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Study of the *cofactor conditions*: Conditions of supercompatibility between phases

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ABSTRACT

The *cofactor conditions*, introduced in James and Zhang(2005), are conditions of compatibility between phases in martensitic materials. They consist of three subconditions: (i) the condition that the middle principal stretch of the transformation stretch tensor $\mathbf{U}$ is unity ($\lambda_2 = 1$), (ii) the condition $\mathbf{a} \cdot \mathbf{U}\mathrm{cof}(\mathbf{U}^2 - \mathbf{I})\mathbf{n} = 0$, where the vectors $\mathbf{a}$ and $\mathbf{n}$ are certain vectors arising in the specification of the twin system, and (iii) the inequality $\mathrm{tr}\mathbf{U}^2 + \det \mathbf{U}^2 - (1/4)|\mathbf{a}|^2|\mathbf{n}|^2 \geq 2$. Together, these conditions are necessary and sufficient for the equations of the crystallographic theory of martensite to be satisfied for the given twin system but for any volume fraction f of the twins, $0 \leq f \leq 1$. This contrasts sharply with the generic solutions of the crystallographic theory which have at most two such volume fractions for a given twin system of the form f^* and $1-f^*$. In this paper we simplify the form of the cofactor conditions, we give their specific forms for various symmetries and twin types, we clarify the extent to which the satisfaction of the cofactor conditions for one twin system implies its satisfaction for other twin systems. In particular, we prove that the satisfaction of the cofactor conditions for either Type I or Type II twins implies that there are solutions of the crystallographic theory using these twins that have *no elastic transition layer*. We show that the latter further implies macroscopically curved, transition-layer-free austenite/martensite interfaces for Type I twins, and planar transition-layer-free interfaces for Type II twins which nevertheless permit significant flexibility (many deformations) of the martensite. We identify some real material systems nearly satisfying the cofactor conditions. Overall, the cofactor conditions are shown to dramatically increase the number of deformations possible in austenite/martensite mixtures without the presence of elastic energy needed for coexistence. In the context of earlier work that links the special case $\lambda_2 = 1$ to reversibility (Cui et al., 2006; Zhang et al., 2009; Zarnetta et al., 2010), it is expected that satisfaction of the cofactor conditions for Type I or Type II twins will lead to further lowered hysteresis and improved resistance to transformational fatigue in alloys whose composition has been tuned to satisfy these conditions.

1. Introduction

This paper gives a precise derivation and implications of the cofactor conditions (James and Zhang , 2005), defined briefly in the abstract. These conditions are appropriate to a material that undergoes an austenite to martensitic phase transformation having symmetry-related variants of martensite. The cofactor conditions represent a degeneracy of the

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equations of the crystallographic theory of martensite (Lieberman et al., 1955; Bowles and Mackenzie, 1954a, 1954b), under which this theory possesses solutions with any volume fraction $0 \le f \le 1$ of the twins (James and Zhang , 2005).

For the special cases $f=0$ and $f=1$ the equations of the crystallographic theory reduce to the equations of compatibility between austenite and the appropriate single variant of martensite. Hence, as also can be seen from the conditions themselves (in particular, the condition $\lambda_2 = 1$), the cofactor conditions imply perfect compatibility between austenite and each single variant of martensite. The solutions of the crystallographic theory for the intermediate volume fractions $0 < f < 1$ imply the existence of the standard low energy transition layers between austenite and finely twinned martensite.

The main result of this paper is that in many cases, the cofactor conditions imply that the transition layer can be eliminated altogether, resulting in the coexistence of austenite and twinned martensite with zero elastic energy. Examples are shown in Figs. 2(right), 3, 4, 6 and 7. These include macroscopically curved austenite/martensite interfaces and natural mechanisms of nucleation (Figs. 6, 7). The latter are continuous families of deformations in which the austenite grows from zero volume in a matrix of martensite, or the martensite grows in a matrix of austenite, all having zero elastic energy. Said differently, while the crystallographic theory implies that the energy due to elastic distortion can be reduced as close to zero as desired by making the twins finer and finer, the elastic energy in the cases studied here is eliminated at all length scales. From a physical viewpoint, the only remaining energy is then a small interfacial energy. We describe explicitly the cases in which the transition layer can be eliminated in Section 4.

The value of λ_2 can be modified by changing composition, and the special case $\lambda_2 = 1$ (up to experimental error in the measurement of lattice parameters) has been achieved in many systems. As reviewed in detail below, satisfaction of only the condition $\lambda_2 = 1$ has a dramatic effect on hysteresis and transformational fatigue (Cui et al., 2006; Zhang et al., 2009; Zarnetta et al., 2010; Delville et al., 2009; Srivastava et al., 2010; see also Buschbeck et al., 2011; Meethong et al., 2007; Louie et al., 2010; Srivastava et al., 2011). A theory for the width of the hysteresis loop that predicts this sensitivity was given in Zhang et al. (2009), Knüpfer et al. (2011), and Zwicknagl (2013). It is based on the idea that transformation is delayed, say on

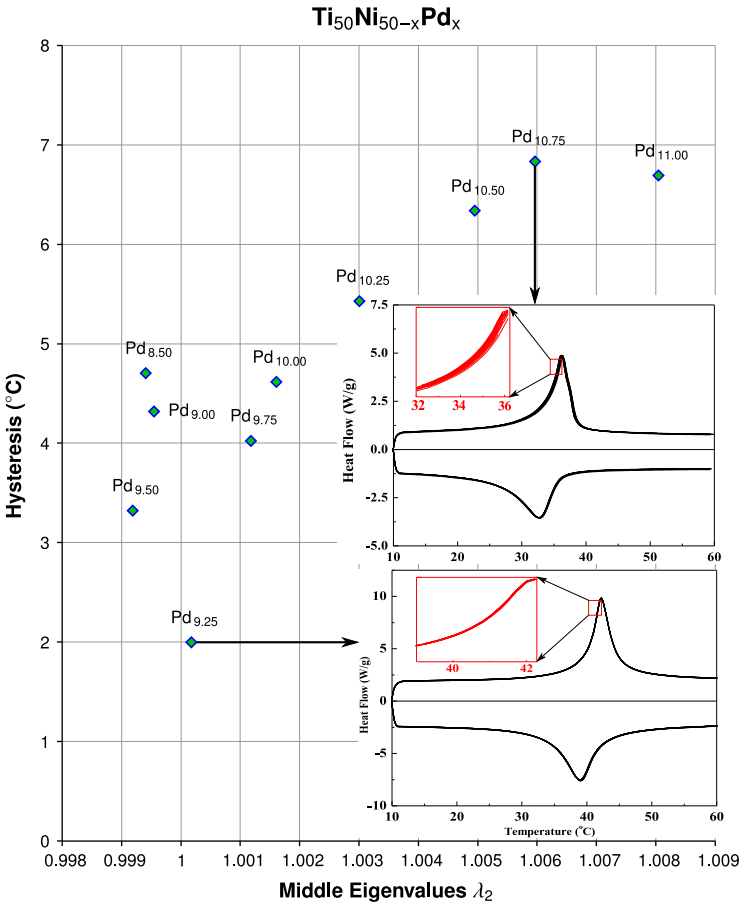

Fig. 1. Reduced hysteresis of $Ti_{50}Ni_{50-x}$ Pd $_x$ alloy system as the composition is tuned to achieve $\lambda_2 = 1$. A thermal hysteresis of 2 °C is obtained at $x=9.25$. The insets show a comparison of thermal hysteresis under repeated cycling through the transformation (30 cycles) measured by differential scanning calorimetry at $x=9.25$ vs. $x=10.75$. A careful comparison of these graphs shows an average migration of transformation temperature of 0.16 °C/cycle at $x=10.75$ is reduced to 0.030 °C/cycle at $x=9.25$. These values should be contrasted to ordinary TiNi which exhibits an average migration over 30 cycles of about 0.6 °C/cycle.

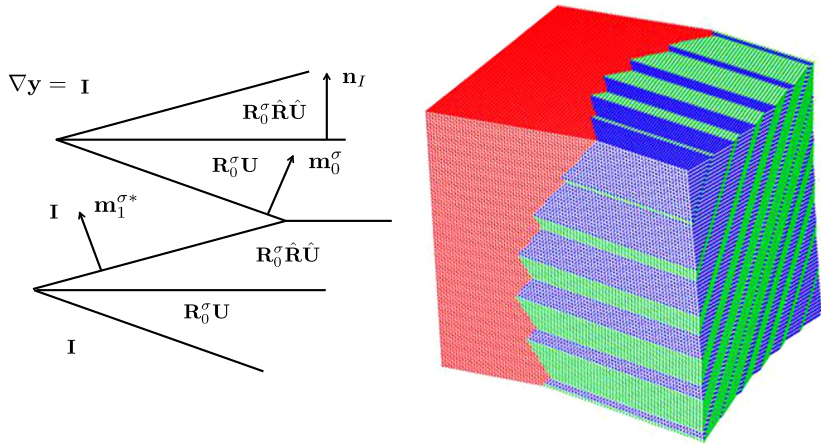

Fig. 2. Left diagram is a schematic of three triple conjunctions using the deformation gradients in (33). A macroscopically curved austenite/martensite interface with zero elastic energy is plotted on the right for a material satisfying the cofactor conditions (Type I domain).

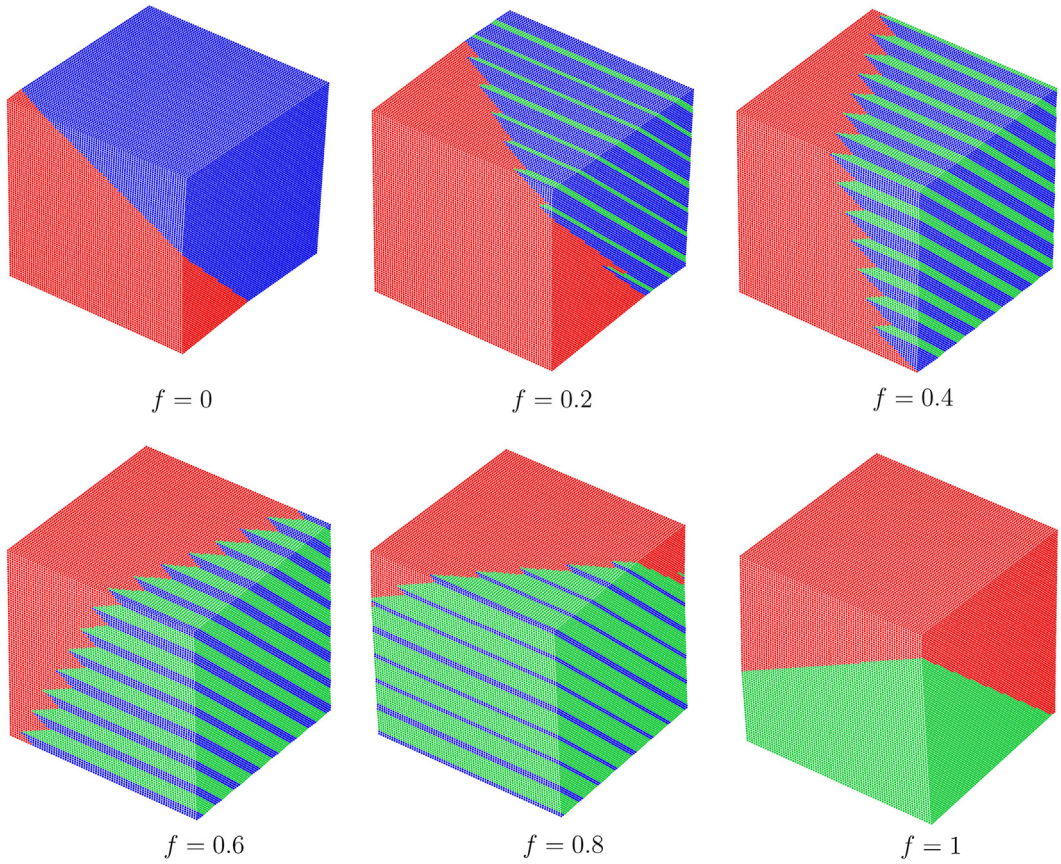

Fig. 3. Zero elastic energy austenite/martensite interfaces for a material satisfying the cofactor conditions (Type I domain) at various f from 0 to 1.

cooling, because the additional bulk and twin-boundary energy at the austenite/martensite interface has to be compensated by a further lowering of the energy wells of the martensite phase, so as to have a free energy decreasing transformation path. This bulk and interfacial energy is eliminated by tuning composition to make $\lambda_2 = 1$. Both this theory and broad collection of measurements of hysteresis demonstrate extreme sensitivity of the width of the hysteresis to λ_2 (and composition), which also explains why this was not observed previously. For example, as shown in Fig. 1, 1/4% changes of composition in the $Ti_{50}Ni_{50-x}Pd_x$ system give a minimum width of the hysteresis loop at x=9.25 with a remarkable value $(1/2)(A_f + A_s - M_f - M_s) = 2\ ^\circ C$. This is accompanied by improvements of the reversibility of the phase transformation as measured by the migration of the transformation temperature under repeated cycling.

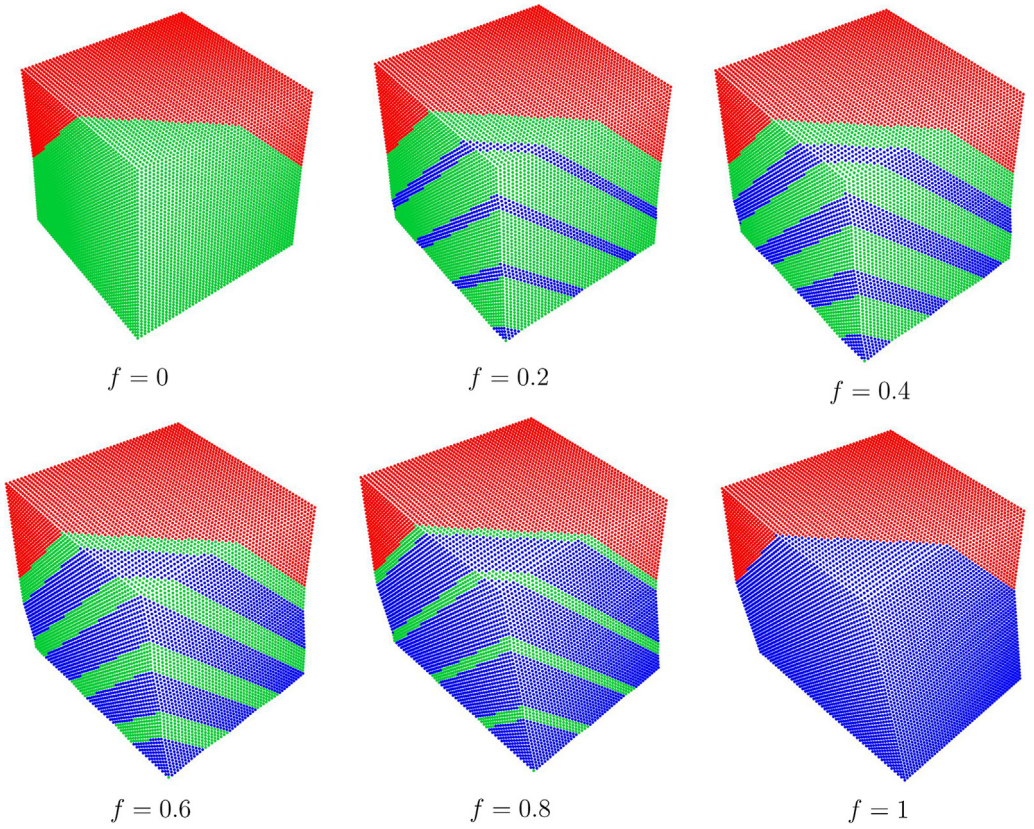

Fig. 4. Zero elastic energy austenite/martensite interfaces for a material satisfying the cofactor conditions (Type II domain) at various f from 0 to 1.

Tuning λ_2 to 1 actually entails a reduction of the number of deformations that belong to solutions of the crystallographic theory in many cases. This can be seen in the following way. In general, for λ_2 near 1 but $\lambda_2 \neq 1$, the crystallographic theory implies the existence of four solutions per twin system (Ball and James, 1987), resulting in four average deformation gradients of twinned laminates that participate in austenite/martensite interfaces. As $\lambda_2 \to 1$, these four solutions converge to four perfect austenite/single-variant martensite interfaces. (This is consistent with the fact that when the middle eigenvalue λ_2 of a positive-definite symmetric tensor $\mathbf{U}$ is 1, there are two solutions $\mathbf{R}_1, \mathbf{a}_1 \otimes \mathbf{n}_1$ and $\mathbf{R}_2, \mathbf{a}_2 \otimes \mathbf{n}_2$ of the equation of perfect compatibility $\mathbf{RU}-\mathbf{I} = \mathbf{a} \otimes \mathbf{n}$, $\mathbf{R} \in \mathrm{SO}(3)$, $\mathbf{a}, \mathbf{n} \in \mathbb{R}^3$, Ball and James, 1992.) However, some of these four also result from other solutions of the crystallographic theory, because a variant can belong to many twin systems. In fact, a simple counting exercise shows that the number of deformation gradients participating in exact interfaces equals the number of generic twin systems (Pitteri and Zanzotto, 1998). For example, in a classic cubic to orthorhombic phase transformation (Zhang et al., 2009) as in the material TiNiPd (Fig. 1), there are 6 variants of martensite, resulting generically in 30 twin systems and 24 (resp., 96) solutions of the crystallographic theory for $\lambda_2 \lesssim 1$ (resp., $\lambda_2 \gtrsim 1$). If $\lambda_2 = 1$ in this case, there are only 30 deformation gradients corresponding to exact austenite/martensite interfaces.

