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Compatibility conditions for microstructures and the austenite–martensite transition

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Abstract

We explore theoretically the possibility of austenite–martensite transformations more complicated than those envisaged by the crystallographic theory, and make corresponding experimental predictions. The use of the Hadamard jump condition in this context is justified, and leads also to results on non-attainment of minimum energy. © 1999 Elsevier Science S.A. All rights reserved.

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1. Introduction

The crystallographic theory of martensite [1] assumes that the martensitic microstructure in contact with the austenite is a simple laminate. We relax this requirement so as to allow more general martensitic microstructures. In particular, we give necessary and sufficient conditions on lattice parameters for the existence in single crystals of planar non-classical austenite–martensite interfaces separating a pure phase of austenite from a homogeneous martensitic microstructure, that is one whose macroscopic deformation gradient, or weak limit, namely the deformation gradient observed on a length-scale sufficiently large for the underlying microstructure not to be seen, is constant.

The classical Hadamard jump condition states that there exists a continuous deformation having constant gradients A, B on opposite sides of a planar interface with normal m if and only if:

$$A - B = a \otimes m \tag{1.1}$$

for some vector a. To study non-classical interfaces we need to know if we can use this condition when the deformation on the martensite side of the interface is more complex, such as a layers-within-layers structure (perhaps involving several variants), or even a non-homogeneous structure with fractal refinement as the interface is approached (see Fig. 1). (Fractal structures have been observed in quartz [2] and CuAlNi [3].) As a by-product, our analysis of this issue leads to statements on non-attainment of minimum energy and the formation of microstructure.

We use the non-linear elasticity approach to martensitic transformations developed in [4], [5], in which microstructures are identified with 'minimizing sequences' for the total free energy:

$$I_\theta(y) = \int_\Omega \varphi(\nabla y(x), \theta)\mathrm{d}x, \tag{1.2}$$

where interfacial energy contributions are ignored. Here, $y(x)$ denotes the deformed position of the particle at $x \in \Omega$, where the reference configuration Ω represents undistorted austenite. The free energy function $\varphi(F, \theta)$ depends on the deformation gradient F and the temperature θ. By frame-indifference, $\varphi(RF, \theta) = \varphi(F, \theta)$ for all F, θ and for all rotations R, i.e. for all 3×3 matrices in the set $SO(3) := \{R : R^{\mathrm{T}}R = \mathbf{1}, \det R = 1\}$. Adding a suitable function of θ we may assume that $\min_F \varphi(F, \theta) = 0$. At the transformation temperature θ_c the energy wells of φ are given by $SO(3)$ for the austenite, and by $SO(3)U_i$ for each of the N different variants of martensite, with $U_i = U_i^{\mathrm{T}} > 0$ for each i. Thus $\varphi(F,\theta_c) \geq 0$ with $\varphi(F,\theta_c) = 0$ precisely for those F in the set $SO(3) \cup \cup_{i=1}^{N} SO(3)U_i$. For $\theta > \theta_c$, φ is minimized just

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at the austenite well $SO(3)\alpha(\theta)\mathbf{1}$, while for $\theta < \theta_c$ the martensite wells minimize energy. Here $\alpha(\theta)$, $\alpha(\theta_c) = 1$, describes the thermal expansion of the austenite; the U_i also depend on temperature.

Following [7], p. 402 ff we consider various transformations. For an orthorhombic to monoclinic transformation we have $N = 2$ and in a suitable basis:

$$U_1 = \mathrm{diag}(\eta_1, \eta_2, \eta_3), \qquad U_2 = \mathrm{diag}(\eta_2, \eta_1, \eta_3), \tag{1.3}$$

with lattice parameters $\eta_i > 0$, $\eta_1 \neq \eta_2$ For a cubic to tetragonal transformation we have $N = 3$ and:

$$U_1 = \mathrm{diag}(\eta_2, \eta_1, \eta_1), \qquad U_2 = \mathrm{diag}(\eta_1, \eta_2, \eta_1),$$
$$U_3 = \mathrm{diag}(\eta_1, \eta_1, \eta_2), \tag{1.4}$$

