Non-Laminate Microstructures in Monoclinic-I Martensite

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Abstract

We study the symmetrised rank-one convex hull of monoclinic-I martensite (a twelve-variant material) in the context of geometrically-linear elasticity. We construct sets of $T_3$s, which are (non-trivial) symmetrised rank-one convex hulls of three-tuples of pairwise incompatible strains. In addition, we construct a five-dimensional continuum of $T_3$s and show that its intersection with the boundary of the symmetrised rank-one convex hull is four-dimensional. We also show that there is another kind of monoclinic-I martensite with qualitatively different semi-convex hulls which, as far as we know, has not been experimentally observed. Our strategy is to combine understanding of the algebraic structure of symmetrised rank-one convex cones with knowledge of the faceting structure of the convex polytope formed by the strains.

1. Introduction

Shape-memory alloys are materials that undergo a diffusionless solid-to-solid phase transformation due to change of temperature. They are capable of large macroscopic deformations and recover their original shape upon heating. While such materials usually form a cubic lattice (austenite) above a critical temperature, they develop microstructures at lower temperatures (martensite). In this article we are interested in the cubic-to-monoclinic-I phase transformation which occurs, for example, in NiTi, which is one of the most important industrial shape-memory alloys. In this case, there are twelve transformation strains, see Section 5 for details.

Of interest is the set of all strains that can be recovered upon heating. In the variational approach to martensite [1] this set is modelled by the quasiconvex hull (Definition 2.8) of the transformation strains. Unfortunately, the quasiconvex hull of a set is difficult to calculate.

BHATTACHARYA and KOHN [5] consider various phase transformations (cubic to tetragonal, cubic to trigonal, cubic to orthorhombic and cubic to monoclinic)
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in the context of geometrically-linear elasticity and observe that, except for cubic-to-monoclinic martensite, the symmetrised quasiconvex hull coincides with the convex hull. For cubic-to-monoclinic martensite they show that the symmetrised quasiconvex hull is strictly smaller than the convex hull and they present an inner bound for it.

We aim to find a better approximation of the symmetrised quasiconvex hull, again in the context of geometrically-linear elasticity. To this end, we are interested in the symmetrised lamination convex hull and the symmetrised rank-one convex hull of the transformation strains; these give inner bounds on the symmetrised quasiconvex hull, see Section 2.3.

Our analysis shows that there are points in the symmetrised rank-one convex hull of monoclinic-I martensite which are attained by \textit{non-laminate} microstructures. This suggests (see below) that the symmetrised rank-one convex hull is strictly larger than the lamination convex hull of the twelve transformation strains. Since the symmetrised rank-one convex hull is a subset of the symmetrised quasiconvex hull (Remark 2.9), the strains attained by these non-laminate microstructures belong to the set of recoverable strains.

Next, we give more details on the strategy we use, our results and the organisation of the paper. Finally, we will fix some notation.

\textit{Strategy.} Our strategy is first to exploit the algebraic structure of symmetrised rank-one convex cones, second, the faceting structure of the convex hull of a finite set, and third, the interaction between the two.

That rank-one convex cones are varieties has been exploited to develop algorithms to calculate semi-convex hulls [21, 22]. The relevance of convex polytopes to semi-convex hulls (compare Lemma 2.10 with Theorem 2.11) has been noticed in [35, 39] but has not, to our knowledge, been exploited to determine semi-convex hulls. This paper represents a first attempt in this direction.

The central idea is the following: Given a finite set whose symmetrised rank-one convex hull we wish to compute, we proceed as follows. First we compute the symmetrised rank-one convex hulls of all its one-dimensional facets, that is, edges in the language of convex polytopes; this is trivial, see (2.2) below. We use this, together with knowledge of the structure of symmetrised rank-one convex cones on two-dimensional affine subspaces (Section 3), to determine the symmetrised rank-one convex hulls of all its two-dimensional facets. We then repeat this for higher dimensions.

When the finite set we are interested in is the set of transformation strains of a material capable of a phase transformation from austenite to martensite, the set lies in the five-dimensional affine plane of strains with constant trace. Thus, the process above terminates when the symmetrised rank-one convex hull of the five-dimensional facet of the set (which is the convex hull of the set) is computed.

In this bootstrapping strategy the steps become progressively more difficult as the dimension increases. Indeed, while we can completely implement the two-dimensional step (Section 3 and [10]) and have partial results for the three-dimensional step [9], we have a reason to believe that the steps for dimensions four and five are considerably more difficult than those for dimensions two and three: unlike in
lower dimensions, the symmetrised rank-one convex cone in the higher dimensions is an algebraic surface of a polynomial which is necessarily irreducible [10].

**Results.** We have three main results:

First we show that there are two kinds of monoclinic-I martensites which differ qualitatively with regard to the polytope-structure of their convex hulls. It follows that their semi-convex hulls are qualitatively different as well. Curiously, all known monoclinic-I martensites belong to one of these kinds, which we name monoclinic-Ia (the other being monoclinic-Ib).

$T_3$s are non-trivial symmetrised rank-one convex hulls of 3-tuples of pairwise incompatible strains, which are attained by non-laminate microstructures, see Section 4. The question as to whether $T_3$s can be formed from the twelve variants of Monoclinic-II martensite is raised in [6, p. 863]. There it is shown that this is possible when a certain lattice parameter is sufficiently small. Here we prove a stronger result: In Section 4 we present a simple test for $T_3$s (Lemma 4.3) that shows that, in fact, $T_3$s can form for all (non-zero) values of the lattice parameter, and that the same is true for Monoclinic-I martensite as well. This is our second main result.

Our third result is a consequence of this: We show that for Monoclinic-Ia martensite, the symmetrised rank-one convex hull of the twelve transformation strains contains a five-dimensional continuum of points which are attained by non-laminate microstructures. Moreover, the intersection of this continuum with the boundary of the convex hull is four-dimensional. This suggests that the symmetrised rank-one convex hull of the transformation strains is strictly larger than the symmetrised lamination convex hull. This would then imply that the symmetrised quasiconvex envelope of the energy density of this material is different from the symmetrised lamination convex envelope. It is well known that lamination convex envelopes can differ from rank-one convex envelopes, see [11, Sect. 4], and (in dimensions larger than two) that rank-one convex envelopes can differ from quasiconvex envelopes [33]. However, in the context of materials science, all quasiconvex and rank-one convex envelopes that have been evaluated so far have, in fact, coincided with lamination convex envelopes; Monoclinic-Ia martensite is the first material for which we now have a strong indication that they differ.

**Organisation of the paper.** In Section 2 we refresh the reader’s memory of some basic facts and results about strain compatibility, convex sets (in particular, convex polytopes) and semi-convex functions and sets.

In Section 3 we study the structure of symmetrised rank-one convex cones on two-dimensional affine subspaces of $S_c^{3\times 3}$ (Lemma 3.1), see below for notation. The results presented here enable the computation of the symmetrised rank-one convex hull of any finite set in two-dimensional affine subspaces of $S_c^{3\times 3}$ and the characterisation of those compact sets in these spaces that possess non-trivial symmetrised rank-one convex hulls; we present some results in Section 4 but postpone a more extensive discussion to [10]. We extend these results to higher dimensions in [9], but Lemma 4.10 and Section 7 provide a glimpse of the utility of the results in Section 4, even in higher dimensions.

We then turn from abstract results to the specific class of materials of interest to us, monoclinic-I martensite. After some preliminary observations in Section 5 on
the compatibility and symmetry relations between the twelve transformation strains of materials in this class, we determine, in Section 6, the facets of the convex hull of the twelve transformation strains of monoclinic-I martensite (Observations 6.6, 6.8 and 6.7). This leads to the discovery that there are, in fact, two kinds of monoclinic-I martensitic materials.

With this foundation behind us, in Section 7 we investigate the (theoretical) possibility of non-laminate zero-energy microstructures occurring in these materials. We construct an open set in the symmetrised rank-one convex hull of the transformation strains for which $T_3$-microstructures are optimal (Construction 7.5). We then deduce that in monoclinic-Ia martensite this set intersects the boundary of the convex hull, and thus the boundary of the symmetrised rank-one convex hull.