Fewer deformation gradients mean fewer ways that nontransforming impurities, defects, triple junctions and precipitates can be accommodated by a growing austenite/martensite interface. This intuition on the beneficial effects of having more deformations, which is prevalent in the literature on phase transformations, is quantified in random polycrystals by Bhattacharya and Kohn (1996). This line of thought also plays an important role in the concept of non-generic twins of Pitteri and Zanzotto (1998). As summarized above, if the cofactor conditions are satisfied, there are infinitely many deformation gradients participating in austenite/twinned-martensite interfaces. As mentioned above, in some cases (Type I or Type II but generally not Compound twins, see below) the elastic transition layer can be eliminated. Particularly in these cases, the demonstrated advantages with regard to hysteresis and reversibility of having no transition layer are combined with the benefits of having a great many deformations. The precise nature of these possible benefits with regard to the shape memory effect or transformational fatigue awaits further theoretical and experimental study.

This paper unifies the treatment of compatibility of variants of martensite, by including automatically Type I/II and Compound twins, the "domains" of Li (Li and Wayman, 1995; Li and James, 1997), and the non-conventional and non-generic twins of Pitteri and Zanzotto (1998) and Soligo et al. (1999). All of these cases can satisfy the cofactor conditions, and all of these cases are analyzed here.

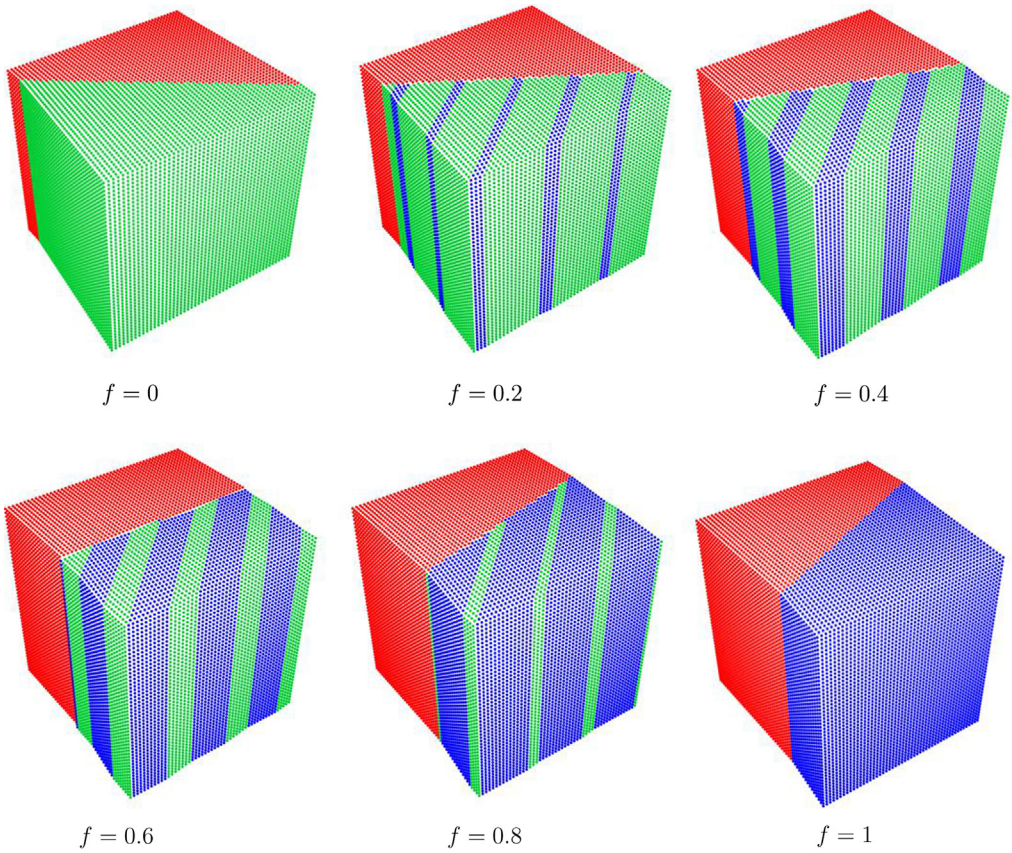

Fig. 5. Austenite/martensite interfaces for Compound twin system satisfying the cofactor conditions at various f from 0 to 1. The deformation is a plane strain. In this case there is an elastic distortion near the habit plane.

Geometrically linear theory is often used in the literature. We present a treatment of the cofactor conditions in that case. They can be obtained either by direct linearization of the cofactor conditions of the geometrically nonlinear theory, or by starting over and imposing the condition of "any volume fraction of the twins" in the geometrically linear form of the crystallographic theory.

Notation and method of visualization: As general background for this paper, including most notation, see the book of Bhattacharya (2003). $\mathbb{R}^{3\times 3}$ is the set of 3×3 real matrices, $\mathbb{R}^{3\times 3}_{+}$ is the subset of $\mathbb{R}^{3\times 3}$ with positive determinant, $\mathbb{R}^{3\times 3}_{+\mathrm{sym}}$ is positive-definite, symmetric real 3×3 matrices, and $\mathrm{SO}(3)$ denotes the group of all 3×3 orthogonal matrices with determinant 1. The notation cof $\mathbf{A}$ denotes the cofactor of the matrix $\mathbf{A}$: in components relative to an orthonormal basis, $(\mathrm{cof}\mathbf{A})_{ij} = (-1)^{i+j}\det(\hat{\mathbf{A}}_{ij})$, where $\hat{\mathbf{A}}_{ij}$ is the determinant of the submatrix obtained by removing the ith row and jth column of $\mathbf{A}$. The pictures of microstructures shown in this paper are plotted using the following algorithm: (a) A deformation $\mathbf{y}(\mathbf{x})$ defined on a cube Ω and having the given values of $\nabla\mathbf{y}$, e.g., those arising from materials satisfying the cofactor conditions, is constructed analytically.[1] (b) Suitable rectangular arrays of points $\mathbf{x}_1, \mathbf{x}_2, \ldots \in \partial\Omega$ are specified. (c) Dots at the points $\mathbf{y}(\mathbf{x}_1), \mathbf{y}(\mathbf{x}_2), \ldots$ are plotted, colored by their phase or variant. This is a direct visualization via the Cauchy–Born rule.

2. Geometrically nonlinear theory of martensite and the crystallographic theory

The cofactor conditions arise as degeneracy conditions in the crystallographic theory of martensite, but they have wider implications for the existence of energy minimizing microstructures within the geometrically nonlinear theory of martensitic transformations. Thus we present a brief summary of the parts of the theory that are needed in this paper. As general references we cite Bhattacharya (2003), James and Hane (2000) and Ball and James (1987).

The domain $\Omega \subset \mathbb{R}^3$, interpreted as a region occupied by undistorted austenite at the transformation temperature, serves as reference configuration for deformations $\mathbf{y} : \Omega \to \mathbb{R}^3$ arising from transformation or elastic distortion. The total energy of

[1] In cases that this deformation contains a transition layer at an interface, linear interpolation of the deformation across this layer is used, unless otherwise noted.

an unloaded body subjected to a deformation $\mathbf{y}:\Omega\to\mathbb{R}^3$ at a temperature θ is given by

$$\int_\Omega \varphi(\nabla\mathbf{y}(\mathbf{x}),\theta)\,d\mathbf{x}. \tag{1}$$

The Helmholtz free energy per unit reference volume, $\varphi(\mathbf{F},\theta)$, depends on the deformation gradient $\mathbf{F}\in\mathbb{R}^{3\times3}_+$ and the absolute temperature $\theta>0$. This energy density can be related to atomistic theory by the Cauchy–Born rule (Pitteri and Zanzotto, 2003). In this scenario $\mathbf{F}$ is interpreted as a linear transformation locally mapping a Bravais lattice representing undistorted austenite to the martensite lattice. If the austenite is represented by a complex lattice consisting of the union of several Bravais lattices, all having the same lattice vectors but having different base points $\mathbf{a}_1,\dots,\mathbf{a}_m$, the appropriate version of the Cauchy–Born rule – the *weak Cauchy–Born rule* in the terminology of Pitteri and Zanzotto (1998) and Ericksen (2008) – gives an energy density of the form $\hat\varphi(\mathbf{F},\mathbf{a}_m-\mathbf{a}_1,\dots,\mathbf{a}_2-\mathbf{a}_1,\theta)$. In that case the free energy density given above is defined by

$$\varphi(\mathbf{F},\theta)=\min_{\mathbf{s}_1,\dots,\mathbf{s}_{m-1}}\hat\varphi(\mathbf{F},\mathbf{s}_1,\dots,\mathbf{s}_{m-1},\theta). \tag{2}$$

The free energy density φ is frame-indifferent, $\varphi(\mathbf{RF},\theta)=\varphi(\mathbf{F},\theta)$ for all $\theta>0$, $\mathbf{R}\in\mathrm{SO}(3)$ and $\mathbf{F}\in\mathbb{R}^{3\times3}_+$, and its energy-well structure is restricted by conditions of symmetry which are not repeated here.

The result is that there is a set of *transformation stretch matrices* $\mathbf{U}_1,\dots,\mathbf{U}_n$, each in $\mathbb{R}^{3\times3}_{+\mathrm{sym}}$, that are related by symmetry, $\mathbf{U}_i=\mathbf{Q}_i\mathbf{U}_1\mathbf{Q}_i^T$, $i=1,\dots,n$, where $\mathcal{P}=\{\mathbf{Q}_1,\dots,\mathbf{Q}_n\}$, $\mathbf{Q}_i\in\mathrm{O}(3)$ is the point group of undistorted austenite at θ_c. $\mathbf{U}_1,\dots,\mathbf{U}_n$ define the energy wells of the *variants of martensite*. That is, there is a *transformation temperature* θ_c such that

$$\varphi(\mathbf{U}_1,\theta)=\cdots=\varphi(\mathbf{U}_n,\theta)\le\varphi(\mathbf{F},\theta),\quad \theta\le\theta_c. \tag{3}$$

The matrices $\mathbf{U}_i=\mathbf{Q}_i\mathbf{U}_1\mathbf{Q}_i^T$, $i=1,\dots,n$ depend weakly on temperature, due to ordinary thermal expansion, but this dependence is suppressed.

For $\theta=\theta_c$, the identity $\mathbf{I}$, representing the austenite, is also a minimizer

$$0=\varphi(\mathbf{I},\theta_c)=\varphi(\mathbf{U}_1,\theta_c)\le\varphi(\mathbf{F},\theta_c). \tag{4}$$

Without loss of generality we have put the minimum value of the energy at θ_c equal to zero. As θ is increased from θ_c the austenite well persists, but it is perturbed slightly away from $\mathbf{I}$ due again to ordinary thermal expansion. $\mathbf{U}_1,\dots,\mathbf{U}_n$ also can be continued as local minimizers of the energy density for $\theta>\theta_c$. While there are various obvious generalizations of our results, in this paper we nominally discuss energy minimizers and minimizing sequences at θ_c. In summary, the full set of minimizers of the free energy density φ at θ_c includes

$$\mathrm{SO}(3)\mathbf{I}\cup\mathrm{SO}(3)\mathbf{U}_1\cup\cdots\cup\mathrm{SO}(3)\mathbf{U}_n \tag{5}$$

for given symmetry-related tensors $\mathbf{U}_1,\dots,\mathbf{U}_n$ in $\mathbb{R}^{3\times3}_{+\mathrm{sym}}$. To avoid degeneracy we assume that $\mathbf{I},\mathbf{U}_1,\dots,\mathbf{U}_n$ are distinct. A general algorithm that can be used to obtain the transformation stretch matrices directly from x-ray measurements, applicable also to complex lattices, is presented in a forthcoming paper (Chen and James, 2013).

2.1. Twins and domains

Accounting for frame-indifference, the equation of compatibility for two variants of martensite is

$$\hat{\mathbf{R}}\mathbf{U}_i-\overline{\mathbf{R}}\mathbf{U}_j=\mathbf{a}\otimes\mathbf{n}, \tag{6}$$

which is to be solved for $\hat{\mathbf{R}},\overline{\mathbf{R}}\in\mathrm{SO}(3)$ and $\mathbf{a},\mathbf{n}\in\mathbb{R}^3$. Without loss of generality, we can put $\overline{\mathbf{R}}=\mathbf{I}$ and $j=1$. The former is accomplished by premultiplying (6) by $\overline{\mathbf{R}}^T$ (corresponding to an overall rigid rotation) and suitably redefining $\hat{\mathbf{R}}$ and $\mathbf{a}$. The latter is accomplished by subsequently pre- and post-multiplying (6) by $\mathbf{Q}_j,\dots,\mathbf{Q}_j^T$ and using the symmetry relations above. Thus we consider

$$\hat{\mathbf{R}}\mathbf{U}_i-\mathbf{U}_1=\mathbf{a}\otimes\mathbf{n}. \tag{7}$$

To recover the general case (6) we multiply (7) by $\mathbf{Q}_j,\dots,\mathbf{Q}_j^T$ and then premultiply by an arbitrary $\overline{\mathbf{R}}\in\mathrm{SO}(3)$ and make the obvious notational changes.

Because of results given in the Appendix and described in the following paragraphs, it is seen that the details of symmetry relations, the number of variants, point groups, etc., do not play a direct role in the analysis. So we simplify the notation. Let $\mathbf{U}=\mathbf{U}_1\in\mathbb{R}^{3\times3}_{+\mathrm{sym}}$ and $\hat{\mathbf{U}}\in\mathbb{R}^{3\times3}_{+\mathrm{sym}}$. Let $\hat{\mathbf{R}}\in\mathrm{SO}(3),\mathbf{a},\mathbf{n}\in\mathbb{R}^3$ satisfy

$$\hat{\mathbf{R}}\hat{\mathbf{U}}-\mathbf{U}=\mathbf{a}\otimes\mathbf{n}. \tag{8}$$

It is known that the solutions of the equation of compatibility (8) between martensite variants can be classified into five types: Type I, Type II, Compound, non-conventional but generic and non-generic twins. The terminology non-generic twins and non-conventional twins was introduced by Pitteri and Zanzotto (1998) and Soligo et al. (1999) in the context of cubic to monoclinic transformations. Briefly, Type I/II twins are the well-known solutions generated by a two-fold $\mathbf{Q}\in\mathcal{P}$ such that $\mathbf{U}_j=\mathbf{Q}\mathbf{U}_1\mathbf{Q}^T\neq\mathbf{U}_1$. Compound twins are possible when there are two distinct two-fold transformations relating $\mathbf{U}_j$ and $\mathbf{U}_1$ and can be considered as both Type I and Type II simultaneously. Non-conventional twins are solutions of (8) that are not generated by a two-fold transformation in $\mathcal{P}$ but that persist under arbitrary small perturbations of $\mathbf{U}_1$, and non-generic

twins are solutions of (8) that do not persist under arbitrary small perturbations of $\mathbf{U}_1$ and therefore can be considered as associated to special choices of the lattice parameters. Both non-generic and non-conventional twins do not in general have a mirror symmetry relation across the interface. Or, more precisely, if atom positions on each side of interface are constructed using the Cauchy–Born rule and non-generic or non-conventional solutions of (8), then generally there will be no mirror symmetry relating the atom positions across the interface. Noticing this fact from a purely experimental viewpoint in $LaNbO_4$, Li and Wayman (1995) referred to these structures as "domains" rather than twins in their thesis.

In the Appendix we show that all solutions of (8) can be expressed in a common form by simple formulas. In particular, these formulas include Types I/II, Compound, non-conventional and non-generic twins, as well as cases that may occur with other symmetries that have not yet been classified. Our analysis of the cofactor conditions below relies only on the presence of these formulas, so we use this framework below. Our formulas have the same form as for Type I/II twins with an associated two-fold rotation (which is given by an explicit formula), but this two-fold rotation is not generally in $\mathcal{P}$. For this reason we here use the terminology of Li and call these general solutions *Type I domains* and *Type II domains* (see also the case of *Compound domains* defined below). It can be seen from the Appendix that these domains are twins with respect to a mythical symmetry, not the symmetry of lattices of austenite and martensite consistent with the framework above.

The analysis, under the hypotheses on $\mathbf{U}, \hat{\mathbf{U}}$ given above, that all solutions of (8) (and therefore of (6)) are Type I, Type II or Compound domains is given in the Appendix. The proposition given there implies that if $\hat{\mathbf{R}}, \mathbf{a}, \mathbf{n}$ satisfy (8), then there is a unit vector $\hat{\mathbf{e}}$ such that

$$\hat{\mathbf{U}} = (-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}), \tag{9}$$

and it therefore follows by standard results (see Bhattacharya, 2003) that there are two solutions $(\mathbf{R}_I, \mathbf{a}_I\otimes\mathbf{n}_I)$ and $(\mathbf{R}_{II}, \mathbf{a}_{II}\otimes\mathbf{n}_{II})$ of (8) given by

$$\begin{aligned}&\text{Type I}\quad \mathbf{n}_I = \hat{\mathbf{e}},\quad \mathbf{a}_I = 2\left(\frac{\mathbf{U}^{-1}\hat{\mathbf{e}}}{|\mathbf{U}^{-1}\hat{\mathbf{e}}|^2} - \mathbf{U}\hat{\mathbf{e}}\right),\\ &\text{Type II}\quad \mathbf{n}_{II} = 2\left(\hat{\mathbf{e}} - \frac{\mathbf{U}^2\hat{\mathbf{e}}}{|\mathbf{U}\hat{\mathbf{e}}|^2}\right),\quad \mathbf{a}_{II} = \mathbf{U}\hat{\mathbf{e}}.\end{aligned} \tag{10}$$

Following this specification of $\mathbf{a}_I\otimes\mathbf{n}_I$ and $\mathbf{a}_{II}\otimes\mathbf{n}_{II}$, the corresponding rotations $\mathbf{R}_I$ and $\mathbf{R}_{II}$ can be calculated from (8). Note that by changing $\mathbf{a}\to\rho\mathbf{a}$ and $\mathbf{n}\to(1/\rho)\mathbf{n}$, $\rho\neq 0$, we do not change $\mathbf{a}\otimes\mathbf{n}$, so these individual vectors are not uniquely determined by the solution. This situation occurs widely below, and so statements about uniqueness or numbers of solutions always refer to the diadic $\mathbf{a}\otimes\mathbf{n}$ rather than the individual vectors. This observation can be used to normalize $\mathbf{n}$, up to $\pm$, but we do not do that in this paper.