where the lattice parameters $\eta_1 > 0$, $\eta_2 > 0$, $\eta_1 \neq \eta_2$. For cubic to orthorhombic transformations $N = 6$, and there are two different types. The first corresponds to the change of point group $\mathscr{P}^{(432)} \to \mathscr{P}^{(222)}$, where $\mathscr{P}^{(432)}$ denotes the group of rotations of a cube into itself and $\mathscr{P}^{(222)}$ the orthorhombic subgroup with axes consisting of three face normals, with $U_1 = \mathrm{diag}\ (\eta_1, \eta_2, \eta_3)$ and $U_2, \ldots, U_6$ obtained by permuting the distinct $\eta_i > 0$. However, we do not know of examples in which this type of transformation occurs in the absence of stress. The other type, observed in materials such as AgCd and CuAlNi, corresponds to the change of point group $\mathscr{P}^{(432)} \to \mathscr{P}^{(222)'}$, where $\mathscr{P}^{(222)'}$ is an orthorhombic subgroup of $\mathscr{P}^{(432)}$ with axes consisting of two face diagonals and one face normal. In this case:

$$U_1 = \frac{1}{2}\eta_1(e_1 + e_2) \otimes (e_1 + e_2) + \frac{1}{2}\eta_2(e_1 - e_2) \otimes (e_1 - e_2) + \eta_3\, e_3 \otimes e_3, \tag{1.5}$$

where (e_1, e_2, e_3) is an orthonormal basis of unit vectors in the cubic directions, and $U_2, \ldots, U_6$ are obtained by permuting and changing the sign of the e_i.

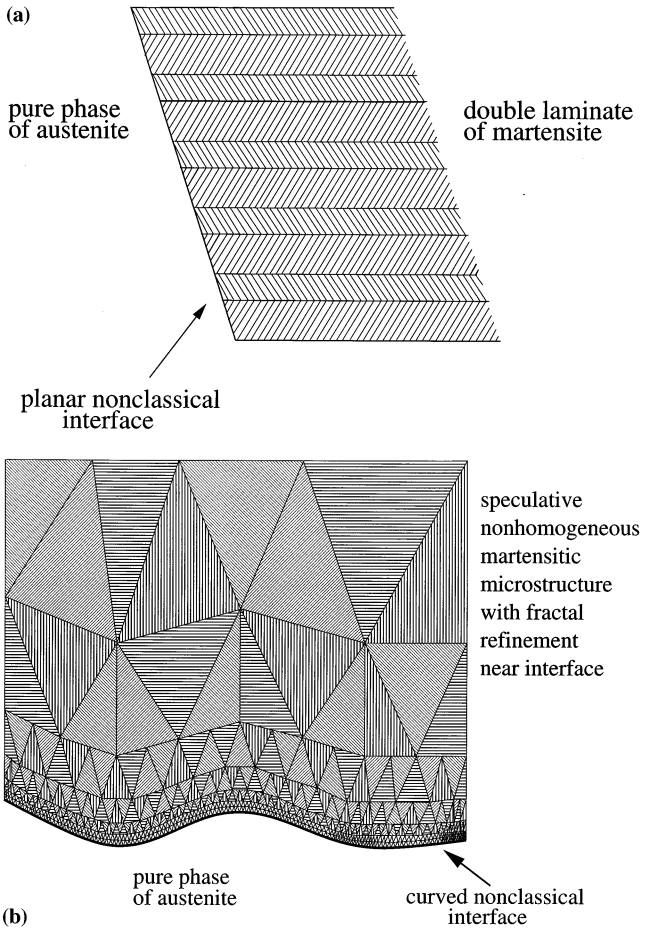

Fig. 1. Non-classical austenite–martensite interfaces in which the martensite has (a) a layers-within-layers structure with constant deformation gradient in each sublayer, (b) a speculative fractal structure.

2. Microscopic and macroscopic deformation gradients

Given a set $\mathscr{K}$ of energy wells, an important related set is the quasiconvexification $Q(\mathscr{K})$ of $\mathscr{K}$, that is the set of macroscopic deformation gradients corresponding to microstructures with gradients in $\mathscr{K}$. One of several equivalent precise definitions is that $Q(\mathscr{K})$ is the set of matrices F for which there exists a sequence $z^{(j)}$ of deformations satisfying $z^{(j)}(x) = Fx$ for x belonging to the boundary $\partial\Omega$ of Ω, and such that $\nabla z^{(j)}(x)$ is bounded independently of x and j with $\nabla z^{(j)} \to \mathscr{K}$ in the sense of measure (i.e. the volume of the set of points x with $\nabla z^{(j)}(x)$ lying outside any prescribed neighbourhood of $\mathscr{K}$ tends to zero as $j \to \infty$). Another equivalent definition is given after Eq. (4.2) below.