(In Sections 6 and 7 we use Mathematica to simplify computations but these computations are non-numerical. The Mathematica code that we have used, together with explanatory notes, can be found in the electronic supplementary material accompanying this article [8].)

We conclude with Section 8 with some questions raised by the preceding two sections. One of these is whether monoclinic-Ib martensite might have a larger set of recoverable strains (that is, quasiconvex hull) than monoclinic-Ia martensite (modulo appropriate normalisation of the lattice parameters). This naturally leads to the question as to whether a material that lies at the boundary of monoclinic-Ia and monoclinic-Ib martensite might demonstrate the best behaviour of all.

**Notation.** In the geometrically linear theory of elasticity, the strains (pointwise) belong to the space of real symmetric $3 \times 3$ matrices denoted by $S^{3 \times 3}$. We phrase some of our results for real symmetric $d \times d$ matrices and then use the symbol $S^{d \times d}$. The space of real symmetric $d \times d$ matrices whose trace is an arbitrary (but fixed) constant $c$ is denoted by $S^{d \times d}_c$.

We introduce an inner product $\langle \cdot, \cdot \rangle$ on $S^{d \times d}$ by $S^{d \times d} \ni A, B \mapsto \langle A, B \rangle = \text{Tr}(AB)$; the norm induced by this inner product is $\| \cdot \|$.

For $e_1, e_2 \in S^{d \times d}$ we set

$$(e_1, e_2) := \{\lambda e_1 + (1 - \lambda)e_2 \mid \lambda \in (0, 1)\},$$

$$[e_1, e_2] := \{\lambda e_1 + (1 - \lambda)e_2 \mid \lambda \in [0, 1]\}.$$  

By a direction in $S^{d \times d}$ we mean a one-dimensional affine subspace of $S^{d \times d}$. We denote the affine span of $S \subset S^{d \times d}$ by aff span$(S)$, the relative boundary of $S \subset S^{d \times d}$ by rel $\partial S$ and its relative interior by rel int $S$.

## 2. Preliminaries

### 2.1. Strain Compatibility

**Definition 2.1.** (Strain compatibility) Let $e_1, e_2 \in S^{3 \times 3}$ and $S_1, S_2 \subset S^{3 \times 3}$.

1. $e_1$ is compatible with $e_2$ (or $e_1$ and $e_2$ are compatible), $e_1 \parallel e_2$, if there exist $a, b \in \mathbb{R}^3$ such that $e_1 - e_2 = \frac{1}{2}(a \otimes b + b \otimes a)$, where $\otimes$ denotes the dyadic product.
2. $e_1$ is compatible with 0 (or compatible for short) if $e_1 \parallel 0$.
3. $e_1$ is incompatible with $e_2$ (or $e_1$ and $e_2$ are incompatible), $e_1 \parallel e_2$, if $e_1$ and $e_2$ are not compatible.
4. $e_1$ is incompatible with 0 (or incompatible for short) if $e_1 \parallel 0$.
5. $S_1$ is totally compatible with $S_2$ (or $S_1$ and $S_2$ are totally compatible), $S_1 \parallel S_2$, if for all $e_1 \in S_1$ and for all $e_2 \in S_2$, $e_1 \parallel e_2$.
6. $S_1$ is compatible if $S_1 \parallel S_1$, that is, if for all $e_1, e_2 \in S_1, e_1 \parallel e_2$.
7. $S_1$ is totally incompatible with $S_2$ (or $S_1$ and $S_2$ are totally incompatible), $S_1 \parallel S_2$, if for all $e_1 \in S_1$ and for all $e_2 \in S_2, e_1 \parallel e_2$.

We observe that $[e_1, e_2]$ is compatible if and only if $e_1 \parallel e_2$. An alternative term for compatibility is symmetrised rank-one connectedness.

The following lemma follows immediately from [20, Lemma 4.1].

**Lemma 2.2.** (Compatibility in $S^{3 \times 3}_c$) Let $e_1, e_2 \in S^{3 \times 3}_c$. Then $e_1 \parallel e_2$ if and only if $\det(e_1 - e_2) = 0$.

**Definition 2.3.** (Compatible cone) Let $S \subset S^{3 \times 3}_c$ and $x \in S$. The compatible cone in $S$ at $x$ is the set

$$
\Lambda_{S,x} := \{ y \in S \mid y \parallel x \}.
$$

When $0 \in S$ we set $\Lambda_S := \Lambda_{S,0}$.

Note that the compatible cone $\Lambda_{S,x}$ is an affine cone with vertex $x$ in the linear algebraic sense, that is, it is closed under multiplication by positive reals. However, the compatible cone is not geometrically a cone.

### 2.2. Convex Sets

We recall some elementary definitions and results from convex analysis. For more details see, for example [29].

Let $E$ be a subset of a vector space. We denote the convex hull of $E$ by $C(E)$.

**Definition 2.4.** (Extreme subsets of convex sets) Let $S \subset \mathbb{R}^d$ be convex. Then $S' \subseteq S$ is an extreme subset of $S$ if $S'$ is convex and satisfies: If $x, y \in S$ and $\exists \lambda \in (0, 1)$ such that $\lambda x + (1 - \lambda) y \in S'$, then $x, y \in S'$.

Of special interest to us are convex polytopes which are convex hulls of finite sets. Definition 2.5 and Remark 2.6 suffice for us. For an introduction to convex polytopes we refer the reader to, for example [2, 7, 12, 15, 14, 40].

**Definition 2.5.** (Vertices, edges and facets of convex polytopes) The vertices of a convex polytope are its extreme points, its edges are its one-dimensional extreme subsets and its facets are its extreme subsets with co-dimension one.

Let $E$ be a finite set. We denote the set of $n$-dimensional extreme subsets of $C(E)$ by $F_n(E)$. Thus the set of vertices of $C(E)$ is $F_0(E)$, the set of its edges is $F_1(E)$, and the set of facets is $F_{\dim C(E) - 1}(E)$ and $F_{\dim C(E)}(E) = \{C(E)\}$.

**Remark 2.6.** For $S \in F_n(E), n = 1, \ldots, \dim(C(E))$, the relative boundary $\partial S$ is a union of elements of $F_{n-1}(E)$. 
2.3. Semi-Convex Functions and Sets

Next, we recall some elementary definitions and results about semi-convex functions and sets. For more details see, for example [11,23]. Since we work in the context of $S^{d \times d}$ (as opposed to $\mathbb{R}^{d \times d}$) we have appended the qualifier “symmetrised” to the various notions of semi-convexity. The qualifier “symmetric” is also used in the literature.

The term “symmetrised rank-one convex” (Definition 2.8 below) might be misleading in that the matrices involved need not be of rank one, but rather are the symmetric parts of rank-one matrices. An alternative name could be “wave-cone convex”, because the symmetric tensor products form the wave cone of a second-order linear differential operator whose kernel is the symmetrised gradients [24,36].

**Definition 2.7. (Semi-convex functions)**

1. $f : S^{d \times d} \to \mathbb{R}$ is symmetrised rank-one convex if, for all $\lambda \in [0, 1]$

   \[ f(\lambda e_1 + (1 - \lambda)e_2) \leq \lambda f(e_1) + (1 - \lambda)f(e_2) \quad \forall e_1, e_2 \in S^{d \times d} \text{ with } e_1 \parallel e_2. \]

2. A locally-bounded Borel function $f : S^{d \times d} \to \mathbb{R}$ is symmetrised quasiconvex if, for an open and bounded set $U \subset \mathbb{R}^d$ with $|\partial U| = 0$, one has

   \[ f(e) \leq \frac{1}{|U|} \int_U f(e + D_s\varphi) \, dx \quad \forall \varphi \in W^{1,\infty}_0(U, \mathbb{R}^d), \]

   whenever the integral on the right-hand side exists, where $D_s\varphi$ is the symmetrised gradient of $\varphi$.