As seen from Corollary 13 of the Appendix, there are cases in which $\mathbf{U}$ and $\hat{\mathbf{U}}$ are related as in (9) by *two* nonparallel unit vectors $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2$. This apparently gives rise to four solutions of (8) via (10), but these solutions cannot be distinct due to the fact that there are at most two solutions $\hat{\mathbf{R}}, \mathbf{a}\otimes\mathbf{n}$ of (8) according to Prop. 4 of Ball and James (1987). One solution can be considered Type I for $\hat{\mathbf{e}}_1$ and Type II for $\hat{\mathbf{e}}_2$ and the other is Type II for $\hat{\mathbf{e}}_1$ and Type I for $\hat{\mathbf{e}}_2$. In the conventional cases of twins, these degenerate solutions are interpreted as Compound twins. Corollary 13 and (10) show that the same situation can arise in the general case of the Appendix. Therefore we use the following terminology throughout the rest of this paper. We call the solutions given in (10) *Type I/II domains* in the case that there is one and only one unit vector $\hat{\mathbf{e}}$ satisfying (9) (up to $\pm$) and $\mathbf{a}_I\otimes\mathbf{n}_I/\mathbf{a}_{II}\otimes\mathbf{n}_{II}$ is given by the first line/second line of (10). In cases where there are two nonparallel unit vectors satisfying (9), we call the resulting pair of solutions *Compound domains*.

Compound domains are characterized below.

Proposition 1 (*Compound domains*). *Assume that* $\mathbf{U}\in\mathbb{R}^{3\times3}_{+\mathrm{sym}}$. *Let* $|\hat{\mathbf{e}}_1|=1$ *be given, define* $\hat{\mathbf{U}} = (-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)$ *and suppose* $\hat{\mathbf{U}}\neq\mathbf{U}$. *There is a second unit vector* $\hat{\mathbf{e}}_2$, *not parallel to* $\hat{\mathbf{e}}_1$, *satisfying* $\hat{\mathbf{U}} = (-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2)\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2)$ *if and only if* $\hat{\mathbf{e}}_1$ *is perpendicular to an eigenvector of* $\mathbf{U}$. *In the case that* $\hat{\mathbf{e}}_1$ *is perpendicular to an eigenvector of* $\mathbf{U}$, $\hat{\mathbf{e}}_2$ *is unique up to* $\pm$ *and is perpendicular to both* $\hat{\mathbf{e}}_1$ *and that eigenvector.*

Supposing that $\hat{\mathbf{e}}_1$ *is perpendicular to an eigenvector* $|\mathbf{v}|=1$ *of* $\mathbf{U}$ $(\neq\hat{\mathbf{U}})$ *and* $\hat{\mathbf{e}}_2=\mathbf{v}\times\hat{\mathbf{e}}_1$, *then the two solutions* $\mathbf{a}^1_C\otimes\mathbf{n}^1_C$, $\mathbf{a}^2_C\otimes\mathbf{n}^2_C$ *of* (8) *can be written as*

$$\begin{aligned}&\mathbf{n}^1_C = \hat{\mathbf{e}}_1,\quad \mathbf{a}^1_C = \xi\mathbf{U}\hat{\mathbf{e}}_2,\quad \text{where } \xi = 2\frac{\hat{\mathbf{e}}_2\cdot\mathbf{U}^{-2}\hat{\mathbf{e}}_1}{\hat{\mathbf{e}}_1\cdot\mathbf{U}^{-2}\hat{\mathbf{e}}_1},\\ &\mathbf{n}^2_C = \hat{\mathbf{e}}_2,\quad \mathbf{a}^2_C = \eta\mathbf{U}\hat{\mathbf{e}}_1,\quad \text{where } \eta = -2\frac{\hat{\mathbf{e}}_2\cdot\mathbf{U}^{2}\hat{\mathbf{e}}_1}{\hat{\mathbf{e}}_1\cdot\mathbf{U}^{2}\hat{\mathbf{e}}_1}.\end{aligned} \tag{11}$$

Proof. Suppose $\hat{\mathbf{e}}_1\cdot\mathbf{v}=0$ for some $|\mathbf{v}|=1$ satisfying $\mathbf{U}\mathbf{v}=\mathbf{v}$. Define $\hat{\mathbf{e}}_2=\hat{\mathbf{e}}_1\times\mathbf{v}$ so that $\hat{\mathbf{e}}_1,\hat{\mathbf{e}}_2,\mathbf{v}=0$ is an orthonormal basis. Then, $(-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2) = -\mathbf{I}+2\mathbf{v}\otimes\mathbf{v}$. Since $(-\mathbf{I}+2\mathbf{v}\otimes\mathbf{v})\mathbf{U}(-\mathbf{I}+2\mathbf{v}\otimes\mathbf{v})=\mathbf{U}$, we have

$$(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2)\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2) = (-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1). \tag{12}$$

Conversely, if there are two nonparallel unit vectors $\hat{\mathbf{e}}_1,\hat{\mathbf{e}}_2$ satisfying (12), then by Corollary 13 of the Appendix, $\hat{\mathbf{e}}_1\cdot\hat{\mathbf{e}}_2=0$. Let $\mathbf{v}=\hat{\mathbf{e}}_1\times\hat{\mathbf{e}}_2$, so that $|\mathbf{v}|=1$ and $(-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2) = -\mathbf{I}+2\mathbf{v}\otimes\mathbf{v}$. Hence it follows from (12) that

$(-\mathbf{I}+2\mathbf{v}\otimes\mathbf{v})\mathbf{U}(-\mathbf{I}+2\mathbf{v}\otimes\mathbf{v})=\mathbf{U}$. Operating the latter on $\mathbf{v}$ it is seen that $\mathbf{v}$ is an eigenvector of $\mathbf{U}$, so $\hat{\mathbf{e}}_1$ is perpendicular to an eigenvector of $\mathbf{U}$.

Suppose that $\hat{\mathbf{e}}_1$ is perpendicular to an eigenvector $|\mathbf{v}|=1$ of $\mathbf{U}$ and $\hat{\mathbf{e}}_2=\mathbf{v}\times\hat{\mathbf{e}}_1$. Then $\hat{\mathbf{U}}:=(-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1)=(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2)\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2)\neq\mathbf{U}$, so that there are by (9) and (10) apparently four solutions of (8): $\mathbf{a}_I^1\otimes\mathbf{n}_I^1$, $\mathbf{a}_{II}^1\otimes\mathbf{n}_{II}^1$ based on $\hat{\mathbf{e}}_1$ and $\mathbf{a}_I^2\otimes\mathbf{n}_I^2$, $\mathbf{a}_{II}^2\otimes\mathbf{n}_{II}^2$ based on $\hat{\mathbf{e}}_2$. By Prop. 4 of Ball and James (1987) these must reduce to two. This can happen in two possible ways:

$$\mathbf{a}_I^1\parallel\mathbf{a}_{II}^2,\mathbf{n}_I^1\parallel\mathbf{n}_{II}^2,\mathbf{a}_{II}^1\parallel\mathbf{a}_I^2,\mathbf{n}_{II}^1\parallel\mathbf{n}_I^2\quad\text{or}\quad\mathbf{a}_I^1\parallel\mathbf{a}_{II}^1,\mathbf{n}_I^1\parallel\mathbf{n}_{II}^1,\mathbf{a}_I^2\parallel\mathbf{a}_{II}^2,\mathbf{n}_I^2\parallel\mathbf{n}_{II}^2. \tag{13}$$

By direct calculation the latter cannot happen, as it contradicts $\hat{\mathbf{U}}\neq\mathbf{U}$. The former leads to the simplification of the formulas (10) given by (11). □

According to the results in the Appendix, there are at most two nonparallel unit vectors $\hat{\mathbf{e}}$ satisfying (9), if $\hat{\mathbf{U}}\neq\mathbf{U}$. The statement to the left of the "or" in (13) may be interpreted by saying that Compound domains are "both Type I and Type II", although our precise definitions above make Types I, II and Compound mutually exclusive.

2.2. Crystallographic theory of martensite

The crystallographic theory of martensite concerns conditions for which a twinned laminate and the austenite phase are interpolated by a transition layer so that the energy in the layer tends to zero as the twins are made finer and finer. The construction yields a sequence of deformations $\mathbf{y}^{(k)}$, $k=1,2,\ldots$, where k can be taken as the inverse width of the transition layer, such that

$$\int_\Omega\varphi(\nabla\mathbf{y}^{(k)}(\mathbf{x}),\theta_c)\,d\mathbf{x}\to 0\quad\text{as } k\to\infty. \tag{14}$$

Under the hypothesis of Ball and James (1987, Prop. 2), a suitable sequence $\mathbf{y}^{(k)}$ satisfying (14) converges strongly in a suitable function space to a deformation $\mathbf{y}$, as $k\to\infty$, such that

$$\nabla\mathbf{y}=f(\mathbf{U}+\mathbf{a}\otimes\mathbf{n})+(1-f)\mathbf{U},\quad\text{a.e.} \tag{15}$$

in the vicinity of the austenite/martensite interface and on the side of martensite.

The equations of the crystallographic theory are built on a solution of (8). Assuming (8) holds, the equations of the crystallographic theory of martensite are

$$\mathbf{R}[f(\mathbf{U}+\mathbf{a}\otimes\mathbf{n})+(1-f)\mathbf{U}]-\mathbf{I}=\mathbf{b}\otimes\mathbf{m}, \tag{16}$$

which are to be solved for the volume fraction $0\le f\le 1$ of the Type I/II or Compound domains, a possible rigid rotation $\mathbf{R}\in\mathrm{SO}(3)$ of the whole martensite laminate, and vectors $\mathbf{b},\mathbf{m}\in\mathbb{R}^3$.

3. Cofactor conditions

The cofactor conditions are necessary and sufficient that (16) has a solution $(f,\mathbf{R},\mathbf{b}\otimes\mathbf{m})$ for every $0\le f\le 1$.

Theorem 2. *Let* $\mathbf{U}\in\mathbb{R}^{3\times3}_{+\mathrm{sym}}$ *and define* $\hat{\mathbf{U}}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})$ *for some* $|\hat{\mathbf{e}}|=1$, *so that there exist* $\hat{\mathbf{R}}\in\mathrm{SO}(3)$ *and* $\mathbf{a},\mathbf{n}\in\mathbb{R}^3$ *such that*

$$\hat{\mathbf{R}}\hat{\mathbf{U}}=\mathbf{U}+\mathbf{a}\otimes\mathbf{n}. \tag{17}$$

Assume $\mathbf{a}\neq 0$, $\mathbf{n}\neq 0$. *Eq.* (16) *of the crystallographic theory has a solution* $\mathbf{R}\in\mathrm{SO}(3)$, $\mathbf{b},\mathbf{m}\in\mathbb{R}^3$ *for each* $f\in[0,1]$ *if and only if the following* cofactor conditions *are satisfied*:

$$\lambda_2=1,\quad\textit{where } \lambda_2 \textit{ is the middle eigenvalue of } \mathbf{U} \tag{CC1}$$

$$\mathbf{a}\cdot\mathbf{U}\,\mathrm{cof}(\mathbf{U}^2-\mathbf{I})\mathbf{n}=0, \tag{CC2}$$

$$\mathrm{tr}\,\mathbf{U}^2-\det\mathbf{U}^2-\frac{|\mathbf{a}|^2|\mathbf{n}|^2}{4}-2\ge 0. \tag{CC3}$$

Proof. The proof follows Section 5 of Ball and James (1987). As is well known, e.g., Ball and James (1987, Prop. 4), given $\mathbf{U}\in\mathbb{R}^{3\times3}_{+\mathrm{sym}}$, there is a solution $\mathbf{R}\in\mathrm{SO}(3)$, $\mathbf{c},\mathbf{d}\in\mathbb{R}^3$ of $\mathbf{RU}-\mathbf{I}=\mathbf{c}\otimes\mathbf{d}$ if and only if the middle eigenvalue of $\mathbf{U}$ is 1. Since $\mathbf{U}$ has middle eigenvalue equal to 1 if and only if $\mathbf{U}^2$ has a middle eigenvalue equal to 1, the satisfaction of (16) for every $0\le f\le 1$ is equivalent to the condition that the middle eigenvalue of the positive-definite symmetric matrix $(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})$ is 1 for every $0\le f\le 1$. An eigenvalue of $(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})$ is 1 for every $0\le f\le 1$ if and only if $g(f)$ vanishes identically on $[0,1]$, where

$$g(f)=\det[(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})-\mathbf{I}]. \tag{18}$$

Taking the determinant of (17), we see that $\mathbf{n}\cdot\mathbf{U}^{-1}\mathbf{a}=0$. Hence, $\det(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})=\det\mathbf{U}\neq 0$ and

$$\begin{aligned} g(f) &= (\det\mathbf{U})\det[\mathbf{U}+f\mathbf{a}\otimes\mathbf{n}-(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})^{-1}] \\ &= (\det\mathbf{U})\det[\mathbf{U}-\mathbf{U}^{-1}+f(\mathbf{a}\otimes\mathbf{n}+\mathbf{U}^{-1}\mathbf{n}\otimes\mathbf{U}^{-1}\mathbf{a})]. \end{aligned} \tag{19}$$

Since the matrix multiplying f is singular, then $g(f)$ is at most quadratic in f. In addition, by the hypothesis (17), it follows that

$$(\mathbf{U}+\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+\mathbf{a}\otimes\mathbf{n})=\hat{\mathbf{U}}^2=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}^2(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}). \tag{20}$$

Hence, putting $\mathbf{Q}=-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}$, we have that

$$g(1)=\det(\mathbf{Q}\mathbf{U}^2\mathbf{Q}^T-\mathbf{I})=\det(\mathbf{U}^2-\mathbf{I})=g(0). \tag{21}$$

A quadratic g satisfying $g(0)=g(1)$ is expressible in the form $g(f)=a(f(f-1))+b$. Hence, g vanishes identically on $[0,1]$ if and only if $a=b=0$. In particular, $b=0$ is (CC1) and $0=a=-g'(0)$ is (CC2). We have therefore shown that (CC1) and (CC2) are necessary and sufficient that an eigenvalue of $(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})$ is 1 for every $0\le f\le 1$. Let the eigenvalues of $(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})$ be $1,\lambda_1(f)^2,\lambda_3(f)^2$ with no particular ordering assumed. Taking the trace of (20) we have the identity $2\mathbf{n}\cdot\mathbf{U}\mathbf{a}+|\mathbf{a}|^2|\mathbf{n}|^2=0$. Using this identity and the relations

$$\begin{aligned} 1+\lambda_1(f)^2+\lambda_3(f)^2 &= \mathrm{tr}((\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})) \\ &= \mathrm{tr}(\mathbf{U}^2)+2f\mathbf{n}\cdot\mathbf{U}\mathbf{a}+f^2|\mathbf{a}|^2|\mathbf{n}|^2, \end{aligned} \tag{22}$$

and $\lambda_1(f)^2\lambda_3(f)^2=\det\mathbf{U}^2$, we get

$$(1-\lambda_1(f)^2)(\lambda_3(f)^2-1)=\mathrm{tr}(\mathbf{U}^2)-\det\mathbf{U}^2+(f^2-f)|\mathbf{a}|^2|\mathbf{n}|^2-2. \tag{23}$$

Assuming (CC1) and (CC2) are satisfied, (CC3) holds as a necessary condition that 1 is the middle eigenvalue at $f=1/2$. Since $f^2-f\ge -1/4$ it is then seen that (CC1), (CC2) and (CC3) are sufficient that the middle eigenvalue of $(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})$ is 1, completing the proof. □

Noticed that $\lambda_1(f)$ and $\lambda_3(f)$ are chosen to be positive values for every $0\le f\le 1$. Then it is clear that $0<\lambda_1=\lambda_1(0)$ and $\lambda_3=\lambda_3(0)$ are eigenvalues of $\mathbf{U}$.

Corollary 3. *Assume the hypotheses of Theorem 2 and suppose the cofactor conditions are satisfied. Then the other two eigenvalues $\lambda_1(f)^2\le 1\le\lambda_3(f)^2$ of $(\mathbf{U}+f\mathbf{n}\otimes\mathbf{a})(\mathbf{U}+f\mathbf{a}\otimes\mathbf{n})$ satisfy $\lambda_1(f)^2<1<\lambda_3(f)^2$ for $0\le f\le 1$ and $f\neq 1/2$. In particular, the eigenvalues λ_1, λ_3 of $\mathbf{U}$ satisfy $\lambda_1<1<\lambda_3$.*

Proof. Suppose we have some $0\le f^*\le 1$ such that $\lambda_1(f^*)^2=1$ or $\lambda_3(f^*)^2=1$. Then, the formula (23) gives

$$0=(1-\lambda_1(f^*)^2)(\lambda_3(f^*)^2-1)=\mathrm{tr}\,\mathbf{U}^2-\det\mathbf{U}^2+((f^*)^2-f^*)|\mathbf{a}|^2|\mathbf{n}|^2-2 \tag{24}$$

That is

$$\mathrm{tr}\,\mathbf{U}^2-\det\mathbf{U}^2-\frac{|\mathbf{a}|^2|\mathbf{n}|^2}{4}-2=-\left((f^*)^2-f^*+\frac{1}{4}\right)|\mathbf{a}|^2|\mathbf{n}|^2. \tag{25}$$

Since $\left(f^2-f+\frac{1}{4}\right)>0$ for $0\le f\le 1$, $f\neq 1/2$, then (25) violates (CC3) except at $f^*=1/2$, completing the proof. □

This result above shows incidentally that the cofactor conditions cannot be satisfied in the classic cubic-to-tetragonal case, for in that case the presence of a repeated eigenvalue would imply that either $\lambda_1=1$ or $\lambda_3=1$, contradicting Corollary 3.