It is known how to compute $Q(\mathscr{K})$ when $\mathscr{K}$ consists of just two martensitic energy wells. Consider the orthorhombic to monoclinic case, with U_1, U_2 given by Eq. (1.3), and set:

$$\mathscr{K} = SO(3)U_1 \cup SO(3)U_2. \tag{2.1}$$

We make use of the following characterization of $Q(\mathscr{K})$ and of the corresponding macroscopic deformations.

Theorem 2.1. *[5–7]* For $\mathscr{K}$ given by Eq. *(2.1)*, $Q(\mathscr{K})$ consists of those $A \in M^{3\times 3}$ with $\det A > 0$ such that $A^{\mathrm{T}}A = \mathrm{diag}\ (a, b, \eta_3^2) + c(e_1 \otimes e_2 + e_2 \otimes e_1)$, where $a > 0$, $b > 0$, $a + b \pm 2c \leq \eta_1^2 + \eta_2^2$, and $ab - c^2 = \eta_1^2\eta_2^2$. Furthermore, any invertible y with $\Delta\, y(x) \in Q(\mathscr{K})$ a.e. is a plane strain, i.e. $y(x) = Q(z_1(x), z_2(x), \eta_3 x_3 + \mu)$ with $Q \in SO(3)$, and $\partial z_1/\partial x_3 = \partial z_2/\partial x_3 = 0$.

Here and below we use the standard abbreviation a.e. for 'almost everywhere', meaning except possibly on a set of zero volume.

3. Non-attainment of minimum energy and the formation of microstructure

Consider the orthorhombic to monoclinic case and let $\partial\Omega$ have a flat piece Γ with unit normal m. More precisely, we may suppose that Γ passes through the origin and is a subset of the plane $\Pi = \{x\in\mathbf{R}^3 : x\cdot m = 0\}$, and that for some $r>0$, $\Omega\cap B_r = \{x\in\mathbf{R}^3 : x\cdot m < 0\}\cap B_r$ and $\Gamma\supset\Pi\cap B_r$, where $B_r = \{x\in\mathbf{R}^3 : |x|<r\}$. Assume linear boundary conditions on Γ, i.e. $y(x) = A\,x$ for all $x\in\Gamma$ for some matrix A. Then we have the following version of the Hadamard jump condition.

Theorem 3.1. Suppose that an invertible $y:\Omega\to\mathbf{R}^3$ satisfies $\nabla y(x)\in Q(\mathscr{K})$ for a.e. $x\in\Omega$ and linear boundary conditions $y|_\Gamma = A\,x$. Then there exists $a\in\mathbf{R}^3$ such that $A + a\otimes m\in Q(\mathscr{K})$. If $m\cdot e_3\neq 0$ then, in addition, $\nabla y(x)$ is constant a.e. for $|x|$ sufficiently small.

The proof is given in [8] and is an easy consequence of the plane strain assertion of Theorem 2.1 provided $m\cdot e_3\neq 0$. However, the case $m\cdot e_3 = 0$ requires a deep mathematical result [9] on quasi-regular mappings.

Theorem 3.1 implies that if $\theta<\theta_c$ and $m\cdot e_3\neq 0$ the minimum of the total energy I_θ subject to the boundary condition $y|_\Gamma = A\,x$ is not in general attained, so that minimizing sequences necessarily develop microstructure. To see this we need only choose A such that $A + b\otimes m\in Q(\mathscr{K})$ for some b, but $A + a\otimes m\notin\mathscr{K}$ for any a. Then it can be shown that the infimum of I_θ subject to the boundary conditions is zero, so that applying the theorem to a minimizer we deduce that $\nabla y(x) = A + a\otimes m$ for $|x|$ sufficiently small, and hence $A + a\otimes m\in\mathscr{K}$, a contradiction.

Using the same techniques it is also shown in [8] that for $\theta=\theta_c$, provided $\eta_3\neq 1$, boundaries between austenite and martensite, if not so highly irregular that they have positive volume, are necessarily locally planar, with the macroscopic deformation gradient locally constant on each side.