**Definition 2.8. (Semi-convex sets)** Let $E$ be a compact set in $S^{d \times d}$.

1. The symmetrised quasiconvex hull of $E$ is defined as

   \[ Q(E) := \left\{ e \in S^{d \times d} \mid f(e) \leq \sup_{e' \in E} f(e') \quad \forall f : S^{d \times d} \to \mathbb{R} \text{ quasiconvex} \right\}. \]

2. The symmetrised rank-one convex hull of $E$ is defined as

   \[ R(E) := \left\{ e \in S^{d \times d} \mid f(e) \leq \sup_{e' \in E} f(e') \quad \forall f : S^{d \times d} \to \mathbb{R} \text{ symmetrised rank-one convex} \right\}. \]

3. The symmetrised lamination convex hull of $E$, $\mathcal{L}(E)$, is the smallest set $\tilde{E} \supseteq E$ such that $e_1, e_2 \in \tilde{E}$, and $e_1 \parallel e_2$ implies that $[e_1, e_2] \subset \tilde{E}$.

We note that symmetrised lamination convex hulls can be constructed as follows: For $n \in \mathbb{N}_0$, let

\[ \mathcal{L}_0(E) := E, \]

\[ \mathcal{L}_{n+1}(E) := \left\{ e \mid \exists e_1, e_2 \in \mathcal{L}_n(E), \ e_1 \parallel e_2, \ e \in [e_1, e_2] \right\}. \]

Then,

\[ \mathcal{L}(E) = \bigcup_{n \in \mathbb{N}_0} \mathcal{L}_n(E). \]
Symmetrised rank-one convex hulls also have an alternate characterisation (see for example [21, Lemma 2.5]):

\[
\mathcal{R}(E) := \{ e \in S^{d \times d} \mid f(e) = 0 \forall f : S^{d \times d} \to [0, \infty) \}
\]

symmetrised rank-one convex with \( f(E) = \{0\} \). (2.1)

We shall repeatedly use Remark 2.9 and Lemma 2.10 without explicitly citing them:

**Remark 2.9.** \( \mathcal{L}(E) \subseteq \mathcal{R}(E) \subseteq \mathcal{Q}(E) \subseteq \mathcal{C}(E) \).

**Lemma 2.10.** ([3, Section 3.4.1, p. 231]) Let \( E \subset S^{d \times d} \) be finite and compatible. Then \( \mathcal{L}(E) = \mathcal{C}(E) \).

In particular,

\[
\forall x, y \in S_c^{3 \times 3}, \quad \mathcal{R}([x, y]) = \begin{cases} [x, y] & \text{if } x \parallel y, \\ \{x, y\} & \text{else}. \end{cases} \quad (2.2)
\]

Lemma 2.10, however, is too weak for our purposes; we present a sharp version [39, p. 38], [35, p. 1266]:

**Theorem 2.11.** Let \( E \subset S^{d \times d} \) be finite. Then \( \mathcal{L}(E) = \mathcal{C}(E) \) if and only if every edge of \( \mathcal{C}(E) \) is compatible, that is, if and only if

\[
\forall e_1, e_2 \in E, \quad e_1 \parallel e_2 \implies [e_1, e_2] \notin \mathcal{F}_1(E).
\]

**Proof.** **Necessity.** Let \([e_1, e_2] \in \mathcal{F}_1(E)\) with \( e_1 \parallel e_2 \). We show that \([e_1, e_2] \notin \mathcal{L}(E)\):

Let \( e \in [e_1, e_2] \) and \( e \in \mathcal{L}(E) \). Then \( \exists n \in \mathbb{N} \) finite, \( f_1, f_2 \in \mathcal{L}_n(E) \) such that \( e \in [f_1, f_2] \). However by extremality of \([e_1, e_2], f_1, f_2 \in [e_1, e_2] \). Applying the same argument to \( f_1 \) and \( f_2 \) we conclude that, in fact, \( e \in \mathcal{L}([e_1, e_2]) \) but from (2.2), \( \mathcal{L}([e_1, e_2]) = [e_1, e_2] \). Thus \( e \in [e_1, e_2] \) and \( e \in \mathcal{L}(E) \implies e \in [e_1, e_2] \).

**Sufficiency.** Let every edge of \( \mathcal{C}(E) \) be compatible. We show by induction that

\[
S \in \mathcal{F}_n(E) \implies S \subseteq \mathcal{L}_n(E)
\]

for \( n = 0, 1, \ldots, \dim(\mathcal{C}(E)) \). Since \((P_{\dim(\mathcal{C}(E))})\) is the statement that \( \mathcal{C}(E) \subseteq \mathcal{L}(E) \), the result follows from Remark 2.9.

\((P_0)\) is trivially true since \( e \in \mathcal{F}_0 \) implies \( e \in E \) and thus \( e \in \mathcal{L}_0(E) \); \((P_1)\) is true since every edge of \( \mathcal{C}(E) \) is compatible by assumption. Now let \((P_n)\) be true for some fixed \( n = 1, \ldots, \dim(\mathcal{C}(E)) - 1 \). We show that \((P_{n+1})\) is true:

Let \( S \in \mathcal{F}_{n+1}(E) \) and \( e \in S \). If \( e \in \text{rel} \partial S \), then \( e \) is contained in an element of \( \mathcal{F}_n(E) \) (Remark 2.6) and thus, by the inductive hypothesis, \( e \in \mathcal{L}_n(E) \subset \mathcal{L}_{n+1}(E) \). We consider the case \( e \in \text{rel} \text{int} \ S \):

Pick \( v \in \mathcal{F}_1(E) \cap \text{rel} \partial S \). We view \( v \) as a vector in \( S^{d \times d} \). Since \( S \) is bounded, the inclusion

\[
e + \lambda v \in \text{rel} \partial S, \quad \lambda \in \mathbb{R},
\]
has two solutions $\lambda_- < 0$ and $\lambda_+ > 0$. Note that $(e + \lambda_+ v) - (e + \lambda_- v)$ is parallel to $v$, which is compatible (by assumption). Thus $e + \lambda_\pm v \in \mathcal{L}_n(E)$ (by $(P_n)$), $e + \lambda_- v \parallel e + \lambda_+ v$ and

$$e = \frac{\lambda_+}{\lambda_+ - \lambda_-}(e + \lambda_+ v) + \frac{-\lambda_-}{\lambda_+ - \lambda_-}(e + \lambda_- v).$$

It follows that $e \in \mathcal{L}_{n+1}(E)$ and thus $S \subseteq \mathcal{L}_{n+1}(E)$. □

3. The Compatible Cone in Two-Dimensional Affine Subspaces of $S_c^{3 \times 3}$

Our first task is to characterise, both geometrically (Lemma 3.1) and algebraically (Remark 3.7), the symmetrised rank-one convex cone in two-dimensional affine subspaces of $S_c^{3 \times 3}$.

Lemma 3.1. Let $S$ be a two-dimensional subspace of $S_c^{3 \times 3}$. Then either

1. $S$ contains precisely one, two or three compatible directions, or
2. $S$ is compatible.