Corollary 4. *Assume the hypotheses of Theorem 2 and suppose the cofactor conditions are satisfied. There are two distinct solutions $(\mathbf{R}_f^\kappa\in\mathrm{SO}(3),\mathbf{b}_f^\kappa\otimes\mathbf{m}_f^\kappa)$, $\kappa\in\{\pm 1\}$, of Eq. (16) of the crystallographic theory for each $0\le f\le 1$, $f\neq 1/2$. The solutions for $\mathbf{b}_f^\kappa,\mathbf{m}_f^\kappa$ are*

$$\begin{aligned} \mathbf{b}_f^\kappa &= \frac{\rho}{\sqrt{\lambda_3(f)^2-\lambda_1(f)^2}}\left(\lambda_3(f)\sqrt{1-\lambda_1(f)^2}\mathbf{v}_1(f)+\kappa\lambda_1(f)\sqrt{\lambda_3(f)^2-1}\mathbf{v}_3(f)\right) \\ \mathbf{m}_f^\kappa &= \frac{1}{\rho}\frac{\lambda_3(f)-\lambda_1(f)}{\sqrt{\lambda_3(f)^2-\lambda_1(f)^2}}\left(-\sqrt{1-\lambda_1(f)^2}\mathbf{v}_1(f)+\kappa\sqrt{\lambda_3(f)^2-1}\mathbf{v}_3(f)\right), \end{aligned} \tag{26}$$

$\kappa\in\{\pm 1\}$, $\rho\neq 0$ and $\mathbf{v}_1(f),\mathbf{v}_3(f)$ are orthonormal. (Note that the presence of ρ does not affect $\mathbf{b}_f^\kappa\otimes\mathbf{m}_f^\kappa$.)

Proof. The existence of a solution of (16) for each $0\le f\le 1$ follows from Theorem 2. The fact that there are two distinct solutions for $f\neq 1/2$ follows from Corollary 3. In particular, the conclusion $\lambda_1(f)^2<1<\lambda_3(f)^2$ for $f\neq 1/2$, and the explicit characterization (26) of the vectors $\mathbf{b}_f^\kappa,\mathbf{m}_f^\kappa$ given by Prop. 4 of Ball and James (1987) shows that $(\mathbf{R}_f^{+1},\ \mathbf{b}_f^{+1}\otimes\mathbf{m}_f^{+1})\neq(\mathbf{R}_f^{-1},\ \mathbf{b}_f^{-1}\otimes\mathbf{m}_f^{-1})$. □

Corollary 5. *Assume the hypotheses of Theorem 2. In the cofactor conditions, (CC2) can be replaced by the simpler form*

$$(\mathbf{a}\cdot\hat{\mathbf{v}}_2)(\mathbf{n}\cdot\hat{\mathbf{v}}_2)=0, \tag{CC2′}$$

where $\hat{\mathbf{v}}_2$ is a normalized eigenvector of $\mathbf{U}$ corresponding to its middle eigenvalue. That is, assuming the hypotheses of Theorem 2, (CC1), (CC2), (CC3) $\Longleftrightarrow$ (CC1), (CC2′), (CC3).

Proof. Assuming the hypotheses of Theorem 2 and (CC1), (CC2), (CC3), we write $\mathbf{U}=\lambda_1\hat{\mathbf{v}}_1\otimes\hat{\mathbf{v}}_1+\hat{\mathbf{v}}_2\otimes\hat{\mathbf{v}}_2+\lambda_3\hat{\mathbf{v}}_3\otimes\hat{\mathbf{v}}_3$ using ordered eigenvalues, which, according to Corollary 3, satisfy $\lambda_1<1<\lambda_3$. Then (CC3) becomes

$$(\lambda_1^2-1)(\lambda_3^2-1)(\mathbf{a}\cdot\hat{\mathbf{v}}_2)(\mathbf{n}\cdot\hat{\mathbf{v}}_2)=0, \tag{27}$$

implying (CC2′). Trivially, (CC1), (CC2′), (CC3) $\Longrightarrow$ (CC1), (CC2), (CC3). □

4. Microstructures possible under the cofactor conditions

Under the mild hypotheses of Theorem 2, the satisfaction of the cofactor conditions implies the existence of low energy transition layers in austenite/martensite interfaces for every volume fraction $0\le f\le 1$, in the sense of (14), i.e., in the sense of the crystallographic theory. In many cases the transition layer can be eliminated altogether, resulting in zero elastic energy in these cases. These cases are identified here.

Let the hypotheses of Theorem 2 be satisfied and write the implied solutions of the crystallographic theory as above in the form $\mathbf{R}_f^\kappa\in\mathrm{SO}(3)$, $\mathbf{b}_f^\kappa,\mathbf{m}_f^\kappa\in\mathbb{R}^3$, $\kappa\in\{\pm 1\}$, so we have

$$\begin{aligned}&\hat{\mathbf{R}}\hat{\mathbf{U}}-\mathbf{U}=\mathbf{a}\otimes\mathbf{n},\quad \hat{\mathbf{U}}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}),\quad |\hat{\mathbf{e}}|=1,\\ &\mathbf{R}_f^\kappa[f(\mathbf{U}+\mathbf{a}\otimes\mathbf{n})+(1-f)\mathbf{U}]=\mathbf{I}+\mathbf{b}_f^\kappa\otimes\mathbf{m}_f^\kappa,\quad 0\le f\le 1,\ \kappa=\pm 1.\end{aligned} \tag{28}$$

At $f=0$ we have

$$\mathbf{R}_0^\kappa\mathbf{U}=\mathbf{I}+\mathbf{b}_0^\kappa\otimes\mathbf{m}_0^\kappa, \tag{29}$$

which describes the implied austenite/single variant martensite interface. According to Corollary 4 specialized to the case $f=0\neq 1/2$, we know that there are two distinct solutions ($\mathbf{R}_0^\kappa\in\mathrm{SO}(3)$, $\mathbf{b}_0^\kappa\otimes\mathbf{m}_0^\kappa$), $\kappa=\pm 1$ of (29). Values of $\mathbf{b}_0^\kappa,\mathbf{m}_0^\kappa$ belonging to these solutions can be written explicitly as

$$\begin{aligned}\mathbf{b}_0^\kappa&=\frac{\rho}{\sqrt{\lambda_3^2-\lambda_1^2}}\left(\lambda_3\sqrt{1-\lambda_1^2}\mathbf{v}_1+\kappa\lambda_1\sqrt{\lambda_3^2-1}\mathbf{v}_3\right)\\ \mathbf{m}_0^\kappa&=\frac{1}{\rho}\frac{\lambda_3-\lambda_1}{\sqrt{\lambda_3^2-\lambda_1^2}}\left(-\sqrt{1-\lambda_1^2}\mathbf{v}_1+\kappa\sqrt{\lambda_3^2-1}\mathbf{v}_3\right),\quad \kappa\in\{\pm 1\},\end{aligned} \tag{30}$$

for some $\rho\neq 0$ by specialization of (26), where $0<\lambda_1<1<\lambda_3$ are the ordered eigenvalues of $\mathbf{U}$ with corresponding orthonormal eigenvectors $\mathbf{v}_1,\mathbf{v}_2,\mathbf{v}_3$.

4.1. Preliminary results for Types I and II domains

Proposition 1 says that if the cofactor conditions are satisfied for Type I or Type II domains, then $\hat{\mathbf{U}}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})$ holds for some $\hat{\mathbf{e}}$ with $\mathbf{v}_2\cdot\hat{\mathbf{e}}\neq 0$. In fact, only one unit vector $\hat{\mathbf{e}}$ satisfies this condition up to $\pm$.

The condition $\mathbf{v}_2\cdot\hat{\mathbf{e}}\neq 0$ implies that the main condition (CC2′) (see Corollary 5) of the cofactor conditions simplifies for Types I and II domains.

Proposition 6. *Assume* $\mathbf{U}=\lambda_1\mathbf{v}_1\otimes\mathbf{v}_1+\mathbf{v}_2\otimes\mathbf{v}_2+\lambda_3\mathbf{v}_3\otimes\mathbf{v}_3$, $0<\lambda_1<1<\lambda_3$, *and* $\hat{\mathbf{U}}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\neq\mathbf{U}$, $|\hat{\mathbf{e}}|=1$. *Recall Corollary 5.*

1. *For Type I domains* $(\mathbf{a}_I\cdot\mathbf{v}_2)(\mathbf{n}_I\cdot\mathbf{v}_2)=0\Longleftrightarrow\mathbf{a}_I\cdot\mathbf{v}_2=0\Longleftrightarrow|\mathbf{U}^{-1}\hat{\mathbf{e}}|=1$.
2. *For Type II domains* $(\mathbf{a}_{II}\cdot\mathbf{v}_2)(\mathbf{n}_{II}\cdot\mathbf{v}_2)=0\Longleftrightarrow\mathbf{n}_{II}\cdot\mathbf{v}_2=0\Longleftrightarrow|\mathbf{U}\hat{\mathbf{e}}|=1$.

Proof. By Proposition 1 and the definitions of Type I and II domains (which exclude the case of Compound domains), we have $\hat{\mathbf{e}}\cdot\mathbf{v}_2\neq 0$. The results then follow from (10) and the condition $\mathbf{U}\mathbf{v}_2=\mathbf{v}_2$. □

Proposition 6 shows that one of the two main cofactor conditions can be interpreted geometrically as the condition that the vector $\hat{\mathbf{e}}$ which defines the twin system (or, more generally, the domain system) lies on the intersection of the strain ellipsoid, or inverse strain ellipsoid, and the unit sphere.

4.2. Elimination of the transition layer in the austenite/martensite interface for some Type I domains

The removal of the transition layer in the case of Type I domains proceeds by proving the existence of a zero-energy triple junction. The key is to prove that $\mathbf{R}_1^{\kappa_*}=\mathbf{R}_0^\kappa$ for suitable choices of $\kappa,\kappa_*\in\{\pm 1\}$.

Theorem 7 (*Type I domains*). *Assume the hypotheses of Theorem 2 and suppose the cofactor conditions are satisfied using Type I domains. There are particular choices of* $\sigma, \sigma_* \in \{\pm 1\}$ *such that* $\mathbf{R}_1^{\sigma_*} = \mathbf{R}_0^{\sigma}$ *and* $\mathbf{b}_1^{\sigma_*} = \xi \mathbf{b}_0^{\sigma}$ *for some* $\xi \neq 0$, *so that*

$$\mathbf{R}_0^{\sigma}\mathbf{U} = \mathbf{I} + \mathbf{b}_0^{\sigma} \otimes \mathbf{m}_0^{\sigma}, \quad \mathbf{R}_0^{\sigma}(\mathbf{U} + \mathbf{a}_I \otimes \mathbf{n}_I) = \mathbf{I} + \mathbf{b}_0^{\sigma} \otimes \xi \mathbf{m}_1^{\sigma_*}, \tag{31}$$

and therefore, by taking a convex combination of the equations in (31), one of the two families of solutions of the crystallographic theory can be written as

$$\mathbf{R}_0^{\sigma}[\mathbf{U} + f\mathbf{a}_I \otimes \mathbf{n}_I] = \mathbf{I} + \mathbf{b}_0^{\sigma} \otimes (f\xi \mathbf{m}_1^{\sigma_*} + (1-f)\mathbf{m}_0^{\sigma}) \quad \text{for all } 0 \le f \le 1. \tag{32}$$

The three deformation gradients $\mathbf{I}$, $\mathbf{R}_0^{\sigma}\mathbf{U}$, $\mathbf{R}_0^{\sigma}\hat{\mathbf{R}}\hat{\mathbf{U}}$ *can form a compatible austenite/martensite triple junction in the sense that*

$$\mathbf{R}_0^{\sigma}\mathbf{U} - \mathbf{I} = \mathbf{b}_0^{\sigma} \otimes \mathbf{m}_0^{\sigma}, \quad \mathbf{R}_0^{\sigma}\hat{\mathbf{R}}\hat{\mathbf{U}} - \mathbf{I} = \mathbf{b}_0^{\sigma} \otimes \xi \mathbf{m}_1^{\sigma_*}, \quad \mathbf{R}_0^{\sigma}\hat{\mathbf{R}}\hat{\mathbf{U}} - \mathbf{R}_0^{\sigma}\mathbf{U} = \mathbf{R}_0^{\sigma}\mathbf{a}_I \otimes \mathbf{n}_I. \tag{33}$$

There is a constant $c \neq 0$ *such that* $c\mathbf{n}_I = \xi \mathbf{m}_1^{\sigma_*} - \mathbf{m}_0^{\sigma}$, *so the three vectors* $\mathbf{m}_0^{\sigma}, \mathbf{m}_1^{\sigma_*}$, *and* $\mathbf{n}_I$ *lie in a plane.*

Proof. By Proposition 6 we have for Type I domains under the cofactor conditions, $\mathbf{a}_I \cdot \mathbf{v}_2 = 0$ and $|\mathbf{U}^{-1}\hat{\mathbf{e}}| = |\hat{\mathbf{e}}| = 1$. The latter can be written, alternatively, as

$$\hat{\mathbf{e}} \cdot (\mathbf{U}^{-2} - \mathbf{I})\hat{\mathbf{e}} = 0 \Longleftrightarrow \lambda_3\sqrt{1-\lambda_1^2}(\mathbf{v}_1 \cdot \hat{\mathbf{e}}) = \pm \lambda_1\sqrt{\lambda_3^2 - 1}(\mathbf{v}_3 \cdot \hat{\mathbf{e}}). \tag{34}$$

Note in passing that $\mathbf{v}_3 \cdot \hat{\mathbf{e}} \neq 0$, because, if this was not the case, then it would follow by (34) and Corollary 3 that also $\mathbf{v}_1 \cdot \hat{\mathbf{e}} = 0$, so $\hat{\mathbf{e}} \parallel \mathbf{v}_2$. But then it would follow that $\hat{\mathbf{U}} = (-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}})\mathbf{U}(-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}}) = \mathbf{U}$ which is forbidden.

By Corollary 4, we have two families of solutions of the crystallographic theory that can be written $(\mathbf{R}_f^{\kappa} \in \mathrm{SO}(3), \mathbf{b}_f^{\kappa} \otimes \mathbf{m}_f^{\kappa})$, $\kappa \in \{\pm 1\}$, $0 \le f \le 1$ and these are distinct if $f \neq 1/2$. Thus, at $f = 1$

$$\mathbf{R}_1^{\kappa}(\mathbf{U} + \mathbf{a}_I \otimes \mathbf{n}_I) = \mathbf{R}_1^{\kappa}\hat{\mathbf{R}}\hat{\mathbf{U}} = \mathbf{I} + \mathbf{b}_1^{\kappa} \otimes \mathbf{m}_1^{\kappa}, \quad \kappa \in \{\pm 1\}. \tag{35}$$

Using that $\hat{\mathbf{U}} = (-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}})\mathbf{U}(-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}})$ and pre- and post-multiplying (35) by the 180° rotation $\hat{\mathbf{Q}} = (-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}}) = \hat{\mathbf{Q}}^T$, we have that

$$\hat{\mathbf{Q}}\mathbf{R}_1^{\kappa}\hat{\mathbf{R}}\hat{\mathbf{Q}}\mathbf{U} = \mathbf{I} + \hat{\mathbf{Q}}\mathbf{b}_1^{\kappa} \otimes \hat{\mathbf{Q}}\mathbf{m}_1^{\kappa}, \quad \kappa \in \{\pm 1\} \tag{36}$$

Comparison of (36) with (29) shows that there is a map $\hat{\sigma} : \{\pm 1\} \to \{\pm 1\}$ and $\delta \neq 0$ such that $\hat{\mathbf{Q}}\mathbf{b}_1^{\hat{\sigma}(\kappa)} = \delta \mathbf{b}_0^{\kappa}, \hat{\mathbf{Q}}\mathbf{m}_1^{\hat{\sigma}(\kappa)} = (1/\delta)\mathbf{m}_0^{\kappa}$, i.e.,

$$\mathbf{b}_1^{\hat{\sigma}(\kappa)} = \delta(-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}})\mathbf{b}_0^{\kappa}, \quad \mathbf{m}_1^{\hat{\sigma}(\kappa)} = \frac{1}{\delta}(-\mathbf{I} + 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}})\mathbf{m}_0^{\kappa}. \tag{37}$$

We note from (29), (30) and (34) that

$$\begin{aligned}\mathbf{b}_0^{\kappa} \cdot \hat{\mathbf{e}} &= \frac{\rho}{\sqrt{\lambda_3^2 - \lambda_1^2}}\left(\lambda_3\sqrt{1-\lambda_1^2}(\mathbf{v}_1 \cdot \hat{\mathbf{e}}) + \kappa\lambda_1\sqrt{\lambda_3^2 - 1}(\mathbf{v}_3 \cdot \hat{\mathbf{e}})\right) \\ &= \frac{\rho\lambda_1\sqrt{\lambda_3^2 - 1}(\mathbf{v}_3 \cdot \hat{\mathbf{e}})}{\sqrt{\lambda_3^2 - \lambda_1^2}}(\pm 1 + \kappa).\end{aligned} \tag{38}$$

Hence there is a particular choice $\kappa = \sigma \in \{\pm 1\}$ such that $\mathbf{b}_0^{\sigma} \cdot \hat{\mathbf{e}} = 0$. Let $\sigma_* = \hat{\sigma}(\sigma)$. For these choices we have from (39) that

$$\mathbf{b}_1^{\sigma_*} = -\delta \mathbf{b}_0^{\sigma}, \tag{39}$$

so, in particular, $\mathbf{b}_1^{\sigma_*} \cdot \hat{\mathbf{e}} = \mathbf{b}_1^{\sigma_*} \cdot \mathbf{v}_2 = 0$.

