SO}(3) \text{ in measure for } x \cdot m < k, \quad (2.1)$$

$$Dy^j \rightarrow K := \bigcup_{i=1}^N \text{SO}(3) U_i(\theta_c) \text{ in measure for } x \cdot m > k, \quad (2.2)$$

i.e. y^j corresponds to a pure phase of austenite and a general zero-energy microstructure of martensite on either side of the interface $\{x \cdot m = k\}$. Above, the convergence in measure of the sequence Dy^j to a compact set L means that for all open neighbourhoods U of L in $\mathbb{R}^{3 \times 3}$,

$$\lim_{j \rightarrow \infty} \text{meas} \{x \in \Omega : Dy^j(x) \notin U\} = 0.$$

In fact, this is equivalent to the Young measure $\nu = (\nu_x)_{x \in \Omega}$ generated by Dy^j being supported in L (see e.g. [16] for details).

Without loss of generality, (2.1) reduces to $Dy^j(x) \rightarrow \mathbf{1}$ a.e. in Ω . As for the martensitic region, $x \cdot m > k$, let us assume for simplicity that the martensitic microstructure is homogeneous; that is, for $x \cdot m > k$, the macroscopic deformation gradient $F = Dy(x)$, i.e. the weak* limit in $L^\infty(\Omega, \mathbb{R}^{3 \times 3})$ of Dy^j satisfying (2.2), is independent of x . We note that such matrices F are precisely the elements of the *quasiconvex hull* of the set K , denoted by K^{qc} . (In general, for a compact set $L \subset \mathbb{R}^{3 \times 3}$, say, its quasiconvex hull L^{qc} is given by the set of matrices F such that there exists a sequence of deformations z^j uniformly bounded in $W^{1,\infty}(\Omega, \mathbb{R}^3)$ with $z^j \xrightarrow{*} Fx$ and $Dz^j(x) \rightarrow L$ in measure².)

To make the overall deformation continuous across the planar interface one needs to satisfy the Hadamard jump condition as in (1.1). Thus, for planar interfaces between austenite and a homogeneous microstructure of martensite, accounting for non-classical interfaces becomes equivalent to establishing rank-one connections between the austenite and the set K^{qc} , i.e. finding vectors b, m such that

$$\mathbf{1} + b \otimes m \in K^{qc}, \quad (2.3)$$

where, by frame indifference, we have chosen the identity matrix $\mathbf{1}$ to represent the austenite energy well. However, in this context, the only known characterization of a quasiconvex hull is for two martensitic wells, that is when $K = \text{SO}(3)U_1 \cup \text{SO}(3)U_2$, in which case any $F \in K^{qc}$ can be obtained as the macroscopic deformation gradient of a double laminate (see [5]). Using this characterization Ball & Carstensen were able to analyze planar non-classical interfaces for cubic-to-tetragonal transformations and the reader is referred to [2] for details.

In the present paper, we wish to work in a more general setting where we allow the martensitic microstructure to depend on the position vector and the interface to be represented by a general (C^1) surface Γ . In this case, one still needs to require that (2.1) and (2.2) hold on either side of Γ but, since we allow the macroscopic deformation gradient Dy of the martensitic microstructure to depend on $x \in \Omega$, we require that $Dy(x) \in K^{qc}$ a.e. in the martensitic region. However, the compatibility condition across the interface Γ no longer suffices and needs to be generalized. An appropriate generalization is provided in the subsequent section along with statements and proofs of our results.

3. CONSTRUCTION OF NON-PLANAR INTERFACES

The first step to constructing a non-planar interface between austenite and an inhomogeneous microstructure of martensite is an appropriate generalization of Hadamard's jump condition; this is Theorem 3.2. However, before stating and proving the generalized jump condition, let us first clarify notation and terminology, as well as prove an auxiliary lemma (Lemma 3.1) used in the proof of Theorem 3.2.

Notation.

- The term *domain* is reserved for an open and connected set in \mathbb{R}^d throughout this paper.
- A function $y : \Omega \rightarrow \mathbb{R}$ belongs to the space $C^1(\overline{\Omega})$ if $y \in C^1(\Omega)$ and y can be extended to a continuously differentiable function on an open set containing $\overline{\Omega}$. The space $C^1(\overline{\Omega}, \mathbb{R}^d)$ consists of those maps $y = (y_1, \dots, y_d) : \Omega \rightarrow \mathbb{R}^d$ such that $y_i \in C^1(\overline{\Omega})$ for all $i = 1, \dots, d$.
- Let $k > 0$. A domain Ω is of class C^k if for each $\xi \in \partial\Omega$ there exist $r > 0$, a Cartesian coordinate system in $B(\xi, r)$, with coordinates (\bar{x}, x_d) where $\bar{x} = (x_1, \dots, x_{d-1})$, and a

²The quasiconvex hull of a compact set L of matrices can be equivalently defined in various ways (see e.g. [16]) but the above definition will suffice for our purposes.

C^k function $g : \mathbb{R}^{d-1} \rightarrow \mathbb{R}$ such that

$$\begin{aligned}\Omega \cap B(\xi, r) &= \{x \in B(\xi, r) : x_d > g(\bar{x})\}, \\ \partial\Omega \cap B(\xi, r) &= \{x \in B(\xi, r) : x_d = g(\bar{x})\}.\end{aligned}$$

- A $(d-1)$ -surface Γ is a relatively compact manifold of dimension $d-1$ embedded in \mathbb{R}^d such that $\Gamma = \text{int}\Gamma$, in the sense that every point of Γ has an open neighbourhood in Γ homeomorphic to a ball in \mathbb{R}^{d-1} . We say that a $(d-1)$ -surface Γ is of class C^k if for each $\xi \in \Gamma$ there exist $r > 0$, a Cartesian coordinate system in $B(\xi, r)$, with coordinates (\bar{x}, x_d) , and a C^k function $g : \mathbb{R}^{d-1} \rightarrow \mathbb{R}$ such that

$$\Gamma \cap B(\xi, r) = \{x \in B(\xi, r) : x_d = g(\bar{x})\}.$$

We note that the reference to the dimension may be dropped when this is obvious.

Lemma 3.1. *Suppose that $\Gamma \subset \mathbb{R}^d$ is a connected $(d-1)$ -surface which is of class C^1 and let $x^0 \in \Gamma$. Then, for all $x \in \Gamma$ there exists a continuous, piecewise continuously differentiable path $\gamma : [0, 1] \rightarrow \Gamma$ such that $\gamma(0) = x^0$ and $\gamma(1) = x$.*

Proof. Let $x^0, x \in \Gamma$; since Γ is a connected manifold, it is also path-connected (see e.g. [14]) and there exists a continuous path connecting x^0 and x . Note that the set of points on the path is compact since it is closed and contained in a relatively compact set. Also, Γ being C^1 , we can cover the path with balls $B(x, r_x)$ centred at x of radius r_x such that $\Gamma \cap B(x, r_x)$ is the graph of a C^1 function $g_x : \mathbb{R}^{d-1} \rightarrow \mathbb{R}$.