Proof. Let $\{e_1, e_2\}$ be a basis for $S$. By Lemma 2.2, an arbitrary non-zero element of $S$, $xe_1 + ye_2$, $(x, y) \neq 0$, is compatible if and only if

$$\det(xe_1 + ye_2) = 0.$$

This is equivalent to

$$x^3 \det(e_1) + x^2 y \langle \text{cof}(e_1), e_2 \rangle + xy^2 \langle e_1, \text{cof}(e_2) \rangle + y^3 \det(e_2) = 0, \quad (3.1)$$

where $\text{cof}(e)$ is the cofactor of $e$:

$$\text{cof} \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \\ e_{31} & e_{32} & e_{33} \end{pmatrix} = \begin{pmatrix} e_{22}e_{33} - e_{32}e_{23} & -e_{21}e_{33} - e_{31}e_{23} & e_{21}e_{32} - e_{31}e_{22} \\ -e_{12}e_{33} - e_{32}e_{13} & e_{11}e_{33} - e_{31}e_{13} & -e_{11}e_{32} - e_{31}e_{12} \\ e_{12}e_{23} - e_{22}e_{13} & -e_{11}e_{23} - e_{21}e_{13} & e_{11}e_{22} - e_{21}e_{12} \end{pmatrix}^T.$$

If the polynomial in (3.1) is the zero-polynomial (that is, $\det(e_1) = 0$, $\langle \text{cof}(e_1), e_2 \rangle = 0$ etc.) then $S$ is compatible. Otherwise:

If either $\det(e_1) = 0$ or $\det(e_2) = 0$ then (3.1) has one or two solutions $(x, y) \neq 0$, and thus $S$ contains one or two compatible directions. Assume, on the contrary, that both $\det(e_1)$ and $\det(e_2) \neq 0$. Since $(x, y) \neq 0$, dividing (3.1) by either $x^3$ or $y^3$ we obtain a polynomial (in either $\frac{x}{y}$ or $\frac{y}{x}$) which, being cubic, has one, two or three distinct real roots. Thus $S$ contains one, two or three compatible directions. □

Corollary 3.2. Let $S$ be a subspace of $S_c^{3 \times 3}$ with $\dim(S) > 1$. Then $S$ contains at least one compatible direction.
The following examples show that each of the possibilities referred to in Lemma 3.1 can occur:

**Example 3.3. (One compatible direction)**

The determinant of these matrices is proportional to \( x(x^2 + y^2) \) so the compatible direction is \( x = 0 \):

\[
\begin{cases}
  x & 0 & 0 \\
  0 & x & y \\
  0 & y & -2x \\
\end{cases} \quad x, y \in \mathbb{R}
\]

The determinant of these matrices is proportional to \( x^3 \) so the compatible direction is \( x = 0 \):

\[
\begin{cases}
  y & x & x \\
  x & -y & x \\
  x & x & 0 \\
\end{cases} \quad x, y \in \mathbb{R}
\]

**Example 3.4. (Two compatible directions)**

The determinant of these matrices is proportional to \( xy^2 \) so the two compatible directions are \( x = 0 \) and \( y = 0 \):

\[
\begin{cases}
  x & 0 & 0 \\
  0 & -x & y \\
  0 & y & 0 \\
\end{cases} \quad x, y \in \mathbb{R}
\]

**Example 3.5. (Three compatible directions)**

The determinant of these matrices is proportional to \( xy(x + y) \) so the three compatible directions are \( x = 0, y = 0 \) and \( x = -y \):

\[
\begin{cases}
  x & 0 & 0 \\
  0 & y & 0 \\
  0 & 0 & -x - y \\
\end{cases} \quad x, y \in \mathbb{R}
\]

The determinant of these matrices is proportional to \( x(x^2 - y^2) \) so the three compatible directions are \( x = 0, x = y \) and \( x = -y \):

\[
\begin{cases}
  -2x & 0 & 0 \\
  0 & x & y \\
  0 & y & x \\
\end{cases} \quad x, y \in \mathbb{R}
\]

**Example 3.6. (Compatible (two-dimensional) plane)**

\[
\begin{cases}
  0 & 0 & 0 \\
  0 & x & y \\
  0 & y & -x \\
\end{cases} \quad x, y \in \mathbb{R}, \quad \begin{cases}
  0 & x & y \\
  x & 0 & 0 \\
  y & 0 & 0 \\
\end{cases} \quad x, y \in \mathbb{R}
\]

We note that Lemma 3.1 follows also from the following characterisation of real homogeneous cubic polynomials in two variables:

**Remark 3.7.** A homogeneous cubic polynomial on \( \mathbb{R}^2 \), by an appropriate choice of basis, can be written in precisely one of the five following forms see for example [16, Sec. 23, pp. 263–266 ], [38] or [26, p. 28]:

\[
\begin{cases}
  0 & 0 & 0 \\
  0 & x & y \\
  0 & y & -x \\
\end{cases} \quad x, y \in \mathbb{R}, \quad \begin{cases}
  0 & x & y \\
  x & 0 & 0 \\
  y & 0 & 0 \\
\end{cases} \quad x, y \in \mathbb{R}
\]
1. \( x(x^2 + y^2) \),
2. \( x^3 \),
3. \( xy^2 \),
4. \( xy(x + y) \) or, equivalently, \( x(x^2 - y^2) \),
5. 0.

The examples above illustrate these possibilities.

Lemma 3.1 shows that from the perspective of symmetrised rank-one convexity there are four kinds of two-dimensional affine subspaces of \( \mathcal{S}_{c}^{3\times 3} \), namely those for which the compatible cone is
1. a line,
2. the union of two (distinct) lines,
3. the union of three (distinct) lines, and
4. the subspace itself.

The next step is to investigate compatible hulls in these subspaces. Cases (1) and (4) are the simplest: In Case (1) compatible hulls are obtained by convexifying in the compatible direction, in Case (4) compatible hulls are identical to convex hulls.

Cases (2) and (3) are reminiscent of separate convexity in \( \mathbb{R}^2 \) [37, 21]: Symmetrised rank-one convexity is geometrically identical to separate convexity in \( \mathbb{R}^2 \) in Case (2), and is similar to separate convexity in \( \mathbb{R}^2 \) in Case (3). As an aside, the inclusion-minimal configurations [34] in these situations are either \( T_3s \) or \( T_4s \) as might be expected. Only \( T_3s \) are relevant to our immediate purposes so we discuss them in Section 4 and leave the rest for [10].

4. \( T_3s \)

\( T_3s \) occur when there are precisely three directions in the compatible cone. Our definition is equivalent/identical to earlier definitions in the literature such as [6, p. 855, (3.9) on p. 862 and Fig. 3.1b on p. 856].

**Definition 4.1.** (\( T_3 \)) Three points \( e_1, e_2, e_3 \in \mathcal{S}_{c}^{3\times 3} \) form a \( T_3 \) if
1. They are pairwise incompatible, and
2. There exist \( e_{1,1} \in (e_2, e_3), e_{2,2} \in (e_3, e_1), e_{3,3} \in (e_1, e_2) \) such that \( e_{i,i} \parallel e_i \), \( i = 1, 2, 3 \).

A schematic representation of a \( T_3 \) is shown in Fig. 1.

**Remark 4.2.** Note that \( \text{span}\{e_1 - e_{1,1}\}, \text{span}\{e_2 - e_{2,2}\} \) and \( \text{span}\{e_3 - e_{3,3}\} \) are distinct compatible directions. By Lemma 3.1 there are no others. It follows that \( e_{1,1}, e_{2,2} \) and \( e_{3,3} \) are unique.

Next we show that it is easy to check whether three points form a \( T_3 \):

**Lemma 4.3.** Three points \( e_1, e_2, e_3 \in \mathcal{S}_{c}^{3\times 3} \) form a \( T_3 \) if and only if

\[
\text{sign det}(e_1 - e_2) = \text{sign det}(e_2 - e_3) = \text{sign det}(e_3 - e_1) \neq 0. \quad (4.1)
\]
Definition 4.4. (Vertices of a $T_3$) Let $e_1, e_2, e_3 \in S^{3 \times 3}_c$ form a $T_3$ as in Definition 4.1. Then $e_1, e_2, e_3$ are referred to as the vertices of this $T_3$. When $e_1, e_2, e_3 \in S^{3 \times 3}_c$ form a $T_3$, then their symmetrised rank-one convex hull $\mathcal{R}([e_1, e_2, e_3])$ is (also) called a $T_3$. The context will make clear whether “$T_3”
Fig. 2. Schematic representations of inner bounds for the rank-one convex hull of three strains forming a $T_3$

refers to the set of three strains $\{e_1, e_2, e_3\}$ or to their symmetrised rank-one convex hull $R(\{e_1, e_2, e_3\})$.