Take the determinant of (35) to observe that $1 + \mathbf{b}_1^{\sigma_*} \cdot \mathbf{m}_1^{\sigma_*} = \det \mathbf{R}_1^{\sigma_*}\hat{\mathbf{R}}\hat{\mathbf{U}} = \det \mathbf{U} > 0$. Premultiply (35) by $(\mathbf{R}_1^{\sigma_*})^T$, take the transpose of the resulting equation, operate the result on $\mathbf{v}_2$, and use that $\mathbf{U}\mathbf{v}_2 = \mathbf{v}_2$ and $\mathbf{a}_I \cdot \mathbf{v}_2 = 0$ (Proposition 6) to get

$$\mathbf{R}_1^{\sigma_*}\mathbf{v}_2 = \mathbf{v}_2 - (\mathbf{b}_1^{\sigma_*} \cdot \mathbf{R}_1^{\sigma_*}\mathbf{v}_2)\mathbf{m}_1^{\sigma_*}. \tag{40}$$

Dot (40) with $\mathbf{b}_1^{\sigma_*}$ and use that $1 + \mathbf{b}_1^{\sigma_*} \cdot \mathbf{m}_1^{\sigma_*} > 0$:

$$\mathbf{b}_1^{\sigma_*} \cdot \mathbf{R}_1^{\sigma_*}\mathbf{v}_2 = \frac{1}{(1 + \mathbf{b}_1^{\sigma_*} \cdot \mathbf{m}_1^{\sigma_*})}\mathbf{b}_1^{\sigma_*} \cdot \mathbf{v}_2 = 0. \tag{41}$$

(The latter follows from (39).) Eqs. (40) and (41) show that $\mathbf{R}_1^{\sigma_*}\mathbf{v}_2 = \mathbf{v}_2$. Using this conclusion and $\mathbf{n}_I = \hat{\mathbf{e}}$, evaluate (35) at $\kappa = \sigma_*$ and operate the result on $\mathbf{v}_2$ to get

$$(\hat{\mathbf{e}} \cdot \mathbf{v}_2)\mathbf{R}_1^{\sigma_*}\mathbf{a}_I = (\mathbf{m}_1^{\sigma_*} \cdot \mathbf{v}_2)\mathbf{b}_1^{\sigma_*} = -\delta(\mathbf{m}_1^{\sigma_*} \cdot \mathbf{v}_2)\mathbf{b}_0^{\sigma}. \tag{42}$$

Proposition 1 shows that $\hat{\mathbf{e}} \cdot \mathbf{v}_2 \neq 0$, so both sides of (42) are nonvanishing. Thus we can condense the constants by writing $\mathbf{R}_1^{\sigma_*}\mathbf{a}_I = c\mathbf{b}_0^{\sigma}$ for some $c \neq 0$. Substitution of the latter back into (35) ($\kappa = \sigma_*$) and use of (39) gives

$$\mathbf{R}_1^{\sigma_*}\mathbf{U} = \mathbf{I} + \mathbf{b}_0^{\sigma} \otimes (-\delta \mathbf{m}_1^{\sigma_*} - c\mathbf{n}_I). \tag{43}$$

Comparison of (43) and (30) (note: $\mathbf{b}_0^{+1} \nparallel \mathbf{b}_0^{-1}$ under our hypotheses) we get that

$$\mathbf{R}_1^{\sigma_*} = \mathbf{R}_0^{\sigma} \quad \text{and} \quad \delta \mathbf{m}_1^{\sigma_*} + c\mathbf{n}_I = -\mathbf{m}_0^{\sigma}. \tag{44}$$

We have proved Theorem 7 up to (31) and (32) is $(1-f)\,(31)_1 + f\,(31)_2$. The three rank-one connections summarized in (33) are from (31) and the basic rank-one relation (8)–(10). The planarity of the three vectors follows from (44). □

Several remarks are worth noting. First, the final statement about the planarity of the three vectors is important for actually making the indicated triple junction. Second, the solutions of the crystallographic theory given by (32) do not necessarily correspond to the choice $\kappa = \sigma$ for all $0 \le f \le 1$ in Corollary 4. In fact, the numerical evidence supports the idea that the solution found in Theorem 7 agrees with different choices of κ in Corollary 4 for different values of f, although this can be fixed by choosing eigenvectors $\mathbf{v}_1(f), \mathbf{v}_2(f), \mathbf{v}_3(f)$ that change continuously with f (this, of course, is not done by most numerical packages). Third, in the arguments of Theorem 7 we have nowhere used the inequality (CC3) of the cofactor conditions. Hence, the particular family solutions of the crystallographic theory found here do not rely on explicitly assuming this inequality. In fact, the inequality (CC3) can be proved as a necessary condition by use of (26) and (35).

The compatibility conditions given in (33) imply the existence of several interesting microstructures using the triple junction as a building block. Fig. 2(left) gives a schematic of three triple junctions. Note that by (33) all the jump conditions across all interfaces are satisfied. Satisfaction of all such jump conditions implies the existence of a continuous deformation with these gradients. Examples of deformations constructed in this way (using the method of visualization described in the introduction) are shown in Figs. 2(right), 3, 6 and 7. Fig. 3 shows the configurations of austenite/martensite interfaces having zero elastic energy for f varying from 0 to 1.

4.3. Elimination of the transition layer in the austenite/martensite interface for some Type II domains

The reason for the elimination of the transition layer in the case of Type II domains is different – it arises from the parallelism of a single variant martensite/austenite interface and a domain wall – but the mathematical argument is dual to the argument for Type I domains.

Theorem 8 (*Type II domains*). *Assume the hypotheses of Theorem 2 and suppose the cofactor conditions are satisfied using Type II domains. There are particular choices of* $\sigma, \sigma_* \in \{\pm 1\}$ *such that* $\mathbf{R}_1^{\sigma_*} = \mathbf{R}_0^{\sigma}$ *and* $\mathbf{m}_1^{\sigma_*} = \xi \mathbf{m}_0^{\sigma}$ *for some* $\xi \neq 0$, *so that*

$$\mathbf{R}_0^{\sigma}\mathbf{U} = \mathbf{I} + \mathbf{b}_0^{\sigma} \otimes \mathbf{m}_0^{\sigma}, \quad \mathbf{R}_0^{\sigma}(\mathbf{U} + \mathbf{a}_{II} \otimes \mathbf{n}_{II}) = \mathbf{I} + \xi \mathbf{b}_1^{\sigma_*} \otimes \mathbf{m}_0^{\sigma}, \tag{45}$$

and therefore, by taking a convex combination of the equations in (45), one of the two families of solutions of the crystallographic theory can be written

$$\mathbf{R}_0^{\sigma}[\mathbf{U} + f\,\mathbf{a}_{II} \otimes \mathbf{n}_{II}] = \mathbf{I} + (f\xi \mathbf{b}_1^{\sigma_*} + (1-f)\mathbf{b}_0^{\sigma}) \otimes \mathbf{m}_0^{\sigma} \quad \text{for all } 0 \le f \le 1. \tag{46}$$

The normal $\mathbf{m}_0^{\sigma}$ *to the austenite/martensite interface is independent of the volume fraction f and is parallel to the domain wall normal*: $\mathbf{n}_{II} = c\mathbf{m}_0^{\sigma}$ *for some* $c \neq 0$.

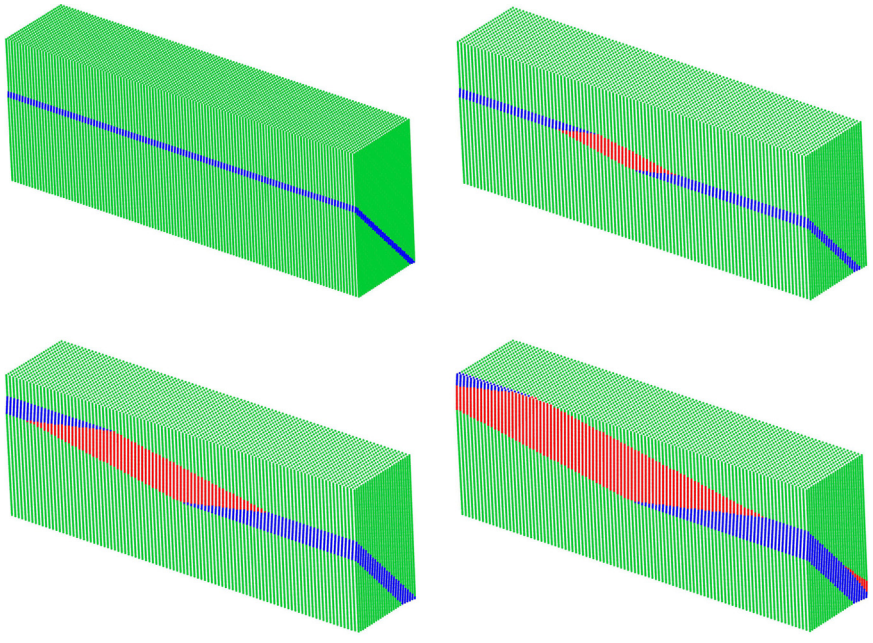

Fig. 6. Example of nucleation of austenite (red) in a band of martensite with zero elastic energy, under the cofactor conditions for Type I domains. The blue and green are two compatible variants of martensite that can form a triple junction with austenite, as described by Theorem 7. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

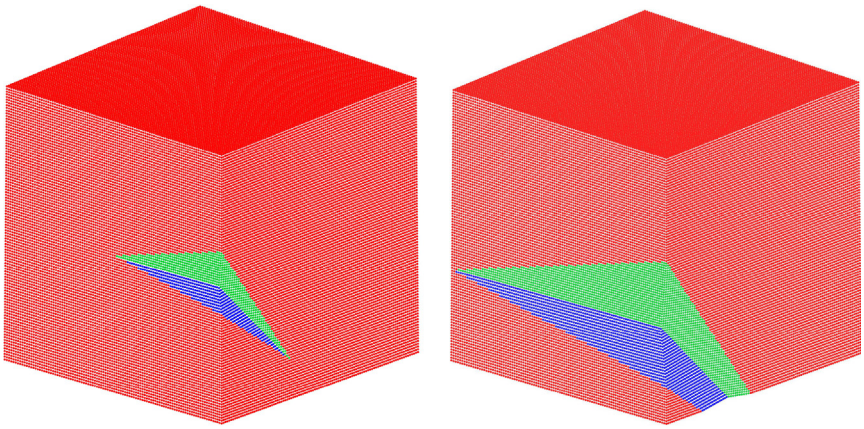

Fig. 7. Example of nucleation of martensite (blue/green bands) in austenite (red lattice) with zero elastic energy, with satisfaction of the cofactor conditions for Type I domains. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Proof. By Proposition 6 we have for Type II domains under the cofactor conditions, $\mathbf{n}_{II}\cdot\mathbf{v}_2=0$ and $|\mathbf{U}\hat{\mathbf{e}}|^2=|\hat{\mathbf{e}}|^2=1$. The latter can be written as

$$\hat{\mathbf{e}}\cdot(\mathbf{U}^2-\mathbf{I})\hat{\mathbf{e}}=0\Longleftrightarrow\sqrt{1-\lambda_1^2}(\mathbf{v}_1\cdot\hat{\mathbf{e}})=\pm\sqrt{\lambda_3^2-1}(\mathbf{v}_3\cdot\hat{\mathbf{e}}),\tag{47}$$

and, as above, $\mathbf{v}_3\cdot\hat{\mathbf{e}}\neq 0$.

Recycling the notation of the Type I case, we have two families of solutions of the crystallographic theory that can be written as $(\mathbf{R}_f^\kappa\in SO(3),\mathbf{b}_f^\kappa\otimes\mathbf{m}_f^\kappa)$, $\kappa\in\{\pm 1\}$, $0\le f\le 1$ and these are distinct if $f\neq 1/2$. Thus, at $f=1$

$$\mathbf{R}_1^\kappa(\mathbf{U}+\mathbf{a}_{II}\otimes\mathbf{n}_{II})=\mathbf{R}_1^\kappa\hat{\mathbf{R}}\hat{\mathbf{U}}=\mathbf{I}+\mathbf{b}_1^\kappa\otimes\mathbf{m}_1^\kappa,\quad\kappa\in\{\pm 1\}.\tag{48}$$

Using that $\hat{\mathbf{U}}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{U}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})$ and pre- and post-multiplying (35) by the 180° rotation $\hat{\mathbf{Q}}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})=\hat{\mathbf{Q}}^T$, we have that

$$\hat{\mathbf{Q}}\mathbf{R}_1^\kappa\hat{\mathbf{R}}\hat{\mathbf{Q}}\mathbf{U}=\mathbf{I}+\hat{\mathbf{Q}}\mathbf{b}_1^\kappa\otimes\hat{\mathbf{Q}}\mathbf{m}_1^\kappa,\quad\kappa\in\{\pm 1\}\tag{49}$$

Comparison of (49) with (29) shows that there is a map $\hat{\sigma}:\{\pm 1\}\to\{\pm 1\}$ and $\delta\neq 0$ such that $\hat{\mathbf{Q}}\mathbf{b}_1^{\hat{\sigma}(\kappa)}=\delta\mathbf{b}_0^\kappa$, $\hat{\mathbf{Q}}\mathbf{m}_1^{\hat{\sigma}(\kappa)}=(1/\delta)\mathbf{m}_0^\kappa$, i.e.,

$$\mathbf{b}_1^{\hat{\sigma}(\kappa)}=\delta(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{b}_0^\kappa,\quad\mathbf{m}_1^{\hat{\sigma}(\kappa)}=\frac{1}{\delta}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{m}_0^\kappa.\tag{50}$$

We note from (29), (30) and (47) that

$$\begin{aligned}\mathbf{m}_0^\kappa\cdot\hat{\mathbf{e}}&=\frac{1}{\rho}\frac{\lambda_3-\lambda_1}{\sqrt{\lambda_3^2-\lambda_1^2}}\left(-\sqrt{1-\lambda_1^2}(\mathbf{v}_1\cdot\hat{\mathbf{e}})+\kappa\sqrt{\lambda_3^2-1}(\mathbf{v}_3\cdot\hat{\mathbf{e}})\right),\\&=\frac{1}{\rho}\frac{\sqrt{\lambda_3^2-1}(\lambda_3-\lambda_1)(\mathbf{v}_3\cdot\hat{\mathbf{e}})}{\sqrt{\lambda_3^2-\lambda_1^2}}(\mp 1+\kappa),\quad\kappa\in\{+1,-1\}.\end{aligned}\tag{51}$$

Hence there is a particular choice $\kappa=\sigma\in\{\pm 1\}$ such that $\mathbf{m}_0^\sigma\cdot\hat{\mathbf{e}}=0$. Let $\sigma_*=\hat{\sigma}(\sigma)$. For these choices we have from (52) that

$$\mathbf{m}_1^{\sigma_*}=-\frac{1}{\delta}\mathbf{m}_0^\sigma,\tag{52}$$

so, in particular, $\mathbf{m}_1^{\sigma_*}\cdot\hat{\mathbf{e}}=\mathbf{m}_1^{\sigma_*}\cdot\mathbf{v}_2=0$.

Following the dual of the Type I case, evaluate (48) at $\kappa=\sigma_*$ and operate on $\mathbf{v}_2$ to get

$$\mathbf{R}_1^{\sigma_*}\mathbf{v}_2=\mathbf{v}_2+(\mathbf{m}_1^{\sigma_*}\cdot\mathbf{v}_2)\mathbf{b}_1^{\sigma_*}=\mathbf{v}_2.\tag{53}$$

Using the formula (10) for $\mathbf{a}_{II}$, evaluate (48) at $\kappa=\sigma_*$ and operate its transpose on $\mathbf{v}_2$ to get

$$(\mathbf{a}_{II}\cdot\mathbf{v}_2)\mathbf{n}_{II}=(\mathbf{b}_1^{\sigma_*}\cdot\mathbf{v}_2)\mathbf{m}_1^{\sigma_*}.\tag{54}$$

Lemma 1 shows that $\mathbf{a}_{II}\cdot\mathbf{v}_2=\hat{\mathbf{e}}\cdot\mathbf{v}_2\neq 0$, so both sides of (54) are nonvanishing. Thus we can condense the constants by writing $\mathbf{n}_{II}=c\mathbf{m}_0^\sigma$ for some $c\neq 0$. Substitution of the latter back into (48) ($\kappa=\sigma_*$) and use of (52) gives

$$\mathbf{R}_1^{\sigma_*}\mathbf{U}=\mathbf{I}+\left(-c\mathbf{R}_1^{\sigma_*}\mathbf{a}_{II}-\frac{1}{\delta}\mathbf{b}_1^{\sigma_*}\right)\otimes\mathbf{m}_0^\sigma.\tag{55}$$

Comparison of (55) and (30) (note: $\mathbf{b}_0^{+1} \nparallel \mathbf{b}_0^{-1}$ under our hypotheses) we get that

$$\mathbf{R}_1^{\sigma_*} = \mathbf{R}_0^{\sigma} \quad \text{and} \quad \mathbf{R}_1^{\sigma_*}\mathbf{a}_{II} + \frac{1}{\delta}\mathbf{b}_1^{\sigma_*} = -\mathbf{b}_0^{\sigma}. \tag{56}$$

We have proved Theorem 8 up to (45) and (46) is $(1-f)\,(45)_1 + f\,(45)_2$. The parallelism of $\mathbf{n}_{II}$ and $\mathbf{m}_0^{\sigma}$ is (54). □

Some of the remarks following the proof of Theorem 7 apply here as well. In a certain sense these results show that, under the cofactor conditions, triple junctions are dual to parallel austenite/twin interfaces. The duality is that which maps Type I into Type II twins.

4.4. The cofactor conditions for Compound domains

We assume in this section the hypotheses of Proposition 1 which gives the basic characterization of Compound domains. Specifically, we assume that there are orthonormal vectors $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2$ such that $\hat{\mathbf{U}} = (-\mathbf{I} + 2\hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_1)\mathbf{U}(-\mathbf{I} + 2\hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_1) = (-\mathbf{I} + 2\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2)\mathbf{U}(-\mathbf{I} + 2\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2) \neq \mathbf{U}$. The two solutions of (8) for Compound domains $\mathbf{a}_C^1 \otimes \mathbf{n}_C^1$, $\mathbf{a}_C^2 \otimes \mathbf{n}_C^2$ are then given by (11).