Extracting a finite subcover, we may assume that there are points $x^0, \dots, x^N = x \in \Gamma$ such that the balls $B(x^j, r_j)$, $j = 0, 1, \dots, N$, cover the path and that there exist local coordinate systems, say $(\bar{x}^{c_j}, x_d^{c_j})$ with $\bar{x}^{c_j} = (x_1^{c_j}, \dots, x_{d-1}^{c_j})$, and C^1 functions $g_j : \mathbb{R}^{d-1} \rightarrow \mathbb{R}$ such that

$$\Gamma \cap B(x^j, r_j) = \{x \in B(x^j, r_j) : x_d^{c_j} = g_j(\bar{x}^{c_j})\}.$$

Above, the superscript c_j denotes the coordinate system in the ball $B(x^j, r_j)$. Trivially, we may also assume that for $j = 0, 1, \dots, N-1$, there exists some $y^{j+1} \in B(x^j, r_j) \cap B(x^{j+1}, r_{j+1})$.

For $j = 0, \dots, N$, we may define N continuously differentiable paths γ_j in each $B(x^j, r_j)$ such that $\gamma_j(0) = y^j$ and $\gamma_j(1) = y^{j+1}$, where we make the identification $x^0 = y^0$ and $x^N = y^{N+1}$, by

$$\gamma_j(t) = (\bar{y}^{j,c_j} + t(\bar{y}^{j+1,c_j} - \bar{y}^{j,c_j}), g(\bar{y}^{j,c_j} + t(\bar{y}^{j+1,c_j} - \bar{y}^{j,c_j}))),$$

where the superscript j, c_j denotes the point y^j expressed in the coordinate system c_j in $B(x^j, r_j)$. Then, the composition of $\gamma_0, \dots, \gamma_N$ gives a continuous, piecewise continuously differentiable path $\gamma : [0, 1] \rightarrow \Gamma$ such that $\gamma(0) = x^0$ and $\gamma(1) = x$. \square

We may now state and prove the generalized jump condition:

Theorem 3.2. *Let $d \geq 2$. Let $\Omega \subset \mathbb{R}^d$ be a bounded C^1 domain and suppose that $\Omega = \Omega^+ \cup \Gamma \cup \Omega^-$ where Ω^+, Ω^- are disjoint open sets and $\Gamma = \Omega \cap \partial\Omega^+ = \Omega \cap \partial\Omega^-$ is a $(d-1)$ -surface of class C^1 . Further, assume that $y^\pm \in C^1(\bar{\Omega}^\pm, \mathbb{R}^d)$ and let $n \in C(\Gamma, \mathbb{R}^d)$ be the outward unit normal to Γ with respect to Ω^+ . If there exists a map $z \in W^{1,\infty}(\Omega, \mathbb{R}^d)$ such that*

$$Dz(x) = \begin{cases} Dy^+(x), & x \in \Omega^+ \\ Dy^-(x), & x \in \Omega^-, \end{cases} \quad (3.1)$$

then, for some $a \in C(\Gamma, \mathbb{R}^d)$ and all $x \in \Gamma$,

$$Dy^+(x) = Dy^-(x) + a(x) \otimes n(x), \quad (3.2)$$

Conversely, suppose that Γ is connected or Ω is simply connected. If (3.2) holds then there exists a map $z \in W^{1,\infty}(\Omega, \mathbb{R}^d)$ satisfying (3.1).

Remark 3.1. Note that, under the hypotheses of Theorem 3.2, Ω^+ and Ω^- locally lie on either side of the surface Γ . Also, for the construction of a non-planar austenite-martensite interface we are interested in the special case where, say, $Dy^- = \mathbf{1}$ represents the pure phase of austenite, whereas Dy^+ represents the macroscopic deformation gradient corresponding to a microstructure of martensite, i.e. $Dy^+(x) \in K^{qc}$ a.e. in Ω^+ for some set K of martensitic wells; see Fig. 3.

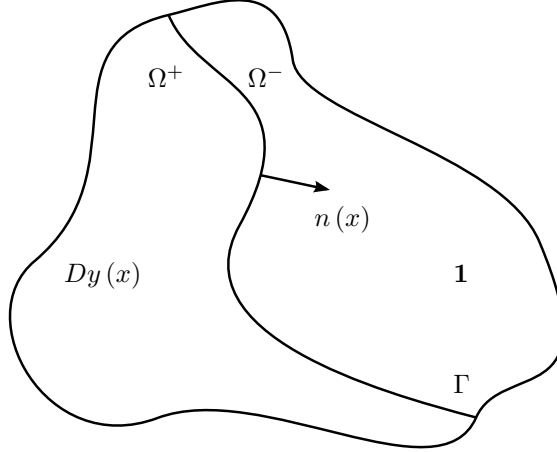


FIGURE 3. Schematic depiction of a deformation gradient Dz taking the values Dy and $\mathbf{1}$ on either side of a non-planar interface Γ ; for an austenite-martensite interface the macroscopic deformation gradient $Dy \in K^{qc}$ a.e. for some appropriate set K of martensitic wells. The deformation z remains continuous across Γ provided that $Dy(x) = \mathbf{1} + a(x) \otimes n(x)$ for all $x \in \Gamma$.

Proof. The necessity of (3.2) for each $x \in \Gamma$ follows from the classical Hadamard jump condition for continuous piecewise C^1 maps, which can be proved by blowing-up about x to reduce the case to that for a continuous piecewise affine map (see e.g. [3] for proofs of much more general statements), while the continuity of $a(\cdot)$ follows from that of Dy^\pm .

To prove sufficiency, assume first that Γ is connected. Let $x_0 \in \Gamma$ fixed and, by adding an appropriate constant, assume that $y^+(x_0) = y^-(x_0) = 0$. It is enough to show that $y^+(x) = y^-(x)$, for all $x \in \Gamma$, as the map

$$z(x) = \begin{cases} y^+(x), & x \in \Omega^+ \\ y^-(x), & x \in \Omega^- \end{cases}$$

is then continuous across Γ and Dz has the required form.

Let $x \in \Gamma$; By Lemma 3.1, we can define a piecewise continuously differentiable path $\gamma : [0, 1] \rightarrow \Gamma$ such that $\gamma(0) = x_0$ and $\gamma(1) = x$. Then,

$$y^+(x) - y^-(x) = \int_0^1 [Dy^+(\gamma(t)) - Dy^-(\gamma(t))] \dot{\gamma}(t) dt.$$

Note that for a.e. $t \in [0, 1]$, $\dot{\gamma}(t)$ is tangential to the path and, in particular, perpendicular to the normal at the point $\gamma(t) \in \Gamma$, i.e. $\dot{\gamma}(t) \cdot n(\gamma(t)) = 0$. On the other hand, we know that for all $x \in \Gamma$, $Dy^+(x) - Dy^-(x) = a(x) \otimes n(x)$ and therefore

$$y^+(x) - y^-(x) = \int_0^1 [n(\gamma(t)) \cdot \dot{\gamma}(t)] a(\gamma(t)) dt = 0.$$

On the other hand, assume that Ω is simply connected. Condition (3.2) now ensures that the map $F \in L^\infty(\Omega, M^{d \times d})$ defined by

$$F(x) = \begin{cases} Dy^+(x), & x \in \Omega^+ \\ Dy^-(x), & x \in \Omega^- \end{cases}$$

is curl-free (in the distributional sense) and Theorem 1 in [1] shows that this is equivalent to the existence of a distribution with a distributional derivative given by F . Then, Maz'ya in Section 1.1.11, [15] shows that a distribution whose derivatives of order k belong to an L^p space must itself be a function and an element of the Sobolev space $W^{k,p}$; sufficiency follows. \square