It is known (see, for example, [6, §3]) that

$$R(\{e_1, e_2, e_3\}) \supseteq [e_1, e_1, 2] \cup [e_2, e_2, 3] \cup [e_3, e_3, 1] \cup C(\{e_1, e_2, e_3, 1\}),$$  \hspace{1cm} (4.4)

where $e_{1,2}, e_{2,3}, e_{3,1}$ are the nodes of the $T_3$ (Definition 4.5 below), see Fig. 2. However, for the convenience of the reader we provide a proof of this in Proposition 4.9 below.

**Definition 4.5. (Nodes of a $T_3$)** Let $e_1, e_2, e_3 \in S_c^{3 \times 3}$ form a $T_3$. Let $e_{1,1}, e_{2,2}, e_{3,3}$ be as defined in (4.2a)–(4.2c). We define the nodes of the $T_3$ to be the three points

$$e_{i,j} := [e_i, e_{i,i}] \cap [e_j, e_{j,j}], \hspace{0.5cm} i \neq j, \hspace{0.2cm} i, \hspace{0.2cm} j = 1, 2, 3$$

(see Fig. 1).

From Definition 4.1(2) the nodes of a $T_3$ are pair-wise compatible and $e_{i,j}$ is compatible with $e_i$ and $e_j$.

Later we will encounter symmetric $T_3$s and similar $T_3$s as defined below:

**Definition 4.6. (Symmetric $T_3$s)** Let $e_1, e_2, e_3 \in S_c^{3 \times 3}$ form a $T_3$. Let $\lambda_{12}, \lambda_{23}, \lambda_{31}$ be as defined in (4.2a)–(4.2c). Then the $T_3$ is symmetric if $\lambda_{12} = \lambda_{23} = \lambda_{31}$.

The following remark is elementary, but we explicitly state it since it arises frequently in applications (see Section 7):

**Remark 4.7.** Let $R \in SO(3)$ such that $R^3$ is the identity. Let $e_1 \in S_c^{3 \times 3}$, $e_2 := R^T e_1 R$ and $e_3 := R^T e_2 R$. Then $\det(e_1 - e_2) = \det(e_2 - e_3) = \det(e_3 - e_1)$ and, if this is non-zero, then $e_1, e_2, e_3$ form a symmetric $T_3$.

**Definition 4.8. (Similar $T_3$s and corresponding points)** Let $e_1, e_2, e_3 \in S_c^{3 \times 3}$ and $e'_1, e'_2, e'_3 \in S_c^{3 \times 3}$ form $T_3$s. Let $\lambda_{ij}, \lambda'_{ij}, j \neq j, i, j = 1, 2, 3$ be defined as in (4.2).
1. We say that these $T_3$s are similar if, for some permutation $\sigma : \{1, 2, 3\} \rightarrow \{1, 2, 3\}$, $\lambda_{12}^\prime = \lambda_{\sigma(1)\sigma(2)}$, $\lambda_{23}^\prime = \lambda_{\sigma(2)\sigma(3)}$ and $\lambda_{31}^\prime = \lambda_{\sigma(3)\sigma(1)}$.

2. Corresponding points in these $T_3$s are points with the same barycentric coordinates: For $\mu_1, \mu_2, \mu_3 \in [0, 1]$, $\sum_{i=1}^3 \mu_i = 1$, $\mu_1 e_1 + \mu_2 e_2 + \mu_3 e_3$ and $\mu_1 e_1 e_{\sigma(1)}^\prime + \mu_2 e_{\sigma(2)}^\prime + \mu_3 e_{\sigma(3)}^\prime$ are corresponding points where $\sigma$ is the permutation in item (1) above.

We now prove (4.4):

**Proposition 4.9.** Let $e_1, e_2, e_3 \in S_3^{3 \times 3}$ form a $T_3$. Then

$$\mathcal{R}(e_1, e_2, e_3) \supseteq [e_1, e_{1,2}] \cup [e_2, e_{2,3}] \cup [e_3, e_{3,1}] \cup \mathcal{C}(e_{1,2}, e_{2,3}, e_{3,1}).$$

(4.4)

**Proof.** We use the same strategy as [21, Proposition 2.7]. Let $e_{1,2}, e_{2,3}, e_{3,1}$ be related to $e_1, e_2, e_3$ as in the left-hand side of Figs. 1 and 2; the proof in the other case is similar.

Let $f$ be non-negative, symmetrised rank-one convex and vanish on $[e_1, e_2, e_3]$. Since $e_1 \parallel e_{1,2}$, it follows from the convexity of $f$ on $[e_1, e_{1,2}]$ that $f(e_{1,2}) \geq f(e_{3,1})$. Similarly, since $e_2 \parallel e_{2,3}$, it follows that $f(e_{2,3}) \geq f(e_{1,2})$. Finally from $e_3 \parallel e_{3,1}$ it follows that $f(e_{3,1}) \geq f(e_{2,3})$. In other words, $f(e_{2,3}) \geq f(e_{1,2}) \geq f(e_{3,1}) = f(e_{2,3})$. We conclude that $f(e_{2,3}) = f(e_{1,2}) = f(e_{3,1})$.

But since $f(e_1) = 0$, convexity of $f$ on $[e_1, e_{1,2}]$ shows that in fact $f(e_{1,2}) = f(e_{2,3}) = f(e_{3,1}) = 0$. From (2.1) we conclude that

$$[e_1, e_{1,2}] \cup [e_2, e_{2,3}] \cup [e_3, e_{3,1}] \subset \mathcal{R}(e_1, e_2, e_3).$$

The last step is to notice that since $e_{1,2}, e_{2,3}, e_{3,1}$ are pair-wise compatible, from Lemma 2.10,

$$\mathcal{C}(e_{1,2}, e_{2,3}, e_{3,1}) \subset \mathcal{R}(e_1, e_2, e_3),$$

which completes the proof. □

We end this section by giving an example of the utility of two-dimensional results in higher dimensions.

**Lemma 4.10.** (A three-dimensional continuum of $T_3$s) Let $e_1, e_2, e_3 \in S_3^{3 \times 3}$ form a $T_3$. Let $e_0 \in S_3^{3 \times 3}$ such that $e_i \parallel e_0$ for $i = 1, 2, 3$. For $\lambda \in \mathbb{R}$ and $i = 1, 2, 3$ let

$$e_i^\lambda := \lambda e_0 + (1 - \lambda)e_i.$$

Then $e_1^\lambda, e_2^\lambda, e_3^\lambda$ also form a $T_3$, and

$$\bigcup_{\lambda \in [0, 1]} \mathcal{R}(e_1^\lambda, e_2^\lambda, e_3^\lambda) \subseteq \mathcal{R}(e_0, e_1, e_2, e_3),$$

(4.5)

which, when $e_0 \notin \text{aff span}\{e_1, e_2, e_3\}$, is a three-dimensional continuum of $T_3$s (Fig. 3).

**Proof.** Let $\lambda \in (0, 1)$ and $i = 1, 2, 3$. Since $e_0 \parallel e_i$ it follows that $e_i^\lambda \in \mathcal{L}(e_0, e_1, e_2, e_3)$. Since sign $\det(e_i^\lambda - e_j^\lambda) = \text{sign} \det(e_i - e_j)$, $i, j = 1, 2, 3$, it follows, from Lemma 4.3, that $e_1^\lambda, e_2^\lambda, e_3^\lambda$ form a $T_3$. The result follows. □
5. The Transformation Strains of Monoclinic-I Martensite

In this and the next section we prepare to apply the results of the preceding sections to monoclinic-I martensite by exploring first the symmetry and the geometry of this material.