Lemma 9. *Suppose that there are orthonormal vectors* $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2$ *such that* $\hat{\mathbf{U}} = (-\mathbf{I} + 2\hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_1)\mathbf{U}(-\mathbf{I} + 2\hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_1) = (-\mathbf{I} + 2\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2)\mathbf{U}(-\mathbf{I} + 2\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2) \neq \mathbf{U}$, *and let* $\mathbf{a}_C^1 \otimes \mathbf{n}_C^1$, $\mathbf{a}_C^2 \otimes \mathbf{n}_C^2$ *be given by* (11). *The cofactor conditions are satisfied for either of these solutions if and only if* $\hat{\mathbf{e}}_1 \cdot \mathbf{v}_2 = 0$, $\hat{\mathbf{e}}_2 \cdot \mathbf{v}_2 = 0$, $\hat{\mathbf{e}}_1$ *is not parallel to either* $\mathbf{v}_1$ *or* $\mathbf{v}_3$, *and the inequality* (CC3) *holds.*

Proof. By Corollary 5, the condition (CC2) of the cofactor conditions for either solution $\mathbf{a}_C^1 \otimes \mathbf{n}_C^1$ or $\mathbf{a}_C^2 \otimes \mathbf{n}_C^2$ reduces to

$$(\hat{\mathbf{e}}_1 \cdot \mathbf{v}_2)(\hat{\mathbf{e}}_2 \cdot \mathbf{v}_2) = 0. \tag{57}$$

Suppose the cofactor conditions are satisfied. According to Proposition 11 both $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ are perpendicular to an eigenvector of $\mathbf{U}$. But this eigenvector cannot be $\mathbf{v}_1$ or $\mathbf{v}_3$, because then (57) would force either $\hat{\mathbf{e}}_1$ or $\hat{\mathbf{e}}_2$ to be parallel to an eigenvector of $\mathbf{U}$ which contradicts $\hat{\mathbf{U}} \neq \mathbf{U}$. Therefore the eigenvector in question must be $\mathbf{v}_2$ and we have both $\hat{\mathbf{e}}_1 \cdot \mathbf{v}_2 = 0$ and $\hat{\mathbf{e}}_2 \cdot \mathbf{v}_2 = 0$. Of course, it also follows from the hypothesis $\hat{\mathbf{U}} \neq \mathbf{U}$ that $\hat{\mathbf{e}}_1$ is not parallel to either $\mathbf{v}_1$ or $\mathbf{v}_3$. The remaining condition of the cofactor conditions is the inequality (CC3). Clearly, these necessary conditions are also sufficient for the cofactor conditions. □

This result says that we satisfy cofactor conditions for Compound domains by putting the orthonormal vectors $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2$ in the $\mathbf{v}_1, \mathbf{v}_3$ plane and satisfying the inequality (CC3), see Fig. 5. If $\mathbf{U}$ is given as above, then there is only one degree-of-freedom, say, the angle θ between $\hat{\mathbf{e}}_1$ and $\mathbf{v}_1$, in the assignment of $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2$. The left hand side of the inequality (CC3) then becomes a function of λ_1, λ_3 and θ. Given θ, it can be seen from numerical examples that there is a domain in $\mathbb{R}^2$ of possible values of λ_1, λ_3 at which (CC3), and therefore the cofactor conditions are satisfied. For many choices of θ this domain seems to be quite large, including many potential alloys, but does not include all of $\lambda_1 < 1 < \lambda_3$. We do not see any general statements one can make about this domain, except the obvious point that if θ is fixed, then the left hand side of the inequality (CC3) tends to 0 as $|\lambda_3 - 1| + |1 - \lambda_1| \to 0$.

It should be noted that except for the possibility of a restricted domain for λ_1, λ_3, Compound domains can satisfy the cofactor conditions *merely by symmetry and* $\lambda_2 = 1$. That is, if the lattice parameters of a potential alloy are first tuned to satisfy $\lambda_2 = 1$, and the symmetry happens to be such that there are two 180° rotations in the point group $\mathcal{P}$ with perpendicular axes that lie in a plane perpendicular to $\mathbf{v}_2$, then the cofactor conditions are satisfied as long as the domain for λ_1, λ_3 is suitable. See the example of VO_2 in Section 8.

There seem to be no general statements about the elimination of the transition layer that one can make that are independent of the choice of $\hat{\mathbf{e}}_1$ (satisfying Lemma 9), as was done in the cases of Types I and II domains. For example, the main condition $\mathbf{R}_0 = \mathbf{R}_1$ that eliminated the transition layer for Type I domains becomes a single scalar equation restricting λ_1, λ_3 and θ in the case of Compound domains. It may well be possible for quite special choices of λ_1, λ_3 and θ to eliminate the transition layer. For practical alloy development such a condition seems not so useful, as usually θ would be given, and the resulting further restriction on λ_1, λ_3 would seem to be difficult to satisfy. But further investigation is warranted.

5. Simultaneous satisfaction of the cofactor conditions for different domain systems

In the Introduction we have argued that the cofactor conditions imply the existence of many deformations consistent with the coexistence of austenite and martensite, and many of these cases also have zero elastic energy. Here we quantify these statements for one of the two types of cubic to monoclinic phase transformations (see, e.g., Soligo et al., 1999; James and Hane, 2000). This case is interesting with regard to applications (see Section 8), and is representative of other high-to-low symmetry cases.

We consider symmetry change from cubic to monoclinic with $\langle 100 \rangle_a$ as the inherited 2-fold axis. There are 12 martensite variants in this case with transformation stretch matrices given by

$$\mathbf{U}_1 = \begin{bmatrix} \alpha & \beta & 0 \\ \beta & \delta & 0 \\ 0 & 0 & \gamma \end{bmatrix}, \quad \mathbf{U}_2 = \begin{bmatrix} \alpha & -\beta & 0 \\ -\beta & \delta & 0 \\ 0 & 0 & \gamma \end{bmatrix}, \quad \mathbf{U}_3 = \begin{bmatrix} \delta & \beta & 0 \\ \beta & \alpha & 0 \\ 0 & 0 & \gamma \end{bmatrix}, \quad \mathbf{U}_4 = \begin{bmatrix} \delta & -\beta & 0 \\ -\beta & \alpha & 0 \\ 0 & 0 & \gamma \end{bmatrix},$$

$$\mathbf{U}_5=\begin{bmatrix}\gamma & 0 & 0\\ 0 & \delta & \beta\\ 0 & \beta & \alpha\end{bmatrix},\quad \mathbf{U}_6=\begin{bmatrix}\gamma & 0 & 0\\ 0 & \delta & -\beta\\ 0 & -\beta & \alpha\end{bmatrix},\quad \mathbf{U}_7=\begin{bmatrix}\alpha & 0 & \beta\\ 0 & \gamma & 0\\ \beta & 0 & \delta\end{bmatrix},\quad \mathbf{U}_8=\begin{bmatrix}\alpha & 0 & -\beta\\ 0 & \gamma & 0\\ -\beta & 0 & \delta\end{bmatrix},$$
$$\mathbf{U}_9=\begin{bmatrix}\delta & 0 & \beta\\ 0 & \gamma & 0\\ \beta & 0 & \alpha\end{bmatrix},\quad \mathbf{U}_{10}=\begin{bmatrix}\delta & 0 & -\beta\\ 0 & \gamma & 0\\ -\beta & 0 & \alpha\end{bmatrix},\quad \mathbf{U}_{11}=\begin{bmatrix}\gamma & 0 & 0\\ 0 & \alpha & \beta\\ 0 & \beta & \delta\end{bmatrix},\quad \mathbf{U}_{12}=\begin{bmatrix}\gamma & 0 & 0\\ 0 & \alpha & -\beta\\ 0 & -\beta & \delta\end{bmatrix}. \tag{58}$$

To avoid degeneracies, we assume for the rest of this section that $\alpha\neq\delta$ and that the eigenvalues of $\mathbf{U}_1$ are distinct. Between these martensite variants, there are 24 Type I twins, 24 Type II twins, 24 Compound twins, 24 Type I domains, 24 Type II domains and 12 Compound domains. These domains with labels of pairs of compatible variants are listed in Table 1. The notation for variants is consistent with (58).

In the case of domains that are not conventional twins (Table 1), the rotation relating each pair of compatible variants is a 90° rotation. The 180 ° rotation that necessarily relates these variants is given by formulas in the Appendix.

The boxes within the dark shaded region in Table 1 have the property that if one pair in the box satisfies the cofactor conditions for a certain type of domain, then all pairs in the box satisfy the cofactor conditions for the same type of domain. For example, if variants 1 and 6 have a Type I twin satisfying the cofactor conditions, then the Type I twin pairs (2,5), (1,5) and (2,6) also satisfy the cofactor conditions. In each of these cases there are compatible triple junctions leading to numerous zero elastic energy microstructures of austenite coexisting with martensite as discussed in Theorem 7.

The light shaded box is particularly interesting. If $\gamma=1$ (only) then the cofactor conditions are satisfied (Lemma 9). As can be seen from Table 1 there are then a very large number of Compound domains that satisfy the cofactor conditions. For each of these there are infinitely many deformation gradients of martensite that coexist with $\mathbf{I}$ in the sense of the crystallographic theory. Thus, there is a huge collection of compatible deformations of austenite and martensite, although none of these have zero elastic energy. Under our hypotheses, Compound twins with $\gamma\neq1$ cannot satisfy the cofactor conditions, and the numerical evidence suggests that this is also true for the Compound domains.

6. Nucleation under the cofactor conditions

The analysis given above suggests simple microstructures with zero elastic energy that allow a continuous increase of the volume of the new phase, starting at zero volume, in a material satisfying the cofactor conditions. In a single crystal there are obviously cases in which a layer of martensite can grow in austenite and *vice versa*, merely due to the condition $\lambda_2=1$. We illustrate some cases in which the set on which nucleation takes place is lower dimensional, e.g., a line. As illustrated and analyzed by Ball et al. (2011b,a) and Seiner and Landa (2009), the geometry of these nuclei is important for nucleation phenomena.

An example of nucleation of austenite in martensite is given in Fig. 6. It is constructed from any Type I domain for which the cofactor conditions are satisfied, and it uses the three deformation gradients $\mathbf{I},\mathbf{R}_0^{\sigma}\mathbf{U},\mathbf{R}_0^{\sigma}\hat{\mathbf{R}}\hat{\mathbf{U}}$ given in Theorem 7.

Table 1
List of all possible twin systems for cubic to monoclinic transformations with $\langle100\rangle_a$ as the inherited 2-fold axis. The notation (i,j) presents domains which are symmetry related by $\mathbf{U}_i=\mathbf{R}\mathbf{U}_j\mathbf{R}^{\mathrm{T}}$, where $\mathbf{R}\in\mathcal{P}$ is characterized by the angle and rotational axis. See the text.

Type	$\mathbf{R}$ $\theta°,[h,k,l]$	Type I/II twins or domains		Compound twins or domains	
				$\gamma=1$	$\gamma\neq1$
Conventional twins	$180°,[1,0,0]$			$(1,2),(7,8)$ $(3,4),(9,10)$	$(1,2),(7,8)$ $(3,4),(9,10)$
	$180°,[0,1,0]$			$(1,2),(5,6)$ $(3,4),(11,12)$	$(1,2),(5,6)$ $(3,4),(11,12)$
	$180°,[0,0,1]$			$(7,8),(11,12)$ $(5,6),(9,10)$	$(7,8),(11,12)$ $(5,6),(9,10)$
	$180°,[1,0,1]$	$(1,6),(2,5),$	$(3,12),(4,11)$	$(7,9),(8,10)$	$(7,9),(8,10)$
	$180°,[1,0,\bar{1}]$	$(1,5),(2,6),$	$(3,11),(4,12)$	$(7,9),(8,10)$	$(7,9),(8,10)$
	$180°,[1,1,0]$	$(5,10),(6,9),$	$(7,12),(8,11)$	$(1,3),(2,4)$	$(1,3),(2,4)$
	$180°,[\bar{1},1,0]$	$(5,9),(6,10),$	$(7,11),(8,12)$	$(1,3),(2,4)$	$(1,3),(2,4)$
	$180°,[0,1,1]$	$(1,8),(2,7),$	$(3,10),(4,9)$	$(5,11),(6,12)$	$(5,11),(6,12)$
	$180°,[0,\bar{1},1]$	$(1,7),(2,8),$	$(3,9),(4,10)$	$(5,11),(6,12)$	$(5,11),(6,12)$
Domains (all are nonconventional twins)	$90°,[0,0,1]$	$(5,9),(6,10),$ $(5,10),(6,9),$	$(7,12),(8,11)$ $(7,11),(8,12)$	$(1,4),(2,3)$	$(1,4),(2,3)$
	$90°,[0,1,0]$	$(1,5),(2,6),$ $(1,6),(2,5),$	$(3,11),(4,12)$ $(4,11),(3,12)$	$(7,10),(8,9)$	$(7,10),(8,9)$
	$90°,[1,0,0]$	$(1,8),(2,7),$ $(1,7),(2,8),$	$(3,10),(4,9)$ $(3,9),(4,10)$	$(5,12),(6,11)$	$(5,12),(6,11)$

Table 2
Potential starting points for an alloy development program whose goal is to satisfy the cofactor conditions.

Candidates	$Cu_{69}Al_{24}Mn_7$[a]	$Au_{25}Cu_{30}Zn_{45}$[b]	VO_2[c]
Crystal structure			
Austenite	DO3	$L2_1$	Rutile
Martensite	6 M	M18R	Rutile monocl.
Bravais lattice			
Austenite	FCC	FCC	Primitive tetragonal
Martensite	Primitive monocl.	Primitive monocl.	Base-centered monocl.
Transformation stretch matrix **U**	$\begin{pmatrix} 1.1098 & 0.0279 & 0 \\ 0.0279 & 1.0062 & 0 \\ 0 & 0 & 0.8989 \end{pmatrix}$	$\begin{pmatrix} 1.0508 & 0 & 0.0142 \\ 0 & 0.9108 & 0 \\ 0.0142 & 0 & 1.0059 \end{pmatrix}$	$\begin{pmatrix} 1.0669 & 0 & 0.0421 \\ 0 & 0.9939 & 0 \\ 0.0421 & 0 & 0.9434 \end{pmatrix}$
$\lvert\lambda_2-1\rvert$	0.0008	0.0018	0.0061
180° axis $\hat{\mathbf{e}}$	[011] or $[01\bar{1}]$	$[10\bar{1}]$	[001]
Cofactor conditions			
Type I, $\lvert\mathbf{U}^{-1}\hat{\mathbf{e}}\rvert-1$	0.0256	0.0263	
Type II, $\lvert\mathbf{U}\hat{\mathbf{e}}\rvert-1$	0.0202	0.029	
Compound			Satisfied if $\lambda_2=1$
Inequality (CC3)	0.0016	0.0175	0.0144

[a] (Zhang, 2007).
[b] (Hiroshi and Shimizu, 1976) The lattice parameters of austenite, which are needed to calculate **U**, were not measured by these authors, so we have supplied this measurement.
[c] (McWhan and Remeika, 1970).

The regions on which these deformation gradients occur are shown as red, green and blue, respectively, in Fig. 6. Nucleation in this case occurs on a line; four triple junctions are simultaneously emitted from this line.

Under the same conditions, a simple mechanism for boundary nucleation of martensite in austenite is shown in Fig. 7. This is seen as a simplified version of Fig. 2.

7. Cofactor conditions in the geometrically linear case

A number of versions of the geometrically linear theory of martensite are in wide use for both fundamental theoretical and computational studies (Khachaturyan and Shatalov, 1969; Roitburd, 1978; Barsch and Krumhansl, 1984; Kohn, 1989; Bhattacharya, 1993; Knüpfer et al., 2011). There is a version of the cofactor conditions in the geometrically linear case. Since the satisfaction of the cofactor conditions is expected to have a dramatic effect on predicted microstructure and behavior in the geometrically linear theory, we give these conditions here.

The cofactor conditions in geometrically linear theory are different from the cofactor conditions in the geometrically nonlinear theory, owing to the fact that the geometrically linear theory is obtained from the geometrically nonlinear theory by Taylor expansion (Bhattacharya, 1993) or asymptotic analysis (Schmidt, 2008). As discussed below, the cofactor conditions in the geometrically linear case should not be used for alloy development in materials with appreciable transformation strain.

The cofactor conditions in the geometrically linear case can be obtained in two ways: (i) by formal linearization of the cofactor conditions in the geometrically nonlinear case following the expansion given in Ball and James (1992), or (ii) by writing down the equations of the crystallographic theory of martensite in the geometrically linear case, and imposing the condition that they be satisfied for any volume fraction $0\leq f\leq 1$. The latter method is preferable because it proves the existence of actual energy minimizing microstructures (or minimizing sequences) for a broad family of geometrically linear theories of martensite. We therefore follow method (ii).

The geometrically linear version of the crystallographic theory of martensite in the cubic-to-tetragonal case first appeared in a paper of Burkart and Read (1953) in the same issue of AIME Journal of Metals as the general version of the crystallographic theory by Wechsler et al. (1953).

The basic kinematics of geometrically linear theory is the same as linearized elasticity: it is based on the displacement gradient $\nabla\mathbf{u}=\mathbf{H}\in\mathbb{R}^{3\times 3}$, which is decomposed into symmetric and skew parts $\mathbf{H}=\mathbf{S}+\mathbf{W}$, $\mathbf{S}=\mathbf{S}^T$, $\mathbf{W}=-\mathbf{W}^T$ representing infinitesimal strain and rotation. A particular strain $\mathbf{S}=\mathbf{E}$ is given as the *transformation strain*, and strains associated with the variants of martensite are obtained by symmetry. As above, we consider another variant defined by the strain $\hat{\mathbf{E}}=\mathbf{QEQ}^T$ where $\mathbf{Q}=-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}$, $|\hat{\mathbf{e}}|=1$. The basic compatibility condition for variants with displacement gradients $\nabla\mathbf{u}=\hat{\mathbf{E}}+\hat{\mathbf{W}}$ and $\nabla\mathbf{u}=\mathbf{E}$ is

$$\hat{\mathbf{E}}+\hat{\mathbf{W}}-\mathbf{E}=\mathbf{a}\otimes\mathbf{n}. \tag{59}$$

(This is also the direct geometric linearization of (8).) Taking the symmetric part of (59) we have the compatibility condition of geometrically linear theory:

$$\hat{\mathbf{E}}-\mathbf{E}=\tfrac{1}{2}(\mathbf{a}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{a}). \tag{60}$$

By taking the trace, we have necessarily that $\mathbf{a}\cdot\mathbf{n}=0$. The basic lemma governing solutions of (60) is the following.