Remark 3.2. (i) Note that if Γ is disconnected and Ω is not simply connected, the result is in general false. As an example, consider $\Omega = A \times (0, 1)$ where A is the annulus

$$\{(x_1, x_2) : 1 < x_1^2 + x_2^2 < 4\}.$$

Let $\Omega^\pm = \{(x_1, x_2, x_3) : \pm x_1 < 0, x_3 \in (0, 1)\}$ and $\Gamma = \Gamma_1 \cup \Gamma_2$ where

$$\Gamma_1 = \{(x_1, x_2, x_3) : x_1 = 0, x_2 > 1, x_3 \in (0, 1)\}$$

$$\Gamma_2 = \{(x_1, x_2, x_3) : x_1 = 0, x_2 < -1, x_3 \in (0, 1)\}.$$

A planar section perpendicular to the x_3 axis is depicted in Fig. 4 below. Let $y^+(x) = 0$ in Ω^+ ,

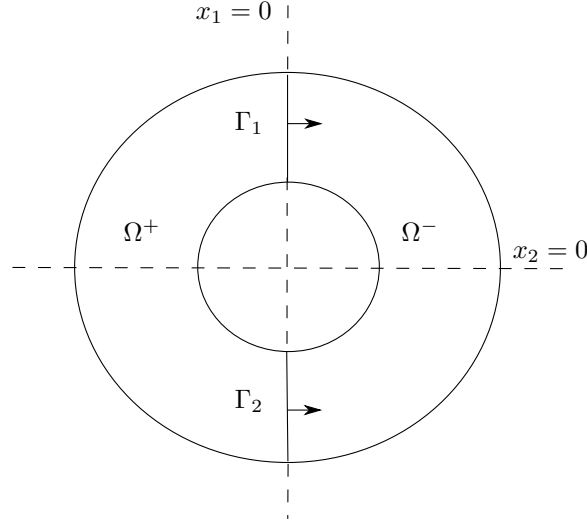


FIGURE 4. The manifold $\Gamma = \Gamma_1 \cup \Gamma_2$ is disconnected, Ω is not simply connected, and the conclusion of Theorem 3.1 no longer holds.

$y^-(x) = 0$ for $x \in \Omega^- \cap \{x_2 > 1\}$, $y^-(x) = ax_1 + e_2$ for $x \in \Omega^- \cap \{x_2 < -1\}$ and interpolate smoothly for $x_2 \in [-1, 1]$, where a is a non-zero vector and $x_1 = x \cdot e_1$, e_i being the standard basis of \mathbb{R}^3 ; trivially, the compatibility condition (3.2) is satisfied across Γ , with $Dy^+ - Dy^- = 0$ on Γ_1 and $Dy^+ - Dy^- = a \otimes e_1$ on Γ_2 . Next suppose that there exists $z \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that

$$Dz(x) = \begin{cases} Dy^+(x), & x \in \Omega^+ \\ Dy^-(x), & x \in \Omega^- \end{cases} = \begin{cases} 0, & x \in \Omega^+ \\ Dy^-(x), & x \in \Omega^- \end{cases}.$$

Then, since Ω^\pm are connected, $z(x) = c$ in Ω^+ for some constant c , whereas, in Ω^- , $z(x) = y^-(x) + d$ for some other constant d . But continuity across Γ_1 requires that $d = c$ and hence on Γ_2 that $c = c + e_2$ - a contradiction.

(ii) For general results concerning the relationship between the gradients of a Lipschitz mapping on either side of an interface see Ball & Carstensen [3], Iwaniec et al. [12].

Next we present a method for constructing non-planar interfaces at zero stress that is applicable to any set of martensitic wells K , provided that there exists a rank-one connection between $\text{SO}(d)$, the austenitic well, and the relative interior of the quasiconvex hull of K , $\text{rint } K^{qc}$. Here, the interior of K^{qc} is taken relative to the set $\mathcal{D} := \{A \in \mathbb{R}^{d \times d} : \det A = \Delta\}$, where Δ denotes the determinant of the martensitic variants.

Lemma 3.3. *Let $K \subset \mathcal{D}$ be a compact set such that $\text{rint } K^{qc} \neq \emptyset$. Further, assume that there exist $\epsilon > 0$ and nonzero vectors $a, n \in \mathbb{R}^d$, $|n| = 1$, such that $\mathbf{1} + a \otimes n \in \mathcal{D}$ and*

$$B(\mathbf{1} + a \otimes n, \epsilon) \cap \mathcal{D} \subset K^{qc}. \quad (3.3)$$

Then, for some open ball $\Omega = B(0, r) \subset \mathbb{R}^d$ and a non-planar $(d-1)$ -surface Γ , as in Theorem 3.2, there exists a deformation $z \in W^{1, \infty}(\Omega, \mathbb{R}^d)$ such that

$$Dz(x) = \begin{cases} Dy(x) & , \quad x \in \Omega^+ \\ \mathbf{1} & , \quad x \in \Omega^- \end{cases}$$

with $y \in C^1(\overline{\Omega^+}, \mathbb{R}^d)$ and $Dy(x) \in K^{qc}$ for all $x \in \overline{\Omega^+}$. That is, there exists a microstructure of martensite represented by Dy which borders compatibly with a pure phase of austenite along the non-planar interface Γ .

Proof. Let $f \in C^1(B(0, 1))$ satisfy the following properties:

- $f(0) = 0$ and $\nabla f(0) = n$;
- $\|\nabla f - n\|_\infty < \epsilon/|a|$;
- $a \cdot \nabla f(x) = a \cdot n$ for all $x \in B(0, 1)$;
- for all sufficiently small $r \in (0, 1)$, $\nabla f/|\nabla f|$ is not constant on $\{x \in B(0, r) : f(x) = 0\}$.

Choose an orthonormal system of coordinates (\bar{x}, x_d) with origin at 0 and $e_d = n$. Consider the map $g : B(0, 1) \rightarrow \mathbb{R}^d$ defined by $g(x) = (\bar{x}, f(x))$. Since $\nabla g(0) = \mathbf{1} \neq 0$ it follows from the inverse function theorem that for $r > 0$ sufficiently small and some neighbourhood V of $0 \in \mathbb{R}^d$ the map $g : B(0, r) \rightarrow V$ is invertible with C^1 inverse g^{-1} , and that

$$\{x \in B(0, r) : f(x) = 0\} = \{x \in B(0, r) : x_d = h(\bar{x})\},$$

where $h(\bar{x}) = g^{-1}(\bar{x}, 0) \cdot n$. Let $\Omega = B(0, r)$, $\Omega^\pm = \{x \in \Omega : \pm f(x) > 0\}$ and $\Gamma = \{x \in \Omega : f(x) = 0\}$. Note that Γ is a $(d-1)$ -surface of class C^1 and that the unit normal $n(x)$ to a point $x \in \Gamma$ is given by $n(x) = \nabla f(x)/|\nabla f(x)|$. Also since on Γ , $\nabla f/|\nabla f|$ cannot be constant, Γ defines a non-planar interface.