We denote the transformation strains of the twelve variants of cubic-to-monoclinic-I martensite, listed in Table 1, by

$$e^{(i)} \in \mathcal{E} := \{e^{(i)} \mid i \in \mathcal{I}\},$$

$$\mathcal{I} := \{1, 2, \ldots, 12\}$$

or simply by $i \in \mathcal{I}$ if the meaning is clear from the context. The transformation strains involve four lattice parameters $\alpha$, $\beta$, $\varepsilon$ and $\delta$. These have been chosen such that $\varepsilon > 0$ and $\delta > 0$. Typical lattice parameters are listed in Table 2. Note that $\text{Tr} \ e = 2\alpha + \beta$ for $e \in \mathcal{E}$; thus $\mathcal{E} \subset S^{3 \times 3}_{2\alpha + \beta}$.

| $i$ | $e^{(i)}$ | $i$ | $e^{(i)}$ | $i$ | $e^{(i)}$ | $i$ | $e^{(i)}$ |
|-----|----------|-----|----------|-----|----------|-----|----------|
| 1   | \[
\begin{pmatrix}
\alpha & \delta & \varepsilon \\
\delta & \alpha & \varepsilon \\
\varepsilon & \varepsilon & \beta \\
\end{pmatrix}
\] | 2   | \[
\begin{pmatrix}
\alpha & \delta & -\varepsilon \\
\delta & \alpha & -\varepsilon \\
-\varepsilon & -\varepsilon & \beta \\
\end{pmatrix}
\] | 3   | \[
\begin{pmatrix}
\alpha & -\delta & -\varepsilon \\
-\delta & \alpha & \varepsilon \\
-\varepsilon & \varepsilon & \beta \\
\end{pmatrix}
\] | 4   | \[
\begin{pmatrix}
\alpha & -\delta & \varepsilon \\
-\delta & \alpha & -\varepsilon \\
\varepsilon & -\varepsilon & \beta \\
\end{pmatrix}
\] |
| 5   | \[
\begin{pmatrix}
\beta & \varepsilon & \delta \\
\varepsilon & \beta & \delta \\
\delta & \varepsilon & \alpha \\
\end{pmatrix}
\] | 6   | \[
\begin{pmatrix}
-\beta & \varepsilon & \delta \\
-\varepsilon & \beta & \delta \\
-\delta & \varepsilon & \alpha \\
\end{pmatrix}
\] | 7   | \[
\begin{pmatrix}
\alpha & -\beta & \varepsilon \\
-\beta & \alpha & -\varepsilon \\
-\varepsilon & \varepsilon & \delta \\
\end{pmatrix}
\] | 8   | \[
\begin{pmatrix}
\alpha & \beta & -\varepsilon \\
-\beta & \alpha & \varepsilon \\
-\varepsilon & \varepsilon & \delta \\
\end{pmatrix}
\] |
| 9   | \[
\begin{pmatrix}
\beta & \varepsilon & \alpha \\
\varepsilon & \beta & \alpha \\
\alpha & \varepsilon & \delta \\
\end{pmatrix}
\] | 10  | \[
\begin{pmatrix}
-\beta & \varepsilon & -\alpha \\
-\varepsilon & \beta & -\alpha \\
-\alpha & \varepsilon & \delta \\
\end{pmatrix}
\] | 11  | \[
\begin{pmatrix}
\beta & -\varepsilon & \alpha \\
-\varepsilon & \beta & -\alpha \\
\alpha & \varepsilon & -\delta \\
\end{pmatrix}
\] | 12  | \[
\begin{pmatrix}
\beta & \varepsilon & -\alpha \\
\varepsilon & \beta & -\alpha \\
-\alpha & \varepsilon & -\delta \\
\end{pmatrix}
\] |

Table 1. The transformation strains of the twelve variants of monoclinic-I martensite, see for example [5, Table 1, p. 119]
Table 2. Typical lattice parameters for monoclinic-I martensite, see for example [32, Table 2, p. 5459] and [4, pp. 55, 184]

| Material | α   | β    | δ    | ε    | References |
|----------|-----|------|------|------|------------|
| NiTi     | 0.0243 | -0.0437 | 0.0580 | 0.0427 | [18,19,27] |
| CuZr     | 0.0348 | 0.0229  | 0.1067 | 0.0929 | [30,31]    |
| TiNiCu   | 0.0232 | -0.0410 | 0.0532 | 0.0395 | [25]       |

Table 3. Compatible and incompatible transformation strains [8, Compatibility.nb]. The signs in the second and third columns depend on the material parameters; the sign in the third column is opposite to the one in the second

| i | det$(e^{(i)} - e^{(i)}) = 0$ | det$(e^{(i)} - e^{(i)}) \geq 0$ | det$(e^{(i)} - e^{(i)}) \leq 0$ |
|---|--------------------------|-----------------------------|-----------------------------|
| 1 | 2, 3, 4, 5, 7, 9, 11     | 8, 12                       | 6, 10                       |
| 2 | 1, 3, 4, 6, 8, 10, 12    | 5, 9                        | 7, 11                       |
| 3 | 1, 2, 4, 5, 7, 10, 12    | 6, 11                       | 8, 9                        |
| 4 | 1, 2, 3, 6, 8, 9, 11     | 7, 10                       | 5, 12                       |
| 5 | 1, 3, 6, 7, 8, 9, 12     | 4, 11                       | 2, 10                       |
| 6 | 2, 4, 5, 7, 8, 10, 11    | 1, 9                        | 3, 12                       |
| 7 | 1, 3, 5, 6, 8, 10, 11    | 2, 12                       | 4, 9                        |
| 8 | 2, 4, 5, 6, 7, 9, 12     | 3, 10                       | 1, 11                       |
| 9 | 1, 4, 5, 8, 10, 11, 12   | 3, 7                        | 2, 6                        |
| 10| 2, 3, 6, 7, 9, 11, 12    | 1, 5                        | 4, 8                        |
| 11| 1, 4, 6, 7, 9, 10, 12    | 2, 8                        | 3, 5                        |
| 12| 2, 3, 5, 8, 9, 10, 11    | 4, 6                        | 1, 7                        |

Compatibility. Compatibility and incompatibility between the transformation strains are of critical importance to us. A simple calculation [8, Compatibility.nb] shows that for $e, f \in \mathcal{E}$,

$$\det(e - f) \in \left\{0, \pm 4\epsilon \left((\alpha - \beta)\delta + \epsilon^2 - \delta^2\right)\right\},$$

which gives the compatibility/incompatibility of the strains by Lemma 2.2.

Note that if the material parameters happen to be such that $(\alpha - \beta)\delta + \epsilon^2 - \delta^2 = 0$, then all strains in $\mathcal{E}$ are pairwise compatible. Then by Lemma 2.10, $\mathcal{L}(\mathcal{E}) = \mathcal{C}(\mathcal{E})$. (In this case the material is able to form many more twins than usual [28].)

Pairs of compatible and incompatible transformation strains in $\mathcal{E}$ are listed in Table 3. Here and henceforth (including in Mathematica calculations) we assume that $(\alpha - \beta)\delta + \epsilon^2 - \delta^2 \neq 0$ and, more generally, that the lattice parameters are generic. We also assume that $\alpha \neq \beta$; the (mathematical) reason for this will become clear in Section 6. There we will also see that the case $\epsilon = \delta$ is special so we shall specifically consider this possibility.

Distances. Also of importance is the distance between the transformation strains [8, Distances.nb]:

**Observation 5.1.** Every pair of incompatible transformation strains is equidistant: For $e, f \in \mathcal{E}$ with $\epsilon \parallel f$,

$$\|e - f\|^2 = 2(\alpha - \beta)^2 + 4\delta^2 + 12\epsilon^2.$$ (5.2a)
Table 4. Distances between compatible transformation strains [8, Distances.nb]

| i | $\|e^{(i)} - e^{(i)}\|^2$ | $\|e^{(i)} - e^{(i)}\|^2$ | $\|e^{(i)} - e^{(i)}\|^2$ |
|---|---|---|---|
| 1 | 16$\epsilon^2$ | 8$\delta^2 + \epsilon^2$ | 2$(\alpha - \beta)^2 + 4(\delta - \epsilon)^2$ |
| 2 | 3,4 | 5,9 | 7,11 |
| 3 | 4,1 | 7,10 | 5,12 |
| 4 | 3,1 | 6,11 | 8,9 |
| 5 | 6,7 | 1,9 | 3,12 |
| 6 | 5,8 | 4,11 | 2,10 |
| 7 | 8,5 | 3,10 | 1,11 |
| 8 | 7,6 | 2,12 | 4,9 |
| 9 | 10,11 | 1,5 | 4,8 |
| 10 | 11,12 | 3,7 | 2,6 |
| 11 | 12,9 | 4,6 | 1,7 |
| 12 | 11,9 | 2,8 | 3,5 |

Remark 5.13 sheds more light on this. However, for pairs of compatible transformation strains the situation is more complex. For $e, f \in \mathcal{E}$ with $e \not= f$,

$$\|e - f\|^2 \in \left\{ 16\epsilon^2, 8(\delta^2 + \epsilon^2), 2(\alpha - \beta)^2 + 4(\delta - \epsilon)^2, 2(\alpha - \beta)^2 + 4(\delta + \epsilon)^2 \right\}.$$  

(5.2b)

Table 4 presents the full picture. (See also Remark 5.11.)