If linear boundary conditions are specified on the entire boundary we obtain the following nonattainment result [8] where Ω is an arbitrary bounded domain with sufficiently regular boundary.

Theorem 3.2. If $A\in Q(\mathscr{K})\backslash\mathscr{K}$ then $\inf_{y|_{\partial\Omega}=Ax}\int_\Omega\psi(D\,y)\mathrm{d}x$ is not attained.

Proof. Suppose $A\in Q(\mathscr{K})$ and that y is a minimizer. Then $D\,y(x)\in\mathscr{K}$ a.e. in Ω. Since $y|_{\partial\Omega}$ is linear, a known invertibility theorem ensures that y is invertible. Hence, by Theorem 2.1, y is a plane strain. Since y is linear on the entire boundary of the three-dimensional region Ω, it follows that y is affine, and hence that $D\,y = A$ a.e. in Q. Hence $A\in\mathscr{K}$, which contradicts $\mathrm{A}\in\mathrm{Q}(\mathscr{K})\backslash\mathscr{K}$.

Theorem 3.2 states that for $A\in Q(\mathscr{K})\backslash\mathscr{K}$, minimizing sequences for I_θ generate microstructure, solving a question in [5]. Note that by Theorem 7.3 in [5], the result also applies to cubic to tetragonal transformations if A belongs to the quasiconvex hull of any pair of tetragonal wells. In two dimensions the corresponding result is false (see [10] and unpublished work of the same authors).

4. Non-classical austenite–martensite interfaces

We let $\theta=\theta_c$ and consider the case of planar non-classical austenite–martensite interfaces separating a region of undistorted austenite (corresponding without loss of generality to $\nabla y = \mathbf{1}$) from a homogeneous microstructure of martensite. Thus we seek vectors b, $m\in\mathbf{R}^3$ with $|m| = 1$, such that:

$$1 + b\otimes m\in Q(\mathscr{K}), \tag{4.1}$$

where $\mathscr{K} = \cup_{i=1}^{N} SO(3)U_i$. To obtain some necessary conditions we need some terminology. A function $\varphi = \varphi(F)$ is polyconvex if it can be expressed in the form $\varphi(G) = h(G, \mathrm{cof}\,G, \det G)$ for some convex h, where $\mathrm{cof}\,G = \det G\cdot G^{-\mathrm{T}}$ denotes the matrix of cofactors of G. The polyconvexification $P(\mathscr{K})$ of $\mathscr{K}$ is defined as the set of F such that:

$$\varphi(F)\le\max_{G\in\mathscr{K}}\varphi(G) \tag{4.2}$$

for every polyconvex function φ. (An alternative definition of $Q(\mathscr{K})$ is that Eq. (4.2) holds for all quasiconvex functions.) We always have that $Q(\mathscr{K})\subset P(\mathscr{K})$. If $\det F>0$, recall that the singular values of F are the square roots of the eigenvalues of the symmetric, positive definite matrix $F^{\mathrm{T}}F$. We write these counting multiplicities as $0<\sigma_{\min}(F)\le\sigma_{\mathrm{mid}}(F)\le\sigma_{\max}(F)$ We suppose that the singular values of each of the U_i are the same and given by $0<\eta_{\min}\le\eta_{\mathrm{mid}}\le\eta_{\max}$. Since $\det F = \sigma_{\min}(F)\sigma_{\mathrm{mid}}(F)\sigma_{\max}(F)$ the determinants of the U_i are all equal to $\delta := \eta_{\min}\,\eta_{\mathrm{mid}}\,\eta_{\max}$.

Let $F = \mathbf{1} + b\otimes m\in P(\mathscr{K})$. Applying Eq. (4.2) with $\varphi(G) = \pm\det G$ we deduce that $\det F = \delta$. We now use the following lemma, which isolates the key mathematical point of the crystallographic theory [1].

Lemma 4.1. *[4,11]* Let F be a non-singular matrix that is not a rotation. Then, the wells $SO(3)$ and $SO(3)F$ are rank-one connected if and only if the middle eigenvalue of $F^{\mathrm{T}}F$ is 1. In this case, $\mathbf{1} + b\otimes m\in SO(3)F$ for some b if and only if m is a non-vanishing multiple of one of the two vectors $\sqrt{1-\lambda_1}\,e_1 \pm \sqrt{\lambda_3 - 1}e_3$, where $0\le\lambda_1\le 1\le\lambda_3$ are the three eigenvalues of $F^{\mathrm{T}}F$ with corresponding orthonormal eigenvectors e_1, e_2, e_3.