We now construct the appropriate deformation. Define $y^- : \Omega^- \rightarrow \mathbb{R}^d$ by $y^-(x) = x$ and $y^+ : \Omega^+ \rightarrow \mathbb{R}^d$ by

$$y^+(x) = x + af(x). \quad (3.4)$$

As $f \in C^1(B(0, 1))$ and $\Omega \subset \subset B(0, 1)$, it follows that $y^+ \in C^1(\overline{\Omega^+}, \mathbb{R}^d)$ and

$$Dy^+(x) = \mathbf{1} + a \otimes \nabla f(x).$$

In particular, $Dy^+(0) = \mathbf{1} + a \otimes n \in \text{rint } K^{qc}$ and, for all other $x \in \Gamma$, $Dy^+(x) = \mathbf{1} + a(x) \otimes n(x)$, where $a(x) = |\nabla f(x)|a$. Also

$$\det Dy^+(x) = 1 + a \cdot \nabla f(x) = 1 + a \cdot n,$$

so that $Dy^+(x) \in \mathcal{D}$ for all $x \in \Omega^+$. Finally, by (3.3) and our assumption that $\|\nabla f - n\|_\infty < \epsilon/|a|$,

$$Dy^+(x) \in B(\mathbf{1} + a \otimes n, \epsilon) \cap \mathcal{D} \subset K^{qc}.$$

Theorem 3.2 now applies and the proof is complete. \square

Depending on the choice of function f defining the implicit surface Γ , one can obtain a variety of interfaces.

Example 3.1. Let $h \in C^1(\mathbb{R})$ be such that \dot{h} is not constant, $h(0) = \dot{h}(0) = 0$ and

$$\|\dot{h}\|_\infty < \frac{\epsilon}{|a|^2}.$$

Assume $a, n \in \mathbb{R}^3$ are nonparallel and define $f \in C^1(\mathbb{R}^3)$ by

$$f(x) = x \cdot n + h(x \cdot (a \wedge n)),$$

where $a \wedge n$ denotes the vector product of a and n . If a and n are parallel, we can proceed similarly replacing $a \wedge n$ by any vector perpendicular to them. Then, $f(0) = 0$ and

$$\nabla f(x) = n + \dot{h}(x \cdot a \wedge n) a \wedge n,$$

so that $\nabla f(0) = n$. Moreover, $a \cdot \nabla f(x) = a \cdot n$. By the orthogonality of the vectors n and $a \wedge n$, $\Gamma := \{f^{-1}(0)\} = \{(-h(x_{a \wedge n}), x_{a \wedge n}, x_m) : (x_{a \wedge n}, x_m) \in \mathbb{R}^2\}$ in some appropriate coordinate system where x_n , $x_{a \wedge n}$ and x_m are coordinates in the directions n , $a \wedge n$ and some vector $m \in \mathbb{R}^3$ perpendicular to both n and $a \wedge n$, respectively. This defines a C^1 surface which extends indefinitely in the direction of $a \wedge n$ and m and $\Omega \subset \mathbb{R}^3$ can be chosen to be any domain intersecting Γ and not just the possibly small neighbourhood of Lemma 3.3. Also, Γ is non-planar as otherwise $\dot{h}(x_{a \wedge n}) = \dot{h}(y_{a \wedge n})$ for all $x, y \in \Gamma$ which is impossible since \dot{h} is not constant.

Moreover, note that $\nabla f(x)$ only changes along the direction $a \wedge n$ and the vector m is always tangential to the surface. Then, the two-dimensional cross-sections of Γ with planes parallel to the one spanned by the vectors n and $a \wedge n$ are the same so that the cross-section with the plane $x \cdot m = k$ is parametrized by $r(t) = (-h(t), t, k)$; see Fig. 5 for an example.

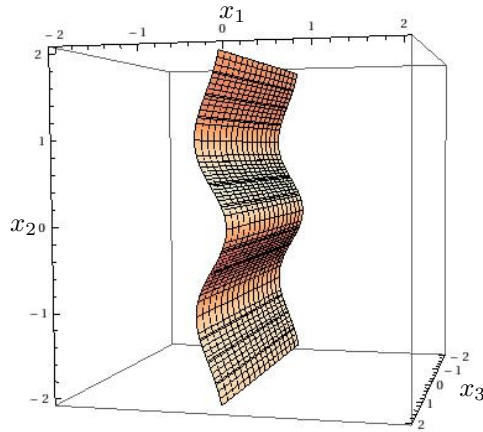


FIGURE 5. Example of a surface produced with $h(t) = t^2 e^{-t^2}$; x_1, x_2, x_3 denote the coordinates in the direction of n , $a \wedge n$ and the vector perpendicular to both n and $a \wedge n$ respectively. The vectors $n = (1, 0, 0)^T$ and $a = (0, 0, 1)^T$ have been chosen arbitrarily for simplicity and there is no smallness assumption imposed on $\|\dot{h}\|_\infty$ so that the curvature of the surface is clearly seen.

Remark 3.3. It is worth noting that if the determinant of the martensitic variants is 1, i.e. $\Delta = 1$ then, at least for martensitic transformations with cubic austenite, the identity matrix is an element of K^{qc} (see Bhattacharya [7]) and the underlying martensitic microstructure can form any non-planar interface with the identity as compatibility is trivial.

In proving Lemma 3.3, we assumed that there exists a relative interior point of K^{qc} which is rank-one connected to $\text{SO}(d)$. This is by no means a trivial assumption and we now address this point.

In the context of martensitic transformations, one is interested in compact subsets of $\mathbb{R}^{d \times d}$ of the form

$$K = \bigcup_{i=1}^N \text{SO}(d) U_i$$

where the matrices U_i are positive definite, symmetric with $\det U_i = \Delta$. For $d = 2$, there is a characterization of K^{qc} (Theorem 2.2.3, in Dolzmann [10]) saying that $K^{qc} = K^{(2)}$, the set of laminates of order up to 2; in fact, it is easy to deduce from the proof that second order laminates are contained in the interior of K^{qc} relative to the determinant constraint. Rank-one connections between second order laminates and $\text{SO}(2)$ indeed exist and the construction of the curved interface is possible in this case. However, the case $d = 3$ is of greater interest and, there, the situation is entirely non-trivial. For instance, in the case of two wells

$$U_1 = \text{diag}(\eta_1, \eta_2, \eta_3), \quad U_2 = \text{diag}(\eta_2, \eta_1, \eta_3),$$

the quasiconvex hull of the set $K = \text{SO}(3)U_1 \cup \text{SO}(3)U_2$ equals $K^{(2)}$ and consists of those matrices F such that

$$F^T F = \begin{pmatrix} a & c & 0 \\ c & b & 0 \\ 0 & 0 & \eta_3^2 \end{pmatrix} \quad (3.5)$$

where $ab - c^2 = \eta_1^2 \eta_2^2$ and $a + b + 2|c| \leq \eta_1^2 + \eta_2^2$ (see [5, 10]). Note that due to the determinant constraint this is a two-dimensional set which implies that K^{qc} is of dimension 5 (since $\text{SO}(3)$ has dimension 3). On the other hand, were the relative interior of K^{qc} non-empty, it would have dimension 8. Therefore, $\text{rint} K^{qc} = \emptyset$ and our construction cannot be applied.