We exclude (until Section 8) the special case $\epsilon = \delta$ for which, for $e, f \in \mathcal{E}$ with $e \neq f$,

$$\|e - f\|^2 \in \left\{ 16\epsilon^2, 2(\alpha - \beta)^2, 2(\alpha - \beta)^2 + 16\epsilon^2 \right\}.$$  

Note that in this case, we can no longer distinguish between compatible and incompatible strains on the basis of the distance between them.

**Symmetry.** Now that we have knowledge of the compatibilities and the distances between the transformation strains we are ready to analyse the symmetry between them.

**Definition 5.2. (Symmetry and symmetry group)**

1. A map $\tau : \mathcal{E} \to \mathcal{E}$ is a symmetry of $\mathcal{E}$ if it preserves distance and compatibility in $\mathcal{E}$. That is, $\forall e, f \in \mathcal{E}$,

$$\|e - f\| = \|\tau e - \tau f\|,$$

$$\det(e - f) = \pm \det(\tau e - \tau f).$$

A symmetry group of $\mathcal{E}$ is a group of symmetries of $\mathcal{E}$. 


2. Let \( n \in \mathcal{I} \setminus \{1\} \) and \( \mathcal{E}_n \) be a set of subsets of \( \mathcal{E} \), all with cardinality \( n \). That is, 
\[
\mathcal{E}_n \subset \{ S \subset \mathcal{E} \mid \#S = n \}.
\]

A map \( \tau : \mathcal{E}_n \to \mathcal{E}_n \) is a symmetry of \( \mathcal{E}_n \) if it preserves distance and compatibility in \( \mathcal{E}_n \). That is, \( \forall S \in \mathcal{E}_n, \forall e, f \in S, \)
\[
\|e - f\| = \|\tau e - \tau f\|, \\
\det(e - f) = \pm \det(\tau e - \tau f).
\]

A symmetry group of \( \mathcal{E}_n \) is a group of symmetries of \( \mathcal{E}_n \).

There are four sets that are of interest to us here. These are: (i) \( \mathcal{E} \) itself, (ii) \( \mathcal{E}^2 \), the set of pairs of compatible transformation strains, (iii) \( \mathcal{E}^2 \), the set of pairs of incompatible transformation strains, and (iv) \( \mathcal{E}^3 \), the set of three-tuples of incompatible transformation strains:
\[
\mathcal{E}^2 := \\{\{e, f\} \mid e, f \in \mathcal{E}, \quad e \neq f, \quad e \parallel f\}, \\
\mathcal{E}^2 := 7\{\{e, f\} \mid e, f \in \mathcal{E}, \quad e \parallel f\}, \\
\mathcal{E}^3 := \{\{e, f, g\} \mid e, f, g \in \mathcal{E}, \quad e \parallel f \parallel g \parallel e\}.
\]

We characterise the symmetry of \( \mathcal{E} \) and \( \mathcal{E}^2 \) in Lemma 5.10 and those of \( \mathcal{E}^2 \) and \( \mathcal{E}^3 \) in Lemma 5.12 below. In order to do so we begin with some observations. For further investigation of these sets see [9].

**Observation 5.3.** (\( S_4 \) is a symmetry group of \( \mathcal{E} \)) Since the transformation strains in \( \mathcal{E} \) are obtained through a phase transformation from a cubic crystal, \( S_4 \), the group of rotational symmetries of a cube, is a symmetry group of \( \mathcal{E} \).

This group and its action on \( \mathcal{E} \) can be generated as follows: Let \( R_1, R_2 \) and \( R_3 \) be anticlockwise rotations of \( \pi/2 \) about the coordinate axes:
\[
R_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad R_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad R_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\]

For \( i = 1, 2, 3 \), let \( r_i \) be the map
\[
\mathcal{S}^{3 \times 3} \ni e \mapsto r_i e := R_i e R_i^T.
\]

It is immediate that these are distance and determinant (and thus, compatibility) preserving: \( \forall i = 1, 2, 3, \forall e, f \in \mathcal{E}, \)
\[
\|e - f\| = \|r_i e - r_i f\|, \\
\det(e - f) = \det(r_i e - r_i f).
\]

Then \( \{r_1, r_2, r_3\} \) generates \( S_4 \). (In fact any two of \( r_1, r_2, r_3 \) generate \( S_4 \), but it is convenient to retain all three.) The action of \( S_4 \) on \( \mathcal{E} \) is listed, for example in [18,
Table 5. The action of $r_1, r_2, r_3$ on $I$

| $i$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|-----|---|---|---|---|---|---|---|---|---|----|----|----|
| $r_1 i$ | 6 | 5 | 8 | 7 | 4 | 3 | 2 | 1 | 11 | 12 | 10 | 9 |
| $r_2 i$ | 12 | 11 | 9 | 10 | 8 | 7 | 5 | 6 | 2 | 1 | 3 | 4 |
| $r_3 i$ | 3 | 4 | 2 | 1 | 10 | 9 | 12 | 11 | 7 | 8 | 5 | 6 |

Table 1, p. 2607], but their numbering of the transformation strains is different from ours.

$S_4$ is isomorphic to a group of permutations on $I$. We denote this group too by $S_4$; the images of $r_1, r_2, r_3$ under this isomorphism are also denoted by $r_1, r_2, r_3$. Table 5 lists the action of $r_1, r_2, r_3$ on $I$ [8, Symmetry.nb].

**Remark 5.4.** Since $S_4$ is the group of rotational symmetries of a cube, it is natural and convenient to identify $E$ (and $I$) with the edges of a cube as shown in Fig. 4. (We could also have identified them with the diagonals of the faces.) Then $r_1, r_2, r_3$ are anticlockwise rotations of $\frac{\pi}{2}$ along an axis perpendicular to the face of the cube and passing through its centre.

From Table 3 we note that the four edges with which an edge is incompatible are precisely the four edges with which it shares a vertex. Thus,

1. The 24 elements of $E_2$ can be identified with the 24 corners of the faces of a cube, and
2. The 8 elements of $E_3$ can be identified with the 8 corners of a cube.

Our next task is to show that $E$ does not have the reflection symmetries of a cube. We will accomplish this in Observation 5.9 below.

**Definition 5.5.** (Inversion) Let $r_0$ be the permutation on $I$ which interchanges 1 and 2, 3 and 4, 5 and 6, 7 and 8, 9 and 10, and 11 and 12.

As can be seen from Fig. 4, $r_0$ is an inversion (reflection through the centre) of the cube. This immediately shows both that $r_0 \notin S_4$ and that \{r_0, r_1, r_2, r_3\} generates $S_4 \times C_2$, the group of symmetries of a cube (including reflections).

**Remark 5.6.** The permutation $r_0$ corresponds to replacing $\varepsilon$ with $-\varepsilon$ in the transformation strains (see Table 1).

**Observation 5.7.** Unlike $r_1, r_2$ and $r_3, r_0$ cannot be identified with a linear operator on $S_{2\alpha + \beta}^{3\times 3}$.