Lemma 10. *Necessary and sufficient conditions that* $\mathbf{S}\in\mathbb{R}^{3\times3}_{\mathrm{sym}}$ *is expressible in the form* $\mathbf{S}=(1/2)(\mathbf{a}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{a})$ *for some nonzero* $\mathbf{a},\mathbf{n}\in\mathbb{R}^3$ *is that the middle eigenvalue of* $\mathbf{S}$ *is zero. If* $\mathbf{S}=s_1\mathbf{e}_1\otimes\mathbf{e}_1+s_3\mathbf{e}_3\otimes\mathbf{e}_3$ *with* $\mathbf{e}_1,\mathbf{e}_3$ *orthonormal and* $s_1\le0\le s_3$, *then solutions* $\mathbf{a},\mathbf{n}$ *of* $\mathbf{S}=(1/2)(\mathbf{a}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{a})$ *can be taken as*

$$\mathbf{a}=\sqrt{-s_1}\mathbf{e}_1+\sqrt{s_3}\mathbf{e}_3,\quad \mathbf{n}=-\sqrt{-s_1}\mathbf{e}_1+\sqrt{s_3}\mathbf{e}_3. \tag{61}$$

These are unique up to switching $\mathbf{a}\to\mathbf{n}$, $\mathbf{n}\to\mathbf{a}$ *and scaling* $\mathbf{a}\to\mu\mathbf{a}$, $\mathbf{n}\to(1/\mu)\mathbf{n}$, $\mu\neq0$.

Proof (*See e.g., Bhattacharya (2003)*). Briefly, it is clear that a necessary condition that $\mathbf{S}$ has the given form is that $\mathbf{S}$ has an eigenvalue equal to zero. By examining the quadratic form $\mathbf{z}\cdot\mathbf{S}\mathbf{z}$ with $\mathbf{z}$ taken as a bisector of $\mathbf{a}$ and $\mathbf{n}$, and as a vector in the $\mathbf{a},\mathbf{n}$ plane that is perpendicular to this bisector, it is seen that the zero eigenvalue is the middle one. The converse is proved by direct calculation using (61). □

In the special case that $\hat{\mathbf{E}}=\mathbf{Q}\mathbf{E}\mathbf{Q}^T$ as given above, an alternative representation of a solution of (60) is possible:

$$\mathbf{a}=4((\hat{\mathbf{e}}\cdot\mathbf{E}\hat{\mathbf{e}})\hat{\mathbf{e}}-\mathbf{E}\hat{\mathbf{e}}),\quad \mathbf{n}=\hat{\mathbf{e}}. \tag{62}$$

This form of the solution can be interpreted as the geometric linearization of the Type I/II domains. That is, due to the switching invariance of Lemma 10, there exist infinitesimal rotations $\hat{\mathbf{W}}_I=-\hat{\mathbf{W}}_I^T$ and $\hat{\mathbf{W}}_{II}=-\hat{\mathbf{W}}_{II}^T$ such that, with $\mathbf{a}$ and $\mathbf{n}$ defined by (62)

$$\hat{\mathbf{E}}+\hat{\mathbf{W}}_I-\mathbf{E}=\mathbf{a}\otimes\mathbf{n},\quad \hat{\mathbf{E}}+\hat{\mathbf{W}}_{II}-\mathbf{E}=\mathbf{n}\otimes\mathbf{a}, \tag{63}$$

i.e., either $\mathbf{a}$ or $\mathbf{n}$ can be considered the interface normal. $\hat{\mathbf{W}}_I=-\hat{\mathbf{W}}_{II}$ as defined by these formulas is necessarily skew.

From these compatibility conditions and the comments of Section 2.2 it is seen that the equations of the crystallographic theory of martensite in the geometrically linear case are the following. Given $\mathbf{E}\in\mathbb{R}^{3\times3}_{\mathrm{sym}}$ and $\hat{\mathbf{E}}=\mathbf{Q}\mathbf{E}\mathbf{Q}^T$ as above, so that $\hat{\mathbf{E}}-\mathbf{E}=\tfrac{1}{2}(\mathbf{a}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{a})$ for some $\mathbf{a},\mathbf{n}\in\mathbb{R}^3$, find $\mathbf{b}_f,\mathbf{m}_f\in\mathbb{R}^3$ and $0\le f\le1$ such that

$$f\hat{\mathbf{E}}+(1-f)\mathbf{E}=\tfrac{1}{2}\left(\mathbf{b}_f\otimes\mathbf{m}_f+\mathbf{m}_f\otimes\mathbf{b}_f\right). \tag{64}$$

The *cofactor conditions in geometrically linear theory* are necessary and sufficient conditions that there exist $\mathbf{b}_f,\mathbf{m}_f\in\mathbb{R}^3$ satisfying (64) for every $0\le f\le1$. An explicit form of these conditions is given in the following theorem.

Theorem 11 (*Cofactor conditions in the geometrically linear theory*). *Let* $\mathbf{E}\in\mathbb{R}^{3\times3}_{\mathrm{sym}}$ *and* $\hat{\mathbf{e}}\in\mathbb{R}^3$, $|\hat{\mathbf{e}}|=1$, *be given. Define* $\hat{\mathbf{E}}=\mathbf{Q}\mathbf{E}\mathbf{Q}^T$ *where* $\mathbf{Q}=-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}$, *suppose that* $\hat{\mathbf{E}}\neq\mathbf{E}$, *and define* $\mathbf{a},\mathbf{n}$ *by* (62). *There exist* $\mathbf{b}_f,\mathbf{m}_f\in\mathbb{R}^3$ *satisfying* (64) *for every* $0\le f\le1$ *if and only if*

$$\varepsilon_2=0,\quad \textit{where } \varepsilon_2 \textit{ is the middle eigenvalue of } \mathbf{E},\ \textit{and rank } \mathbf{E}=2, \tag{CCL1}$$

$$(\mathbf{a}\cdot\mathbf{v}_2)(\mathbf{n}\cdot\mathbf{v}_2)=0,\quad \textit{where } \mathbf{E}\mathbf{v}_2=0,\ |\mathbf{v}_2|=1, \tag{CCL2}$$

$$(\mathrm{tr}(\mathbf{E}+\hat{\mathbf{E}}))^2-\mathrm{tr}((\mathbf{E}+\hat{\mathbf{E}})^2)\le0. \tag{CCL3}$$

Proof. Necessity of the conditions (CCL). Clearly $\varepsilon_2=0$ is a necessary condition at $f=0$. Also, $\mathbf{E}$ cannot vanish because $\hat{\mathbf{E}}\neq\mathbf{E}$. Potentially, $\mathbf{E}$ could be of rank 1, $\mathbf{E}=\mathbf{g}\otimes\mathbf{g}\neq0$, but then we would have $\hat{\mathbf{E}}=\hat{\mathbf{g}}\otimes\hat{\mathbf{g}}$ with $|\mathbf{g}|=|\hat{\mathbf{g}}|$ and $\mathbf{g}\nparallel\hat{\mathbf{g}}$. The unique zero eigenspace of $f\hat{\mathbf{E}}+(1-f)\mathbf{E}$ for $0<f<1$ would then be the 1-D subspace $\delta\,\mathbf{g}\times\hat{\mathbf{g}}$, $\delta\in\mathbb{R}$. The only possibility that the corresponding zero eigenvalue of $f\hat{\mathbf{E}}+(1-f)\mathbf{E}$ would be its middle eigenvalue is that it is a double eigenvalue, because the quadratic form $f\mathbf{z}\cdot\hat{\mathbf{E}}\mathbf{z}+(1-f)\mathbf{z}\cdot\mathbf{E}\mathbf{z}$ is clearly positive semidefinite. This contradicts that the zero eigenspace is one dimensional. Hence, rank $\mathbf{E}=2$.

The necessity of (CCL2) follows by direct calculation of the determinant of $f\hat{\mathbf{E}}+(1-f)\mathbf{E}$. That is, if we write $\mathbf{E}=\mathrm{diag}(\varepsilon_1,0,\varepsilon_3)$ for $\varepsilon_1<0<\varepsilon_3$ (using (CCL1)), a direct calculation gives

$$\det(f\hat{\mathbf{E}}+(1-f)\mathbf{E})=\det(\mathbf{E}+(f/2)(\mathbf{a}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{a}))=4f(1-f)\varepsilon_1\varepsilon_3(\mathbf{a}\cdot\mathbf{v}_2)(\mathbf{n}\cdot\mathbf{v}_2). \tag{65}$$

The remaining necessary condition is that the implied zero eigenvalue is the middle one. Assume (CCL1) and (CCL2) and let $\varepsilon_1^f,0,\varepsilon_2^f$ be the eigenvalues of $f\hat{\mathbf{E}}+(1-f)\mathbf{E}$, with no particular ordering. If 0 is the middle eigenvalue, then $\varepsilon_1^f\varepsilon_2^f\le0$ for $0\le f\le1$. The quantity $\varepsilon_1^f\varepsilon_2^f$ is the second invariant of $f\hat{\mathbf{E}}+(1-f)\mathbf{E}$. This invariant is quadratic in f and has the same values at $f=0,1$, and so it has the form $\mathrm{II}_f=\alpha f(1-f)+\varepsilon_1\varepsilon_3$. The coefficient α can be evaluated from $\alpha=d\mathrm{II}_f(0)/df=-\mathbf{a}\cdot\mathbf{E}\mathbf{n}$. Also, $\alpha\ge0$ by $\mathbf{a}\cdot\mathbf{E}\mathbf{n}=\mathbf{E}\cdot(\hat{\mathbf{E}}-\mathbf{E})$ and the Cauchy–Schwarz inequality, $\hat{\mathbf{E}}\cdot\mathbf{E}\le|\mathbf{E}||\hat{\mathbf{E}}|=|\mathbf{E}|^2=\mathbf{E}\cdot\mathbf{E}$. Therefore, the largest value of $\varepsilon_1^f\varepsilon_2^f\le0$ occurs at $f=1/2$, and so we have the necessary condition $\mathrm{II}_{1/2}\le0$ which is (CCL3). The conditions (CCL1), (CCL2) and (CCL3) are also sufficient for (64) to be satisfied for every $0\le f\le1$, since they imply that the middle eigenvalue of $f\hat{\mathbf{E}}+(1-f)\mathbf{E}$ is zero for all $0\le f\le1$. □

The explicit form of the conditions (CCL1)–(CCL3) in the eigenbasis of $\mathbf{E}$ is

$$\mathbf{E}=\mathrm{diag}(\varepsilon_1,0,\varepsilon_3),\quad \varepsilon_1<0<\varepsilon_3, \tag{CCL1′}$$

$$n_2^2(n_1^2\varepsilon_1+n_3^2\varepsilon_3)=0, \tag{CCL2′}$$

$$\begin{cases}\varepsilon_1\varepsilon_3+n_1^2n_3^2(\varepsilon_3-\varepsilon_1)^2\le 0 & \text{if } n_2=0,\\ \varepsilon_1\varepsilon_3+n_3^2\varepsilon_3(\varepsilon_3-\varepsilon_1)\le 0 & \text{if } n_1^2\varepsilon_1+n_3^2\varepsilon_3=0.\end{cases} \tag{CCL3′}$$

As expected, the elastic transition layer can also be eliminated in the geometrically linear case. This occurs if $n_1^2\varepsilon_1+n_3^2\varepsilon_3=0$. It follows from $n_1^2\varepsilon_1+n_3^2\varepsilon_3=0$ and (CCL1′) and (CCL2′) that $\mathbf{b}_0\parallel\mathbf{b}_1$ or $\mathbf{m}_0\parallel\mathbf{m}_1$, which in turn lead to triple junctions or parallelism, analogous to the nonlinear case.

As mentioned above, one should be cautious on applying the cofactor conditions of geometrically linear theory in alloy development because of the errors of geometric linearization. As a particular example, we can consider the main condition (CC2′) in the case of Types I and II domains. According to Proposition 6, the condition (CC2′) is $|\mathbf{U}^{-1}\hat{\mathbf{e}}|=1$ for Type I domains and $|\mathbf{U}\hat{\mathbf{e}}|=1$ for Type II domains under the general hypotheses given there. Both of these conditions linearize to the same condition $\hat{\mathbf{e}}\cdot\mathbf{E}\hat{\mathbf{e}}=n_1^2\varepsilon_1+n_3^2\varepsilon_3=0$ of (CCL2′) (recall from (62) that $\mathbf{n}=\hat{\mathbf{e}}$). If we use the standard way of evaluating the transformation strain of linearized theory, $\mathbf{E}=\mathbf{U}-\mathbf{I}$, we have

$$\begin{aligned}&\text{Geometrically nonlinear, Type I}: \quad \left(\frac{1}{\lambda_1^2}-1\right)n_1^2+\left(\frac{1}{\lambda_3^2}-1\right)n_3^2=0.\\ &\text{Geometrically nonlinear, Type II}: \quad (\lambda_1^2-1)n_1^2+(\lambda_3^2-1)n_3^2=0.\\ &\text{Geometrically linear}: \quad (\lambda_1-1)n_1^2+(\lambda_3-1)n_3^2=0.\end{aligned} \tag{66}$$

As a numerical example, we can take typical twin systems in a cubic to monoclinic case discussed in Section 5, which is also represented by the particular alloys identified in Section 8 as good starting points for alloy development. For example, we take $\mathbf{n}=\hat{\mathbf{e}}=(1,1,0)/\sqrt{2}$ (in the cubic basis). We take a typical measured value of $\lambda_3=1.08$. Then, the exact satisfaction of the cofactor conditions in the three cases of (66) gives

$$\begin{aligned}&\text{Geometrically nonlinear, Type I}: \quad \lambda_1=0.936,\\ &\text{Geometrically nonlinear, Type II}: \quad \lambda_1=0.913,\\ &\text{Geometrically linear}: \quad \lambda_1=0.920.\end{aligned} \tag{67}$$

In light of the sensitive dependence of hysteresis on the middle eigenvalue seen on the horizontal axis of Fig. 1, the discrepancies seen in (67) may be significant. Of course, it is no more difficult to use the geometrically nonlinear conditions. The present situation with regard to the linearization of the cofactor conditions is similar to a number of other special lattice parameter relationships discussed by Bhattacharya (1993). In geometrically linear theory the elastic energy near the habit plane can also be eliminated in some cases.

8. Implications of the results for alloy development

Although the theory justifying and explaining the cofactor conditions is intricate, the conditions themselves are simple and easy to implement (Table 2). One first chooses a domain system, which is the choice of a unit vector $\hat{\mathbf{e}}$ relating two variants as in (9). Then one calculates $\mathbf{a}$ and $\mathbf{n}$ from (10) or (11), depending on whether the domain system is Type I/II or Compound.

As explained in Section 2.1, this choice also covers the cases of non-conventional and non-generic twins, thus the terminology "domain" throughout this paper. From these choices one identifies whether the domain is Type I, Type II or Compound.

A convenient form of the cofactor conditions for alloy development is then (CC1) and (CC2′) (as further simplified by Proposition 6). The inequality (CC3) also has to be checked. Among the systems identified below that are near to satisfying the cofactor conditions, it seems that this inequality will be automatically satisfied. A useful alloy development procedure is by interpolation:

1. From X-ray measurements determine the transformation stretch matrix $\mathbf{U}$ and unit vector $\hat{\mathbf{e}}$ relating two variants: $\hat{\mathbf{U}}=\mathbf{QUQ}^T$, $\mathbf{Q}=-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}$. See Chen and James (2013) for an algorithm that automates this part. Identify the type of domain. Below, for definiteness, it is assumed that we wish to find an alloy satisfying the cofactor conditions for a Type I twin system. $\mathbf{U}$ depends on composition, and we assume there are two compositional variables x and y.
2. Determine a one-parameter family of alloys satisfying $\lambda_2=1$. We have found the following procedure to be useful. For each x, find and alloy with composition (x,y_1) having $\lambda_2\gtrsim 1$ and another alloy (x,y_2) having $\lambda_2\lesssim 1$. Then interpolate to find a family of alloys with composition $(x,y(x))$ with $\lambda_2=1$.
3. Among alloys with composition $(x,y(x))$, find an alloy with composition $(x_1,y(x_1))$ with $|\mathbf{U}^{-1}\hat{\mathbf{e}}|\gtrsim 1$ and another alloy with composition $(x_2,y(x_2))$ satisfying $|\mathbf{U}^{-1}\hat{\mathbf{e}}|\lesssim 1$. Then interpolate to find an alloy with composition $(x^\star,y(x^\star))$ satisfying $|\mathbf{U}^{-1}\hat{\mathbf{e}}|=1$, where $x^\star$ is between x_1 and x_2. This alloy satisfies (CC1) and (CC2).
4. Check that the inequality (CC3) is satisfied for the alloy $(x^\star,y(x^\star))$.

This procedure relies on the lattice parameters changing smoothly with composition, as in Vegard's law. This is often the case in a suitable domain. It also relies on having good starting points.

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Appendix A. Twin domains

Here it is proved that general solutions of the equation of compatibility (8) between martensite variants are represented as Type I or Type II domains.