Hence, for $K \subset \mathbb{R}^{3 \times 3}$ we follow a different approach to prove the existence of rank-one connections between $\text{SO}(3)$ and the relative interior of K^{qc} ; our argument is based on the following lemma.

Lemma 3.4 (Dolzmann-Kirchheim [11]). *Let $\kappa > 0$, $\kappa \neq 1$ and assume that the set $\tilde{K} \subset \{A \in \mathbb{R}^{3 \times 3} : \det A = 1\}$ is compact and that \tilde{K}^{qc} contains a three-well configuration \tilde{K}_{ct} given by*

$$\begin{aligned} \tilde{K}_{ct} &= \bigcup_{i=1}^3 \text{SO}(3) \tilde{U}_i \quad \text{where} \\ \tilde{U}_1 &= \text{diag}\left(\kappa^2, \frac{1}{\kappa}, \frac{1}{\kappa}\right), \quad \tilde{U}_2 = \text{diag}\left(\frac{1}{\kappa}, \kappa^2, \frac{1}{\kappa}\right), \quad \tilde{U}_3 = \text{diag}\left(\frac{1}{\kappa}, \frac{1}{\kappa}, \kappa^2\right). \end{aligned}$$

Then there exists $\epsilon = \epsilon(\kappa) > 0$ such that

$$B(\mathbf{1}, \epsilon) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = 1\} \subset \tilde{K}^{qc}.$$

In particular, if $\kappa < 3/2$, $\epsilon(\kappa) = (\kappa - 1)^2/62$ suffices.

Remark 3.4. The three well configuration \tilde{K}_{ct} corresponds to a cubic-to-tetragonal transformation for which $\eta_1^2 = 1/\eta_2$. Also, we note that the assumption $\kappa < 3/2$ is realistic as for

shape-memory alloys the lattice parameters are typically close to 1. Henceforth, without loss of generality, we assume that $\epsilon < 1$.

From Lemma 3.4 we deduce the following result providing conditions on K such that rank-one connections between $\text{SO}(3)$ and $\text{rint } K^{qc}$ exist:

Theorem 3.5. *Let $\kappa > 0$, $\kappa \neq 1$ and $\Delta > 0$ be such that*

$$\frac{|\Delta^{1/3} - 1|}{\Delta^{1/3}} \sqrt{\Delta^{4/3} + 2\Delta + \Delta^{2/3} + 2} < \epsilon(\kappa), \quad (3.6)$$

where $\epsilon(\kappa) \in (0, 1)$ is such that $B(\mathbf{1}, \epsilon) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = 1\} \subset \tilde{K}^{qc}$ (see Lemma 3.4). Further, assume that $K \subset \{A \in \mathbb{R}^{3 \times 3} : \det A = \Delta\}$ is compact and that K^{qc} contains a three-well configuration K_{ct} given by

$$K_{ct} = \bigcup_{i=1}^3 \text{SO}(3) U_i, \quad (3.7)$$

where

$U_1 = \text{diag}(\eta_2, \eta_1, \eta_1)$, $U_2 = \text{diag}(\eta_1, \eta_2, \eta_1)$, $U_3 = \text{diag}(\eta_1, \eta_1, \eta_2)$ and $\eta_1 = \Delta^{1/3}/\kappa$, $\eta_2 = \Delta^{1/3}\kappa^2$. Then there exist $a, n \in \mathbb{R}^3$ such that $\mathbf{1} + a \otimes n \in \text{rint } K^{qc}$.

In proving the above theorem, we use two very simple observations which we now prove in the form of a lemma.

Lemma 3.6. *In the notation of Lemma 3.4 and Theorem 3.5 the following hold:*

- (i) $K_{ct}^{qc} = \Delta^{1/3} \tilde{K}_{ct}^{qc}$;
- (ii) $\text{rint } K_{ct}^{qc} = \Delta^{1/3} \text{rint } \tilde{K}_{ct}^{qc}$; in particular, writing $F = \Delta^{1/3} \tilde{F}$,

$$B(\tilde{F}, \epsilon) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = 1\} \subset \tilde{K}_{ct}^{qc}$$

if and only if

$$B(F, \Delta^{1/3} \epsilon) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = \Delta\} \subset K_{ct}^{qc}.$$

Proof. (i) For notational convenience let $K = K_{ct} = \bigcup_{i=1}^3 \text{SO}(3) U_i$ and similarly, $\tilde{K} = \tilde{K}_{ct} = \bigcup_{i=1}^3 \text{SO}(3) \tilde{U}_i$. Note that $\Delta^{1/3} \tilde{K} = K$. To show that $\Delta^{1/3} \tilde{K}^{qc} \subset K^{qc}$, let $\tilde{F} \in \tilde{K}^{qc}$. By the characterization of the elements of \tilde{K}^{qc} as weak* limits (see Section 2), there exists a sequence \tilde{y}^j uniformly bounded in $W^{1,\infty}(\Omega, \mathbb{R}^3)$, for some bounded domain $\Omega \subset \mathbb{R}^3$, such that

$$\begin{aligned} \text{dist}(D\tilde{y}^j, \tilde{K}) &\rightarrow 0 \text{ in measure,} \\ D\tilde{y}^j &\overset{*}{\rightharpoonup} \tilde{F} \text{ in } L^\infty(\Omega, \mathbb{R}^{3 \times 3}). \end{aligned}$$

Define $y^j(x) = \tilde{y}^j(\Delta^{1/3}x)$; by our assumptions on \tilde{y}^j , y^j is uniformly bounded in $W^{1,\infty}(\Delta^{-1/3}\Omega, \mathbb{R}^3)$ and the gradients $Dy^j(x) = \Delta^{1/3} D\tilde{y}^j(\Delta^{1/3}x)$ satisfy

$$\begin{aligned} \text{dist}(Dy^j, \Delta^{1/3} \tilde{K}) &\rightarrow 0 \text{ in measure,} \\ Dy^j &\overset{*}{\rightharpoonup} \Delta^{1/3} \tilde{F} \text{ in } L^\infty(\Delta^{-1/3}\Omega, \mathbb{R}^{3 \times 3}). \end{aligned}$$

But $\Delta^{1/3} \tilde{K} = K$ implying that $\Delta^{1/3} \tilde{F} \in K^{qc}$. That $K^{qc} \subset \Delta^{1/3} \tilde{K}^{qc}$ is proved similarly.