Hence, since $\det F = \delta$:

$$\sigma_{\mathrm{mid}}(F)=1 \quad \textit{and} \quad \sigma_{\min}(F)\sigma_{\max}(F)=\delta. \tag{4.3}$$

Next use the function $\varphi(G)=\sigma_{\max}(G)$. Since $\sigma_{\max}(G)=\max_{|x|=1}|Gx|$, φ is convex and hence polyconvex. Thus from Eq. (4.2):

$$\sigma_{\max}(F)\le\max_{G\in\mathscr{K}}\sigma_{\max}(G)=\eta_{\max}. \tag{4.4}$$

Finally use the function $\varphi(G)=\sigma_{\max}(\mathrm{cof}\ G)$, which is a convex function of cof G and hence also polyconvex. By Eq. (4.2) we therefore have also that:

$$\begin{aligned}\det F\,\sigma_{\min}(F)^{-1}&=\sigma_{\max}(\mathrm{cof}\,F)\le\max_{G\in\mathscr{K}}\sigma_{\max}(\mathrm{cof}\,G)\\&=\delta\eta_{\min}^{-1},\end{aligned}$$

which since $\det F=\delta$ implies that:

$$\eta_{\min}\le\sigma_{\min}(F). \tag{4.5}$$

The inequalities in Eqs. (4.4) and (4.5) and the first identity in Eq. (4.3) yield:

$$\eta_{\min}\le\sigma_{\min}(F)\le 1\le\sigma_{\max}(F)\le\eta_{\max}. \tag{4.6}$$

Straightforward considerations show that Eqs. (4.3) and (4.6) imply that:

$$\eta_{\min}\le\eta_{\mathrm{mid}}^{-1}\le\eta_{\max} \tag{4.7}$$

as necessary conditions for $\mathbf{1}+b\otimes m\in P(\mathscr{K})$ for some b, m.

4.1. Orthorhombic to monoclinic transformations

In this case Theorem 2.1 gives $Q(\mathscr{K})$ explicitly and we can use Lemma 4.1 to derive necessary and sufficient conditions for the existence of b, m satisfying Eq. (4.1). These are that if $\eta_3\le 1$ then:

$$\eta_2^{-1}\le\eta_1\le 1 \quad \text{or} \quad 1\le\eta_2^{-1}\le\eta_1, \tag{4.8}$$

and if $\eta_3\ge 1$ then:

$$\eta_2\le\eta_1^{-1}\le 1 \quad \text{or} \quad 1\le\eta_2\le\eta_1^{-1}. \tag{4.9}$$

For the existence of a classical austenite–martensite interface (Eq. (4.1)) is replaced by $\mathbf{1}+b\otimes m=\lambda\mathrm{A}+(1-\lambda)\mathrm{B}$ for $0<\lambda<1$ and $\mathrm{A},\mathrm{B}\in\mathscr{K}$, and we recover the classical results of the crystallographic theory that this is possible for some b, m if and only if:

$$\begin{aligned}&\eta_1^2+\eta_2^2\le 2 \quad \text{if} \quad \eta_1\eta_2\le 1,\\&\eta_1^{-2}+\eta_2^{-2}\le 2 \quad \text{if} \quad \eta_1\eta_2\ge 1.\end{aligned} \tag{4.10}$$

The details of these calculations, together with a characterization of the non-classical habit-plane normals, are given in [12] for the case $\eta_3\neq 1$ and in [8] for the general case. The results are displayed in Fig. 2(a) and (b).

4.2. Cubic to tetragonal transformations

Let $\mathscr{K}=\bigcup_{i=1}^{3}SO(3)U_i$, where the U_i are given by Eq. (1.4). Then by Eq. (4.7) for a non-classical planar interface between austenite and homogeneous martensite we have the necessary conditions:

$$\begin{aligned}&\eta_1\le\eta_1^{-1}\le\eta_2 \quad \text{if} \quad \eta_1\le\eta_2,\\&\eta_2\le\eta_1^{-1}\le\eta_1 \quad \text{if} \quad \eta_1\ge\eta_2.\end{aligned} \tag{4.11}$$

But these conditions correspond exactly to the necessary and sufficient conditions (Eqs. (4.8) and (4.9)) with $\eta_3=\eta_1$. These latter conditions are shown in Fig. 2(c), together with the regions in (η_1,η_2)-space corresponding to classical austenite–martensite interfaces. We have thus proved:

Theorem 4.2. The following conditions are equivalent: (i) $\mathbf{1}+b\otimes m\in Q(\mathscr{K})$ for some b,m; (ii) $\mathbf{1}+b\otimes m\in P(\mathscr{K})$ for some b, m; (iii) η_1, η_2 satisfy Eq. (4.11).