Proposition 12. *Let* $\mathbf{A}=\mathbf{A}^T$ *and* $\mathbf{B}=\mathbf{B}^T$ *be* 3×3 *positive-definite matrices satisfying* $\mathbf{B}=\mathbf{RAR}^T$ *for some* $\mathbf{R}\in \mathrm{O}(3)$. *Suppose* $\mathbf{A}$ *and* $\mathbf{B}$ *are compatible in the sense that there is a matrix* $\mathbf{Q}\in \mathrm{SO}(3)$ *such that*

$$\mathbf{QB}-\mathbf{A}=\mathbf{a}\otimes\mathbf{n}, \tag{A.1}$$

$\mathbf{a},\mathbf{n}\in\mathbb{R}^3$. *Then there is a unit vector* $\hat{\mathbf{e}}\in\mathbb{R}^3$ *such that*

$$\mathbf{B}=(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{A}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}}). \tag{A.2}$$

Conversely, if 3×3 *matrices* $\mathbf{A}$ *and* $\mathbf{B}$ *satisfy* (A.2) *for some unit vector* $\hat{\mathbf{e}}$, *then there is* $\mathbf{Q}\in \mathrm{SO}(3)$ *so that* (A.1) *is satisfied. A formula for* $\hat{\mathbf{e}}$ *can be given as follows. Under the hypotheses, there is an orthonormal basis* $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$ *such that*

$$\mathbf{A}^{-1}\mathbf{B}^2\mathbf{A}^{-1}=\mu_1\mathbf{e}_1\otimes\mathbf{e}_1+\mathbf{e}_2\otimes\mathbf{e}_2+\mu_3\mathbf{e}_3\otimes\mathbf{e}_3, \tag{A.3}$$

where $0<\mu_1\le 1\le\mu_3$ *and the following identities hold*:

$$\mu_1\mu_3=1,\quad \mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_1=\mu_3\,\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_3,\quad (\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1)^2=\mu_3(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3)^2. \tag{A.4}$$

In the case $\mu_3>1$ *all unit vectors* $\hat{\mathbf{e}}$ *satisfying* (A.2) *are given by*

$$\hat{\mathbf{e}}=\pm(\delta_1\mathbf{Ae}_1+\delta_3\mathbf{Ae}_3), \tag{A.5}$$

where

$$\delta_1=\left(2\left(\mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_1+s\sqrt{\mu_3}\,\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_1\right)\right)^{-1/2}\quad\text{and}\quad \delta_3=s\sqrt{\mu_3}\,\delta_1 \tag{A.6}$$

and $s\in\{\pm 1\}$ *satisfies* $s\sqrt{\mu_3}(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3)=-\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1$. *In the case* $\mu_3=1$ *necessarily* $\mathbf{B}=\mathbf{A}$ *and* $\hat{\mathbf{e}}$ *can be chosen as a normalized eigenvector of* $\mathbf{A}$.

In words: for stretch matrices related by orthogonal similarity as we have for variants of martensite, necessary and sufficient conditions for compatibility are that these matrices are related by a 180° rotation.

Proof. Without loss of generality, by replacing $\mathbf{R}$ by $-\mathbf{R}$ if necessary, we can assume $\mathbf{R}\in\mathrm{SO}(3)$. The condition (A.3), which under the given hypotheses is necessary and sufficient for (A.1), has been proved in Ball and James (1987), Prop. 4. We can assume without loss of generality that $0<\mu_1<1<\mu_3$. That is, if, say, $\mu_3=1$, then by taking det of (A.3) and using $\det\mathbf{A}=\det\mathbf{B}$ we would get necessarily $\mu_1=1$. This would lead to $\mathbf{A}^2=\mathbf{B}^2$. Then by taking the positive-definite square root, we would have $\mathbf{A}=\mathbf{B}$. This, in turn, would imply that (A.2) is satisfied, for example, with $\hat{\mathbf{e}}$ equal to an eigenvector of $\mathbf{A}$. Thus, below we will assume $\mu_1<1<\mu_3$.

There are several identities satisfied by the quantities on the right hand side of (A.3). These follow from the hypothesis that $\mathbf{B}=\mathbf{RAR}^T$ which implies that $\mathbf{A}$ and $\mathbf{B}$ have the same eigenvalues and therefore $\det\mathbf{A}=\det\mathbf{B}$, $\mathrm{tr}\,\mathbf{A}^2=\mathrm{tr}\,\mathbf{B}^2$ and $\mathrm{tr}\,\mathbf{A}^4=\mathrm{tr}\,\mathbf{B}^4$. These in turn yield the following necessary conditions:

1. $\det\mathbf{A}=\det\mathbf{B}\Longrightarrow\mu_1\mu_3=1$. Obvious by taking det of (A.3).
2. $\mathrm{tr}\,\mathbf{A}^2=\mathrm{tr}\,\mathbf{B}^2\Longrightarrow\mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_1=\mu_3\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_3$. This follows by subtracting the identity matrix from (A.3) and then pre- and post-multiplying by $\mathbf{A}$ to get
$$\mathbf{B}^2-\mathbf{A}^2=(\mu_1-1)\mathbf{Ae}_1\otimes\mathbf{Ae}_1+(\mu_3-1)\mathbf{Ae}_3\otimes\mathbf{Ae}_3. \tag{A.7}$$
Taking the trace and using $\mu_1\mu_3=1$ and $\mu_3\neq 1$, we get $\mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_1=\mu_3\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_3$.
3. $\mathrm{tr}\,\mathbf{A}^4=\mathrm{tr}\,\mathbf{B}^4\Longrightarrow(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1)^2=\mu_3(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3)^2$. This follows from (A.3) by pre- and post-multiplying by $\mathbf{A}$ to get $\mathbf{B}^2=\mu_1\mathbf{Ae}_1\otimes\mathbf{Ae}_1+\mathbf{Ae}_2\otimes\mathbf{Ae}_2+\mu_3\mathbf{Ae}_3\otimes\mathbf{Ae}_3$ then squaring this to get $\mathbf{B}^4$. Now write $\mathbf{A}^2=\mathbf{A}\,\mathbf{I}\,\mathbf{A}=\mathbf{A}(\mathbf{e}_1\otimes\mathbf{e}_1+\mathbf{e}_2\otimes\mathbf{e}_2+\mathbf{e}_3\otimes\mathbf{e}_3)\mathbf{A}$ and square this to get $\mathbf{A}^4$. Put $\mathrm{tr}\,\mathbf{A}^4=\mathrm{tr}\,\mathbf{B}^4$ and simplify using items 1 and 2 and $\mu_3\neq 1$ to get the result.

Substituting provisionally the expression (A.2) for $\mathbf{B}$ into (A.3), we get the necessary condition

$$\mathbf{A}^{-1}(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{A}^2(-\mathbf{I}+2\hat{\mathbf{e}}\otimes\hat{\mathbf{e}})\mathbf{A}^{-1}=\mu_1\mathbf{e}_1\otimes\mathbf{e}_1+\mathbf{e}_2\otimes\mathbf{e}_2+\mu_3\mathbf{e}_3\otimes\mathbf{e}_3. \tag{A.8}$$

Multiplying out the tensor products in (A.8) we derive

$$-2\mathbf{A}\hat{\mathbf{e}}\otimes\mathbf{A}^{-1}\hat{\mathbf{e}}-2\mathbf{A}^{-1}\hat{\mathbf{e}}\otimes\mathbf{A}\hat{\mathbf{e}}+4(\hat{\mathbf{e}}\cdot\mathbf{A}^2\hat{\mathbf{e}})\mathbf{A}^{-1}\hat{\mathbf{e}}\otimes\mathbf{A}^{-1}\hat{\mathbf{e}}=(\mu_1-1)\mathbf{e}_1\otimes\mathbf{e}_1+(\mu_3-1)\mathbf{e}_3\otimes\mathbf{e}_3. \tag{A.9}$$

To solve this equation, we try to find a unit vector $\hat{\mathbf{e}}$ of the form

$$\hat{\mathbf{e}}=\sigma_1\mathbf{A}^{-1}\mathbf{e}_1+\sigma_3\mathbf{A}^{-1}\mathbf{e}_3=\delta_1\mathbf{A}\mathbf{e}_1+\delta_3\mathbf{A}\mathbf{e}_3. \tag{A.10}$$

The condition $1=\hat{\mathbf{e}}\cdot\hat{\mathbf{e}}=\mathbf{A}\hat{\mathbf{e}}\cdot\mathbf{A}^{-1}\hat{\mathbf{e}}$ implies that

$$\sigma_1\delta_1+\sigma_3\delta_3=1. \tag{A.11}$$

Substituting the expressions for $\mathbf{A}\hat{\mathbf{e}}$ and $\mathbf{A}^{-1}\hat{\mathbf{e}}$ into Eq. (A.9), we get

$$\begin{aligned}&-2(\sigma_1\mathbf{e}_1+\sigma_3\mathbf{e}_3)\otimes(\delta_1\mathbf{e}_1+\delta_3\mathbf{e}_3)-2(\delta_1\mathbf{e}_1+\delta_3\mathbf{e}_3)\otimes(\sigma_1\mathbf{e}_1+\sigma_3\mathbf{e}_3)\\&+4(\sigma_1^2+\sigma_3^2)(\delta_1\mathbf{e}_1+\delta_3\mathbf{e}_3)\otimes(\delta_1\mathbf{e}_1+\delta_3\mathbf{e}_3)=(\mu_1-1)\mathbf{e}_1\otimes\mathbf{e}_1+(\mu_3-1)\mathbf{e}_3\otimes\mathbf{e}_3.\end{aligned} \tag{A.12}$$

Rearranging similar terms in the above equation results in the following:

$$\begin{aligned}&(-4\delta_1\sigma_1+4(\sigma_1^2+\sigma_3^2)\delta_1^2)\mathbf{e}_1\otimes\mathbf{e}_1\\&\quad+(-2\sigma_1\delta_3-2\delta_1\sigma_3+4(\sigma_1^2+\sigma_3^2)\delta_1\delta_3)(\mathbf{e}_1\otimes\mathbf{e}_3+\mathbf{e}_3\otimes\mathbf{e}_1)\\&\quad+(-4\delta_3\sigma_3+4(\sigma_1^2+\sigma_3^2)\delta_3^2)\mathbf{e}_3\otimes\mathbf{e}_3=(\mu_1-1)\mathbf{e}_1\otimes\mathbf{e}_1+(\mu_3-1)\mathbf{e}_3\otimes\mathbf{e}_3.\end{aligned} \tag{A.13}$$

Comparing the 13 terms on both sides of (A.13) and using (A.11), we get the following expression connecting $\boldsymbol{\sigma}_1,\boldsymbol{\sigma}_3,\boldsymbol{\delta}_1$ and $\boldsymbol{\delta}_3$:

$$(\sigma_1\delta_3-\delta_1\sigma_3)(1-2\sigma_3\delta_3)=0. \tag{A.14}$$

The vanishing of the first factor, $\sigma_1\delta_3-\delta_1\sigma_3=0$, leads to the trivial case $\mu_1=\mu_3=1$ which has been excluded above. The vanishing of the second factor gives that $\sigma_3\delta_3=\frac{1}{2}$ and then from (A.11), $\sigma_1\delta_1=\frac{1}{2}$. This shows that none of the unknowns $\delta_1,\sigma_1,\delta_3,\sigma_3$ vanish. Now the $\mathbf{e}_1\otimes\mathbf{e}_1$ and $\mathbf{e}_3\otimes\mathbf{e}_3$ terms in Eq. (A.13) give

$$\begin{aligned}&4\sigma_3^2\delta_1^2=\mu_1 \quad\Longrightarrow\quad \frac{\delta_1^2}{\delta_3^2}=\mu_1,\\&4\sigma_1^2\delta_3^2=\mu_3 \quad\Longrightarrow\quad \frac{\delta_3^2}{\delta_1^2}=\mu_3.\end{aligned} \tag{A.15}$$

These equations are consistent with $\mu_1\mu_3=1$, and we only need to retain one of them. In summary, (A.8) is satisfied for a unit vector $\hat{\mathbf{e}}$ of the form (A.10) if and only if $\sigma_1,\sigma_3,\delta_1,\delta_3$ satisfy

$$\sigma_1\delta_1=\tfrac{1}{2},\quad \sigma_3\delta_3=\tfrac{1}{2},\quad \delta_3^2=\mu_3\delta_1^2. \tag{A.16}$$

A useful way to write this solution is

$$\delta_3=s\sqrt{\mu_3}\delta_1,\quad \sigma_1=\frac{1}{2\delta_1},\quad \sigma_3=\frac{s}{2\sqrt{\mu_3}\delta_1},\quad s=\pm1. \tag{A.17}$$

So far, $\delta_1\neq0$ and $s=\pm1$ are free parameters.

Although we have solved (A.8) by the choice (A.17), we have to be sure that these values of $\delta_1,\delta_3,\sigma_1,\sigma_3$ satisfy (A.10). This is a vector equation in 3D and therefore is equivalent to the three equations one gets by dotting it with the three linearly independent vectors, $\mathbf{A}\mathbf{e}_1,\mathbf{A}\mathbf{e}_2,\mathbf{A}\mathbf{e}_3$. This gives the three equations

$$\begin{aligned}&\sigma_1=\delta_1(\mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_1)+\delta_3(\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_1),\\&\sigma_3=\delta_1(\mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_3)+\delta_3(\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_3),\\&0=\delta_1(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1)+\delta_3(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3).\end{aligned} \tag{A.18}$$

If we square the last equation and use (A.17) and the nonvanishing of δ_1, we get

$$(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1)^2=\mu_3(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3)^2. \tag{A.19}$$

This is satisfied by virtue of Item 3 above. Hence, the square of the third equation of (A.18) is an identity. So, we can satisfy the third of (A.18) by an appropriate choice of $s=\pm1$ of (A.17). In particular, there exists $s\in\{\pm1\}$ satisfying

$$s\sqrt{\mu_3}(\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3)=-\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1. \tag{A.20}$$

This uniquely determines s unless it happens that $\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_3=0$, in which case also $\mathbf{e}_2\cdot\mathbf{A}^2\mathbf{e}_1=0$ and s can be either ±1. Now we further note that the first two equations in (A.18) are not independent. That is, multiply the first of these by $\delta_1\neq0$ and the second by $\delta_3\neq0$, subtract the equations and use the conditions $\sigma_3\delta_3=\sigma_1\delta_1=\frac{1}{2}$. This leads to

$$\mathbf{e}_1\cdot\mathbf{A}^2\mathbf{e}_1-\mu_3\mathbf{e}_3\cdot\mathbf{A}^2\mathbf{e}_3=0. \tag{A.21}$$

This is automatically satisfied, by virtue of Item 2 above. Hence, there is only one independent equation in (A.18), that we can take to be the first one:

$$\frac{1}{2\delta_1} = \delta_1\left(\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1\right) + s\sqrt{\mu_3}\delta_1\left(\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_1\right), \tag{A.22}$$

that is

$$2\delta_1^2((\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1) + s\sqrt{\mu_3}(\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_1)) = 1. \tag{A.23}$$

We claim that, under our hypotheses, (A.23) can always be solved for $\delta_1 \neq 0$. That is, by the positive definiteness of $\mathbf{A}^2$, we have $\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1 > 0$, $\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_3 > 0$, $(\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1)(\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_3) > (\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_1)^2$. Hence, eliminating $\sqrt{\mu_3}$ using (A.21) (see Item 2), we have for either choice $s = \pm 1$

$$\left(\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1\right) + s\sqrt{\mu_3}\left(\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_1\right) = \sqrt{\frac{\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1}{\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_3}}\left(\sqrt{(\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1)(\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_3)} + s\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_1\right) > 0. \tag{A.24}$$

Hence, δ_1 given by (A.6) is well-defined. Eqs. (A.(23) and A.17) imply that the vector $\hat{\mathbf{e}}$ given by (A.10) is a unit vector and satisfies (A.8) and therefore (A.2).

The sufficiency of the condition (A.2) for compatibility is a standard result, see Bhattacharya (2003) or (10) above. The formula for $\hat{\mathbf{e}}$ follows from (A.10), (A.17) and (A.23) above. □

Corollary 13 (*Compound domains*). *Assume the hypotheses of Proposition 12. There are two unit vectors* $\hat{\mathbf{e}}_+ \nparallel \hat{\mathbf{e}}_-$ *satisfying* (A.2) *if and only if*

$$\mathbf{e}_2 \cdot \mathbf{A}^2\mathbf{e}_3 = \mathbf{e}_2 \cdot \mathbf{A}^2\mathbf{e}_1 = 0. \tag{A.25}$$

If (A.25) *is satisfied and* $\mu_3 > 1$, *there are precisely two such nonparallel unit vectors* (*up to a premultiplied* $\pm$) *that satisfy* (A.2), *and in fact these vectors are orthonormal*, $\hat{\mathbf{e}}_+ \cdot \hat{\mathbf{e}}_- = 0$. *They are given by the formulas*

$$\hat{\mathbf{e}}_\sigma = \delta_1^\sigma \mathbf{A}\mathbf{e}_1 + \delta_3^\sigma \mathbf{A}\mathbf{e}_3, \quad \sigma = \pm, \tag{A.26}$$

where

$$\delta_1^\sigma = \left(2(\mathbf{e}_1 \cdot \mathbf{A}^2\mathbf{e}_1 + \sigma\sqrt{\mu_3}\mathbf{e}_3 \cdot \mathbf{A}^2\mathbf{e}_1)\right)^{-1/2} \quad \text{and} \quad \delta_3^\sigma = \sigma\sqrt{\mu_3}\,\delta_1^\sigma, \quad \sigma = \pm. \tag{A.27}$$

In the case $\mu_3 = 1$ *necessarily* $\mathbf{B} = \mathbf{A}$ *and the solutions* $\hat{\mathbf{e}}$ *of* (A.2) *consist of unit vectors in the eigenspace of* $\mathbf{A}$.

Proof. The proof follows immediately from the statement $s\sqrt{\mu_3}(\mathbf{e}_2 \cdot \mathbf{A}^2\mathbf{e}_3) = -\mathbf{e}_2 \cdot \mathbf{A}^2\mathbf{e}_1$ of Proposition 12, which does not uniquely determine $s \in \{\pm 1\}$ if and only if (A.25) is satisfied. The fact that the two solutions $\mathbf{e}_{\pm 1}$ are nonparallel is seen from their forms (A.6), and the fact that these are the only possible solutions up to premultiplied $\pm$ follows from Proposition 12. The orthonormality of $\hat{\mathbf{e}}_+$ and $\hat{\mathbf{e}}_-$ follows by direct calculation using (A.26) and (A.27). □

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