- (ii) Let $\tilde{F} \in \text{rint } \tilde{K}^{qc}$; then there exists $\epsilon > 0$ such that

$$B(\tilde{F}, \epsilon) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = 1\} \subset \tilde{K}^{qc}.$$

Let $F = \Delta^{1/3} \tilde{F}$; then $F \in K^{qc}$ by part (i). We wish to conclude that $F \in \text{rint } K^{qc}$ and, in particular, that $B(F, \Delta^{1/3} \epsilon) \cap \{A : \det A = \Delta\} \subset K^{qc}$. It is easy to see that for any $G \in B(F, \Delta^{1/3} \epsilon) \cap \{A : \det A = \Delta\}$, $|\Delta^{-1/3} G - \tilde{F}| < \epsilon$ and $\det \Delta^{-1/3} G = 1$. Therefore,

$$\Delta^{-1/3} G \in B(\tilde{F}, \epsilon) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = 1\} \subset \tilde{K}^{qc}$$

so that $\Delta^{-1/3}G \in \tilde{K}^{qc} = \Delta^{-1/3}K^{qc}$ from part (i) and $G \in K^{qc}$. The reverse implication is proved similarly. \square

Proof of Theorem 3.5. We prove the result for the case $K = K_{ct}$ and the general statement then follows. From Lemma 3.4 and Lemma 3.6, we know that the relative interior of K^{qc} is non-empty and, in particular, $\Delta^{1/3}\mathbf{1} \in \text{rint } K^{qc}$. The idea behind the proof is then rather natural: if we choose $\Delta > 0$ close enough to 1, we can surely find a rank-one direction, say $a \otimes n$, such that the line

$$\mathbf{1} + ta \otimes n, \quad t \in \mathbb{R}$$

intersects the relative neighbourhood of $\Delta^{1/3}\mathbf{1}$ lying in K^{qc} , that is the set

$$B\left(\Delta^{1/3}\mathbf{1}, \Delta^{1/3}\epsilon\right) \cap \{A \in \mathbb{R}^{3 \times 3} : \det A = \Delta\}.$$

Then, the point of intersection, say F , will itself be in $\text{rint } K^{qc}$. Choose any vector $n \in \mathbb{R}^3$, $|n| = 1$ and let $a = (\Delta - 1)n$. We claim that $F = \mathbf{1} + a \otimes n$ is the desired point. Trivially

$$\det F = 1 + a \cdot n = \Delta$$

and it remains to show that

$$|F - \Delta^{1/3}\mathbf{1}| < \Delta^{1/3}\epsilon.$$

But, with $a = (\Delta - 1)n$, we obtain that

$$\begin{aligned} |F - \Delta^{1/3}\mathbf{1}|^2 &= |(1 - \Delta^{1/3})\mathbf{1} + a \otimes n|^2 \\ &= 3(1 - \Delta^{1/3})^2 + 2(1 - \Delta^{1/3})a \cdot n + |a|^2 \\ &= (1 - \Delta^{1/3})^2(\Delta^{4/3} + 2\Delta + \Delta^{2/3} + 2) \\ &< \Delta^{2/3}\epsilon^2, \end{aligned}$$

where the last inequality follows from (3.6). This completes the proof. \square

Combining the above result with our construction of the non-planar interface in Lemma 3.3 we deduce that under the hypotheses of Theorem 3.5, we can construct a stress-free curved austenite-martensite interface for a set of martensitic wells containing the three well configuration K_{ct} . As remarked already, the configuration K_{ct} in (3.7) corresponds to a cubic-to-tetragonal transition; nevertheless, such interfaces have not so far been observed in materials with such high symmetry in the martensitic phase. Thus, proving the existence of this relative interior point for transformations with lower martensitic symmetry is desirable. Indeed, through Theorem 3.5, we can prove the existence of rank-one connections between $\text{SO}(3)$ and $\text{rint } K^{qc}$ for any transformation with cubic austenite (with special lattice parameters) through the machinery used by Bhattacharya in [7]; in particular, this includes the cubic-to-orthorhombic transition undergone by Seiner's CuAlNi specimen

To be more specific, let $\mathcal{P}^{24} \subset \text{SO}(3)$ denote the symmetry group of the cube; namely, writing e_1, e_2, e_3 for the standard basis vectors in \mathbb{R}^3 and $R[\theta, e]$ for the rotation by angle θ about the vector $e \in \mathbb{R}^3$, \mathcal{P}^{24} consists of the following rotations:

$$\mathbf{1},$$

$$R[\pm 90^\circ, e_1], R[\pm 90^\circ, e_2], R[\pm 90^\circ, e_3],$$

$$R[\pm 120^\circ, e_1 + e_2 + e_3], R[\pm 120^\circ, -e_1 + e_2 + e_3],$$

$$R[\pm 120^\circ, e_1 - e_2 + e_3], R[\pm 120^\circ, e_1 + e_2 - e_3],$$

$$R[180^\circ, e_1], R[180^\circ, e_2], R[180^\circ, e_3],$$

$$R[180^\circ, e_1 \pm e_2], R[180^\circ, e_2 \pm e_3], R[180^\circ, e_3 \pm e_1].$$

Lemma 3.7. *Let $U \in \mathbb{R}^{3 \times 3}$ be positive definite, symmetric with $\det U = \Delta$ and let*

$$K := \bigcup_{R \in \mathcal{P}^{24}} \text{SO}(3)R^T U R.$$

Then, the set K^{qc} contains the three-well configuration K_{ct} given by

$$K_{ct} = \bigcup_{i=1}^3 \text{SO}(3) V_i \quad (3.8)$$

with

$$V_1 = \text{diag}(\mu, \sqrt{\nu\xi}, \sqrt{\nu\xi}), V_2 = \text{diag}(\sqrt{\nu\xi}, \mu, \sqrt{\nu\xi}), V_3 = \text{diag}(\sqrt{\nu\xi}, \sqrt{\nu\xi}, \mu),$$

and μ, ν, ξ taking distinct values in the set

$$\left\{ \frac{\Delta}{\sqrt{(\text{cof } U^2)_{jj}}}, \sqrt{\frac{(\text{cof } U^2)_{jj}}{(U^2)_{kk}}}, \sqrt{(U^2)_{kk}} \right\},$$

where $j, k = 1, 2, 3$, $j \neq k$, and for $A \in \mathbb{R}^{3 \times 3}$, $(\text{cof } A)_{jj}$ denotes the (j,j) -component of the cofactor matrix of A .

Proof. For much of the proof, we follow Bhattacharya [7]; nevertheless, to retain completeness, we repeat all necessary arguments. Let $R = R[180^\circ, e_1] = -\mathbf{1} + 2e_1 \otimes e_1 \in \mathcal{P}^{24}$; by Mallard's law (see Proposition 2.2 in [7]) there exist $Q \in \text{SO}(3)$, $a \in \mathbb{R}^3$ such that $QUR - U = a \otimes e_1$. In particular, for all $\lambda \in [0, 1]$,

$$F_\lambda = \lambda QUR + (1 - \lambda)U = U + \lambda a \otimes e_1 \in K^{qc}.$$

Set $C_\lambda = F_\lambda^T F_\lambda$; then,

$$C_\lambda = U^2 + \lambda[Ua \otimes e_1 + e_1 \otimes Ua] + \lambda^2|a|^2 e_1 \otimes e_1,$$

$$C_0 = \begin{pmatrix} (C_0)_{11} & (C_0)_{12} & (C_0)_{13} \\ (C_0)_{12} & (C_0)_{22} & (C_0)_{23} \\ (C_0)_{13} & (C_0)_{23} & (C_0)_{33} \end{pmatrix}, \quad C_1 = RC_0R = \begin{pmatrix} (C_0)_{11} & -(C_0)_{12} & -(C_0)_{13} \\ -(C_0)_{12} & (C_0)_{22} & (C_0)_{23} \\ -(C_0)_{13} & (C_0)_{23} & (C_0)_{33} \end{pmatrix},$$

with $C_0 = U^2$. Note that:

- (1) if $ij \neq 11$ then $(C_\lambda)_{ij} = C_\lambda e_j \cdot e_i = (C_0)_{ij} + \lambda a(i, j)$ is affine in λ ;
- (2) if $ij = 12, 21, 31, 13$ then $(C_1)_{ij} = -(C_0)_{ij}$;
- (3) if $i \neq 1, j \neq 1$ then $(C_1)_{ij} = (C_0)_{ij}$.