4.3. Cubic to orthorhombic transformations

In this case we let $\mathscr{K}=\bigcup_{i=1}^{6}SO(3)U_i$ with the U_i given by one of the two possibilities in the introduction. For a non-classical planar interface between austenite and homogeneous martensite we have the necessary conditions (Eq. (4.7)). If $\eta_{\min}\le 1\le\eta_{\mathrm{mid}}^{-1}\le\eta_{\max}$ then we can choose $(\bar\eta_1,\bar\eta_2,\bar\eta_3)=(\eta_{\max},\eta_{\mathrm{mid}},\eta_{\min})$, while if $\eta_{\min}\le\eta_{\mathrm{mid}}^{-1}\le 1\le\eta_{\max}$ we can choose $(\bar\eta_1,\bar\eta_2,\bar\eta_3)=(\eta_{\min},\eta_{\mathrm{mid}},\eta_{\max})$ so that the conditions in Eq. (4.8) or Eq. (4.9) hold for the $\bar\eta_i$. This implies that $\mathbf{1}+b\otimes m\in Q(SO(3)U_i\cup SO(3)U_j)$ for some b, m and some i, j. In fact, supposing for example that $\eta_{\mathrm{mid}}\ge 1$, we can take $U_i=\mathrm{diag}\,(\eta_{\min},\eta_{\mathrm{mid}},\eta_{\max})$, $U_j=\mathrm{diag}\,(\eta_{\mathrm{mid}},\eta_{\min},\eta_{\max})$, in the basis (e_1,e_2,e_3). In the case $\mathscr{P}^{(432)}\to\mathscr{P}^{(222)'}$ we make the extra assumption that either $\eta_3=\eta_{\max}$, $\eta_{\mathrm{mid}}\ge 1$ or $\eta_3=\eta_{\mathrm{mins}}$, $\eta_{\mathrm{mid}}\le 1$. We can then apply the same argument using the basis $\left(\frac{1}{\sqrt{2}}(e_1+e_2),\frac{1}{\sqrt{2}}(e_1-e_2),e_3\right)$. Under these hypotheses we have thus proved:

Theorem 4.3. The following conditions are equivalent: (i) $\mathbf{1}+b\otimes m\in Q(\mathscr{K})$ for some b,m; (ii) $\mathbf{1}+b\otimes m\in\mathscr{P}(\mathscr{K})$ for some b, m; (iii) η_1, η_2, η_3 satisfy Eq. (4.7).

Theorems 4.2, 4.3 are striking in that in neither case are characterizations of $Q(\mathscr{K})$, $\mathscr{P}(\mathscr{K})$ known. In particular, it is not known whether $Q(\mathscr{K})=\mathscr{P}(\mathscr{K})$. They assert that if the lattice parameters allow a non-classical planar interface between austenite and homogeneous martensite, they allow one involving just two martensitic variants. Of course they could simultaneously allow such interfaces involving more than two variants, and this can be expected to increase the set of possible habit-plane normals. Non-classical interfaces in CuAlNi involving four variants in a double laminate have in fact been observed by Chu and James [3]; at the microscopic level the non-classical interface has a zig-zag structure formed by