By (1) and (2), evaluating for $\lambda = 1$, we infer that $a(i, j) = -2(C_0)_{ij}$ for $ij = 12, 21, 31, 13$ and hence $(C_{1/2})_{ij} = 0$; similarly, by (1) and (3), we find that $(C_{1/2})_{ij} = (C_0)_{ij}$ for $i \neq 1, j \neq 1$. This implies that

$$C_{1/2} = \begin{pmatrix} (C_{1/2})_{11} & 0 & 0 \\ 0 & (C_0)_{22} & (C_0)_{23} \\ 0 & (C_0)_{23} & (C_0)_{33} \end{pmatrix}.$$

But $F_{1/2} \in K^{qc}$ implies $\det F_{1/2} = \Delta$ and thus

$$(C_{1/2})_{11} = \frac{\Delta^2}{(\text{cof } U^2)_{11}}. \quad (3.9)$$

Now let $R = R[180^\circ, e_2] \in \mathcal{P}^{24}$. We can find $Q \in \text{SO}(3)$, $a \in \mathbb{R}^3$ such that $QF_{1/2}R - F_{1/2} = a \otimes e_2$ and, for all $\lambda \in [0, 1]$,

$$G_\lambda = \lambda QF_{1/2}R + (1 - \lambda)F_{1/2} = F_{1/2} + \lambda a \otimes e_2 \in K^{qc}.$$

Setting $D_\lambda = G_\lambda^T G_\lambda$ and repeating the above process, we deduce that

$$D_{1/2} = \begin{pmatrix} \frac{\Delta^2}{(\text{cof } U^2)_{11}} & 0 & 0 \\ 0 & \frac{(\text{cof } U^2)_{11}}{(U^2)_{33}} & 0 \\ 0 & 0 & (U^2)_{33} \end{pmatrix},$$

where, we have used (3.9) and the determinant constraint to calculate $(D_{1/2})_{22}$. It follows that $\sqrt{D_{1/2}} \in K^{qc}$. However, for any $Q \in \text{SO}(3)$, $R \in \mathcal{P}^{24}$, $Q\sqrt{D_{1/2}}R \in K^{qc}$ (see [7]) and using $Q = R$ with $R = R[180^\circ, e_2 + e_3]$, $R = R[180^\circ, e_1 + e_3]$ and $R = R[180^\circ, e_1 + e_2]$, we find that

$$\bigcup_{i=1}^6 \text{SO}(3)\tilde{V}_i \subset K^{qc}, \text{ where}$$

$$\tilde{V}_1 = \sqrt{D_{1/2}} = \begin{pmatrix} \frac{\Delta}{\sqrt{(\text{cof } U^2)_{11}}} & 0 & 0 \\ 0 & \sqrt{\frac{(\text{cof } U^2)_{11}}{(U^2)_{33}}} & 0 \\ 0 & 0 & \sqrt{(U^2)_{33}} \end{pmatrix} =: \text{diag}(\alpha, \beta, \gamma)$$

and \tilde{V}_i , $i = 2, \dots, 6$ are given by permuting the components of \tilde{V}_1 on the diagonal. Next consider, for example, the matrices $\tilde{V}_1 = \text{diag}(\alpha, \beta, \gamma)$, $\tilde{V}_2 = \text{diag}(\alpha, \gamma, \beta)$; Then $\text{SO}(3)\tilde{V}_1 \cup \text{SO}(3)\tilde{V}_2 \subset K^{qc}$ and by the two-well problem - see the comment at (3.5) - we infer that

$$\text{diag}(\alpha, \sqrt{\beta\gamma}, \sqrt{\beta\gamma}) \in K^{qc}.$$

In particular, using the 180° rotations about the diagonals as above, we see that the three-well configuration

$$\text{SO}(3)\text{diag}(\alpha, \sqrt{\beta\gamma}, \sqrt{\beta\gamma}) \cup \text{SO}(3)\text{diag}(\sqrt{\beta\gamma}, \alpha, \sqrt{\beta\gamma}) \cup \text{SO}(3)\text{diag}(\sqrt{\beta\gamma}, \sqrt{\beta\gamma}, \alpha)$$

belongs to K^{qc} . It is easy to see that, by considering the other possible pairs of \tilde{V}_i , we can interchange the roles of α , β and γ , to get another two three-well configurations belonging to K^{qc} . We have now obtained our result with $j = 1$, $k = 2$ in the expressions for μ , ν , ξ . This is because we reached the diagonal element $\tilde{V}_1 \in K^{qc}$ by first applying $R = R[180^\circ, e_1]$ and then $R = R[180^\circ, e_2]$. Alternatively, one can do the diagonalization by first applying $R = R[180^\circ, e_1]$ and then $R = R[180^\circ, e_3]$ or any of the other four possibilities and the result follows. \square

Theorem 3.5 now allows us to deduce the existence of rank-one connections between $\text{SO}(3)$ and $\text{rint } K^{qc}$ for any transition with cubic austenite as in Lemma 3.7:

Corollary 3.8. *Let $U \in \mathbb{R}^{3 \times 3}$ be positive definite, symmetric with $\det U = \Delta$ and satisfy*

$$\frac{|\Delta^{1/3} - 1|}{\Delta^{1/3}} \sqrt{\Delta^{4/3} + 2\Delta + \Delta^{2/3} + 2} < \epsilon(\kappa), \quad (3.10)$$

for some $\kappa \in \mathcal{S}(U)$, $\kappa > 0$, $\kappa \neq 1$, where

$$\mathcal{S}(U) := \bigcup_{j \neq k} \left\{ \frac{\Delta^{1/3}}{(\text{cof } U^2)_{jj}^{1/4}}, \frac{(\text{cof } U^2)_{jj}^{1/4}}{(U^2)_{kk}^{1/4} \Delta^{1/6}}, \frac{(U^2)_{kk}^{1/4}}{\Delta^{1/6}} \right\}$$

and $0 < \epsilon(\kappa) < 1$ is as in Lemma 3.4. Let

$$K := \bigcup_{R \in \mathcal{P}^{24}} \text{SO}(3)R^T U R.$$

Then there exist $a, n \in \mathbb{R}^3$ such that $\mathbf{1} + a \otimes n \in \text{rint } K^{qc}$.

Proof. The proof follows immediately by Theorem 3.5 and Lemma 3.7. For example, suppose that (3.10) holds for $\kappa = \Delta^{1/3}/(\text{cof } U^2)_{jj}^{1/4}$ and some $j \neq k$ fixed; by Lemma 3.7 the three-well configuration in (3.8) is contained in K^{qc} where $\mu = \Delta/\sqrt{(\text{cof } U^2)_{jj}}$, $\nu = \sqrt{(\text{cof } U^2)_{jj}/(U^2)_{kk}}$ and $\xi = \sqrt{(U^2)_{kk}}$. But then

$$\mu = \Delta^{1/3}\kappa^2, \quad \sqrt{\nu\xi} = \frac{\Delta^{1/3}}{\kappa}$$

and Theorem 3.5 applies to give the result. \square

Unfortunately for the CuAlNi specimen of Seiner the value of κ given in Theorem 3.5 is not large enough for Corollary 3.8 to apply and establish the existence of a non-planar interface. To see this note that CuAlNi undergoes a cubic-to-orthorhombic transition and the corresponding transformation strain U is given by

$$U = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}.$$

In accordance with [17], let $\alpha = 1.06372$, $\beta = 0.91542$ and $\gamma = 1.02368$ be the lattice parameters; then $\Delta^{1/3} = (\alpha\beta\gamma)^{1/3} = 0.998935$ and it turns out that the value of κ in the set $\mathcal{S}(U)$ that maximizes $(\kappa - 1)^2$ is $\kappa^* = \beta^{1/3}(\alpha\gamma)^{-1/6} = 0.957286$. In particular, $\kappa^* < 3/2$ and we may take $\epsilon = (\kappa^* - 1)^2/62 = 2.94277 \times 10^{-5}$. But then

$$2.60824 \times 10^{-3} = \frac{|\Delta^{1/3} - 1|}{\Delta^{1/3}} \sqrt{\Delta^{4/3} + 2\Delta + \Delta^{2/3} + 2} > \epsilon = 2.94277 \times 10^{-5},$$

so that (3.10) does not hold. For other materials Δ might be closer to 1 so that Corollary 3.8 applies.

4. CONCLUDING REMARKS

Our method of constructing a non-planar interface for a set of martensitic wells K depends on the existence of rank-one connections between $\text{SO}(3)$ and $\text{rint } K^{qc}$. Since K^{qc} is not known for more than two martensitic energy-wells, establishing the existence of such rank-one connections is a difficult problem. Above, we gave conditions for the existence of such rank-one connections for any transition with cubic austenite, but the method of doing so relied on finding an embedded cubic-to-tetragonal configuration and did not exploit the potentially rich structure of K^{qc} . The resulting restriction on the determinant seems much too strong for typical values of the lattice parameters. Possibly, via enlarging the neighbourhood of $\mathbf{1} \in \mathbb{R}^{3 \times 3}$ from Lemma 3.4, we might be able to predict non-planar interfaces for existing alloys or even Seiner's specimen. There could also be entirely new ways of constructing non-planar interfaces which come with less stringent assumptions on the lattice parameters. This is ultimately a problem on quasiconvex hulls and appropriate jump conditions, both of which pose deep and interesting questions. Moreover, we note that the analysis does not reveal much about the microstructure corresponding to the relative interior point. Based on [11], this interior point must be a (potentially high order) laminate but we cannot be more explicit.

Lastly, we mention that R. D. James and others [9, 13] have extensively investigated the case when the middle eigenvalue $\lambda_2(U_i)$ of the martensitic variants equals 1 and the so-called *cofactor condition* (see e.g. [13]) holds, both theoretically, and experimentally by appropriately 'tuning' the lattice parameters of alloys. This work has established a strong connection between these conditions and low thermal hysteresis. Under the cofactor condition, one is able to theoretically construct non-planar interfaces with a pure phase of austenite, without the need for a boundary

layer; however, this is restricted to this special case and the fact that martensitic twins are directly compatible with the austenite [8].

ACKNOWLEDGEMENT

The research of both authors was supported by the EPSRC Science and Innovation award to the Oxford Centre for Nonlinear PDE (EP/E035027/1) and the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement n° 291053. The research of JMB was also supported by a Royal Society Wolfson Research Merit Award. We would like to thank Bernd Kirchheim and Hanuš Seiner for very useful discussions.

REFERENCES

- [1] C. Amrouche, P. G. Ciarlet and P. Ciarlet Jr, Vector and scalar potentials, Poincaré's theorem and Korn's inequality, *C. R. Math. Acad. Sci. Paris*, 345 (2007), 603–608.
- [2] J. M. Ball and C. Carstensen, Non-classical austenite-martensite interfaces, *J. Phys. IV France* 7 (1997), 35–40
- [3] J. M. Ball and C. Carstensen, *in preparation*.
- [4] J. M. Ball and R. D. James, Fine phase mixtures as minimizers of energy, *ARMA* **100** no. 1 (1987) 13–52.
- [5] J. M. Ball and R. D. James, Proposed experimental tests of a theory of fine microstructure and the two-well problem, *Phil. Tran. R. Soc. Lond. A* 338 (1992), 389–450.
- [6] J. M. Ball, K. Koumatos, and H. Seiner, An analysis of non-classical austenite-martensite interfaces in CuAlNi, Proceedings ICOMAT08, TMS, (2010), 383–390 (at arXiv:1108.6220v1).
- [7] K. Bhattacharya, Self-accommodation in martensite, *ARMA* 120 (3) (1992), 201–244.
- [8] X. Chen, V. Srivastava, V. Dabade and R. D. James, Study of the cofactor conditions: conditions of super-compatibility between phases, preprint.
- [9] J. Cui, Y. S. Chu, O. Famodu, Y. Furuya, J. Hattrick-Simpers, R. D. James, A. Ludwig, S. Thienhaus, M. Wuttig, Z. Zhang and I. Takeuchi, Combinatorial search of thermoelastic shape-memory alloys with extremely small hysteresis width, *Nature materials*, 5 (4) (2006), 286–290.
- [10] G. Dolzmann, *Variational methods for crystalline microstructure—analysis and computation*, Lecture Notes in Math., Springer-verlag, 2003.
- [11] G. Dolzmann and B. Kirchheim, Liquid-like behavior of shape memory alloys, *C. R. Math. Acad. Sci. Paris*, 336 (5) (2003), 441–446.
- [12] T. Iwaniec, G. C. Verchota and A. L. Vogel, The failure of rank-one connections, *ARMA* 163 (2) (2002), 125–169.
- [13] R. D. James and Z. Zhang, A way to search for multiferroic materials with “unlikely” combinations of physical properties, *Magnetism and structure in functional materials* (2005), 159–175.
- [14] J. M. Lee, *Introduction to smooth manifolds*, Springer, 2012
- [15] V. G. Maz'ya, *Sobolev spaces*, Springer-Verlag, 1985.
- [16] S. Müller, *Variational models for microstructure and phase transitions*, Lecture Notes in Math., 1999.
- [17] P. Sedláč, H. Seiner, M. Landa, V. Novák, P. Šittner, Ll. Mañosa, Elastic constants of bcc austenite and 2H orthorhombic martensite in CuAlNi shape memory alloy, *Acta Materialia* 53 (2005), 3643–3661.
- [18] H. Seiner and M. Landa, Non-classical austenite-martensite interfaces observed in single crystals of Cu–Al–Ni, *Phase Transitions* **82** no. 18 (2009) 793–807.

KONSTANTINOS KOUMATOS: MATHEMATICAL INSTITUTE, UNIVERSITY OF OXFORD, 24–29 ST GILES', OXFORD OX1 3LB, UNITED KINGDOM.

E-mail address: koumatos@maths.ox.ac.uk

JOHN M. BALL: MATHEMATICAL INSTITUTE, UNIVERSITY OF OXFORD, 24–29 ST GILES', OXFORD OX1 3LB, UNITED KINGDOM.

E-mail address: ball@maths.ox.ac.uk