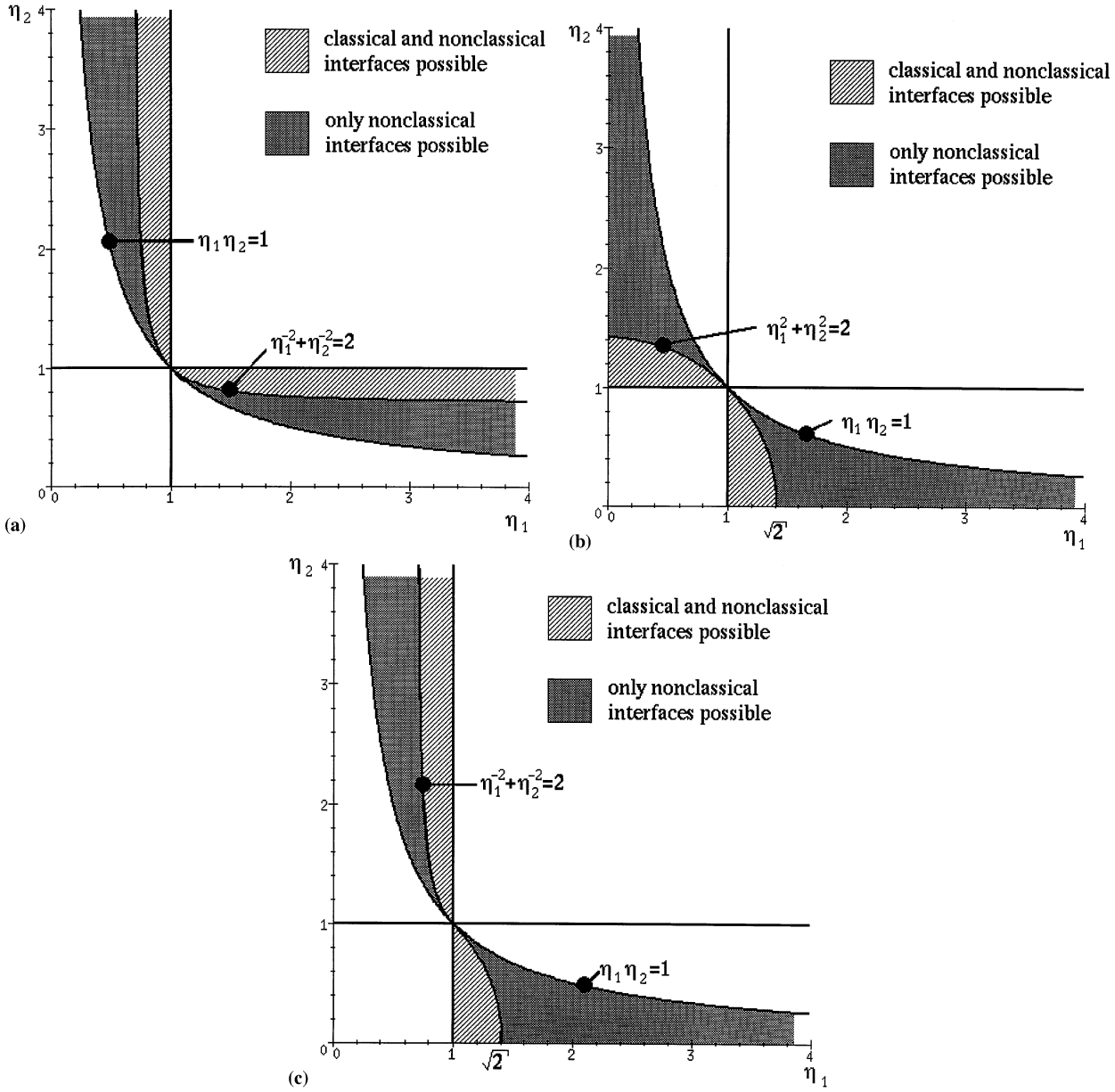

Fig. 2. Lattice parameters allowing classical and non-classical austenite–martensite interfaces. (a) Orthorhombic to monoclinic in case $\eta_3 \leq 1$. (b) Orthorhombic to monoclinic in case $\eta_3 \geq 1$. (c) Cubic to tetragonal, where the martensite microstructure is assumed to be homgeneous.

wedge microstructures of the type analyzed by Bhattacharya [13].

An earlier attempt to understand non-classical austenite–martensite interfaces is the 'double-shear' theory of Acton and Bevis [14] and Ross and Crocker [15]. While it is not straightforward to make a precise comparison with [14,15], it should be noted that our theory allows for martensitic microstructures more complicated than double laminates, and takes proper account of geometric compatibility.

4.4. Experimental predictions

The experimental predictions of our theory are cleanest in the case of orthorhombic to monoclinic transformations. If the η_i satisfy Eq. (4.8) or Eq. (4.9) but not Eq. (4.10) (see Fig. 2(a) and (b)) then austenite is predicted to transform to martensite by planar and locally homogeneous non-classical austenite–martensite interfaces. For η_i not satisfying Eq. (4.8) or Eq. (4.9) we would expect no zero-energy path from austenite to martensite, though it remains a theoretical possibility that such a path could exist with a wild geometrical structure of the austenite and martensite regions. For cubic to tetragonal transformations, if η_1, η_2 satisfy Eq. (4.11) but not Eq. (4.10) then a zero-energy path between austenite and martensite is predicted, and the transformation cannot take place via a classical austenite–martensite interface. Note that the region in the (η_1,

η_2) – plane for which only non-classical interfaces exist has a pair of cusps at $\eta_1 = \eta_2 = 1$, so that for lattice parameters very near 1 the region corresponding to the existence of a classical interface is much larger. While a transformation via a non-classical planar interface between austenite and homogeneous martensite is consistent with the theory, other possibilities are not excluded. If η_1, η_2 satisfy neither Eq. (4.11) nor Eq. (4.10) zero-energy configurations in which smooth or even planar interfaces separate austenite from non-homogeneous martensite are not excluded. The predictions for cubic to orthorhombic transformations are similar. A zero-energy path between austenite and martensite is guaranteed under our hypotheses when Eq. (4.7) holds which could involve a non-classical planar interface between austenite and homogeneous martensite, but the existence of such a zero-energy path is not excluded even if Eq. (4.7) does not hold. Unfortunately we do not know of (and would be very interested in) any experimental work that involves materials with lattice parameters in the non-classical regions described above.

5. Towards a new crystallographic theory of martensite

A satisfying theory of the austenite–martensite transition should not make a priori geometrical assumptions about shapes of the austenite and martensite regions. Of course such a theory should be dynamic, but one can still ask for a geometrically unprejudiced static theory. The results described here, while being fairly close to such a theory for orthorhombic to monoclinic transformations, stop well short for transformations involving more than two martensitic variants. A completely geometrically unprejudiced, but very partial, result can be obtained using the theory of Young measure disjoint sets in [16]. It says that for any of the three changes of symmetry considered here, if the lattice parameters η_i are all sufficiently close to some constant $\bar{\eta} \neq 1$ then there is no zero-energy microstructure involving both austenite and martensite (for the precise statement see [16]). The techniques of the same theory enables one [17] to prove that, for any lattice parameters, if Ω is convex then the existence of any zero-energy microstructure involving both austenite and martensite implies the existence of such a microstructure in which the volume fraction of martensite can take any given value between 0 and 1.

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References

[1] M.S. Wechsler, D.S. Lieberman, T.A. Read, Trans. AIME J. Metals 197 (1953) 1503.
[2] J. Van Landuyt, G. Van Tendeloo, S. Amelinckx, Ultramicroscopy 23 (1987) 371.
[3] C. Chu, R.D. James (personal communication).
[4] J.M. Ball, R.D. James, Arch. Rat. Mech. Anal. 100 (1987) 13.
[5] J.M. Ball, R.D. James, Phil. Trans. Roy. Soc. London A 338 (1992) 389.
[6] J.M. Ball, R.D. James (book in preparation).
[7] J.M. Ball, R.D. James, Proc. Roy. Soc. London A 432 (1991) 93.
[8] J.M. Ball, C. Carstensen, Hadamard's compatibility condition for microstructures (to appear).
[9] Y.G. Reshetnyak, Space mappings of bounded distortion, vol. 73, American Mathematical Society, Providence, 1989.
[10] S. Müller, V. Šverák, Attainment results for the two-well problem by convex integration, in: J. Jost (Ed.), Geometric Analysis and the Calculus of Variations, International Press, 1996, p. 239.
[11] A.G. Khachaturyan, Theory of Structural Transformations in Solids, John Wiley, 1983.
[12] J.M. Ball, C. Carstensen, J. Phys. (France) IV 7 (1997) C5–35.
[13] K. Bhattacharya, Acta Metall. Mater. 39 (1991) 2431.
[14] A.F. Acton, M. Bevis, Mater. Sci. Eng. 5 (1969) 19.
[15] N.D.H. Ross, A.G. Crocker, Acta Metall. 18 (1970) 405.
[16] J.M. Ball, R.D. James, Young measure disjoint sets of gradients and metastability (in preparation).
[17] J.M. Ball, R.D. James (to appear).