**Proof.** Assume, on the contrary, that there exists $L: S_{2\alpha + \beta}^{3\times 3} \rightarrow S_{2\alpha + \beta}^{3\times 3}$, linear, such that $\forall i \in I$, $L e^{(i)} = e^{(r_0 i)}$. Then,

$$L \left( e^{(1)} + e^{(2)} + e^{(3)} + e^{(4)} \right) = e^{(1)} + e^{(2)} + e^{(3)} + e^{(4)}$$

$$\Rightarrow L \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}.$$
Fig. 4. The oriented cube representing the symmetries of $E$ [8, Symmetry.nb]

\[
\mathcal{L} \left( e^{(5)} + e^{(6)} + e^{(7)} + e^{(8)} \right) = e^{(5)} + e^{(6)} + e^{(7)} + e^{(8)}
\]

\[
\implies \mathcal{L} \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix},
\]

\[
\mathcal{L} \left( e^{(9)} + e^{(10)} + e^{(11)} + e^{(12)} \right) = e^{(9)} + e^{(10)} + e^{(11)} + e^{(12)}
\]

\[
\implies \mathcal{L} \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix} = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}.
\]
Thus (i) \( L \) is an identity on the diagonal components of \( S_{2\alpha + \beta}^3 \). Moreover

\[
L \left( e^{(1)} + e^{(3)} \right) = e^{(2)} + e^{(4)} \implies L \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & \epsilon \\ 0 & \epsilon & \beta \end{pmatrix} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & -\epsilon \\ 0 & -\epsilon & \beta \end{pmatrix},
\]

\[
L \left( e^{(5)} + e^{(8)} \right) = e^{(6)} + e^{(7)} \implies L \begin{pmatrix} \alpha & \epsilon & 0 \\ \epsilon & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix} = \begin{pmatrix} \alpha & -\epsilon & 0 \\ -\epsilon & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix},
\]

\[
L \left( e^{(9)} + e^{(11)} \right) = e^{(10)} + e^{(12)} \implies L \begin{pmatrix} \beta & 0 & \epsilon \\ 0 & \alpha & 0 \\ \epsilon & 0 & \alpha \end{pmatrix} = \begin{pmatrix} \beta & 0 & -\epsilon \\ 0 & \alpha & 0 \\ -\epsilon & 0 & \alpha \end{pmatrix}.
\]

Thus (ii) \( L \) is a negative of the identity on the off-diagonal components of \( S_{2\alpha + \beta}^3 \).

It is easy to check that (i) and (ii) are contradictory, for example \( Le^{(1)} = e^{(2)} \).

\( \square \)

Now we address the question of whether \( r_0 \) is a symmetry of \( \mathcal{E} \):

**Observation 5.8. (Inversions preserve compatibility)** As can be verified \cite[Symmetry.nb]{8} from Table 3 and (5.1), \( r_0 \) is compatibility preserving: \( \forall e, f \in \mathcal{E} \),

\[
det(e - f) = -det(r_0e - r_0f).
\]

**Observation 5.9. (Effect of inversions on distance)** From Observation 5.1 and Remark 5.6 it follows that \( r_0 \) is distance-preserving on pairs of incompatible transformation strains. However, it is distance-preserving only on some pairs of compatible transformation strains: For \( e, f \in \mathcal{E} \),

\[
\|e - f\|^2 = \|r_0e - r_0f\|^2 \iff \|e - f\|^2 \neq 2(\alpha - \beta)^2 + 4(\delta \pm \epsilon)^2. \tag{5.5}
\]

This is easy to verify in view of the following: Let \( e, f \in \mathcal{E} \) with \( e \parallel f \). Then,

\[
\|e - f\|^2 = \begin{cases} 
16\epsilon^2 & \text{if } e = r_0f, \\
8\delta^2 + 8\epsilon^2 & \text{if } \exists i \in \{1, 2, 3\}, e = r_i f, \\
2(\alpha - \beta)^2 + 4(\delta \pm \epsilon)^2 & \text{else}.
\end{cases} \tag{5.6}
\]

(The middle case corresponds to parallel edges of the cube that share a face.)

Thus \( r_0 \) is not a symmetry of \( \mathcal{E} \), nor is it a symmetry of \( \mathcal{E}^2 || \). In light of Observation 5.3 we conclude that \( \mathcal{E} \) and \( \mathcal{E}^2 || \) have the rotation symmetries of a cube but not its reflection symmetries:

**Lemma 5.10.** \( S_4 \) is a symmetry group of \( \mathcal{E} \) and \( \mathcal{E}^2 || \), whereas \( S_4 \times C_2 \) is not a symmetry group of \( \mathcal{E} \) or \( \mathcal{E}^2 || \).

**Remark 5.11.** From (5.2b) we deduce that the orbits of \( S_4 \) partition \( \mathcal{E}^2 || \) into four equivalence classes. (Equation (5.6) relates this to the edges of a cube.)
Observations 5.1, 5.3 and 5.8 show that $E^2\|_1$ and $E^3\|_1$ have the symmetries of a cube:

**Lemma 5.12.** $S_4 \times C_2$ is a symmetry group of $E^2\|_1$ and of $E^3\|_1$.

**Remark 5.13.** From Remark 5.4(1) it is clear that $S_4 \times C_2$ (or indeed $S_4$) acts transitively on $E^2\|_1$, that is, the orbit of any element of $E^2\|_1$ under $S_4 \times C_2$ equals $E^2\|_1$. This explains Observation 5.1. Likewise, from Remark 5.4(2) it is clear that $S_4 \times C_2$ (or indeed $S_4$) acts transitively on $E^3\|_1$.

6. The Convex Polytope Formed by the Transformation Strains

In this section we study $C(E)$, the convex hull of $E$, which is a five-dimensional polytope [8, Dimension.nb], when, as we have assumed, $\alpha \neq \beta$ (otherwise it is a three-dimensional polytope). We are interested in the facets of $C(E)$. However the vertices and edges of $C(E)$ are also of interest and we begin with them.

For convenience, we set $\Lambda_1 = \{\lambda \in [0, 1]^{12}, \sum_{i=1}^{12} \lambda_i = 1\}$. The following linear functionals will be helpful in studying $C(E)$:

**Definition 6.1.** The linear functionals $H_i : S^{3 \times 3} \rightarrow \mathbb{R}$, $i = 0, 1, 2, 3$, are defined by

- $H_0 e = -e_{12} - e_{23} - e_{31}$,
- $H_1 e = H_0 r_1 e = -e_{12} + e_{23} + e_{31}$,
- $H_2 e = H_0 r_2 e = e_{12} - e_{23} + e_{31}$,
- $H_3 e = H_0 r_3 e = e_{12} + e_{23} - e_{31}$;

and $H_{ij} : S^{3 \times 3} \rightarrow \mathbb{R}$, $i, j = 1, 2, 3$, by

$H_{ij} e = e_{ij}$,

where $e_{ij}$ denotes the $(i, j)$-component of the matrix $e$.

For the convenience of the reader we summarise the images of the transformation strains under the functionals $H_i$, $i = 0, 1, 2, 3$, in Table 6. We also list the extremisers of these functionals; note that the extremisers when $\varepsilon = \delta$ are the union of the extremisers when $\varepsilon < \delta$ and when $\varepsilon > \delta$.

**Vertices.** The vertices of $C(E)$ are the transformation strains:

**Lemma 6.2.** The set of vertices of $C(E)$ is $E$.

**Proof.** We show this explicitly for $e^{(1)}$, the proof for the other vertices follows from symmetry.

Let $\lambda \in \Lambda$ such that $e^{(1)} = \sum_{i=1}^{12} \lambda_i e^{(i)}$. Then,

$$\beta = H_{33} e^{(1)} = \sum_{i=1}^{12} \lambda_i H_{33} e^{(i)} = \sum_{i=1}^{4} \lambda_i \beta + \sum_{i=5}^{12} \lambda_i \alpha,$$
Table 6. The images of the transformation strains under the linear functionals $H_i, i = 0, 1, 2, 3$, along with their extremisers [8, Linear_Functionals.nb]

| $i$ | $H_0 e^{(i)}$ | $H_1 e^{(i)}$ | $H_2 e^{(i)}$ | $H_3 e^{(i)}$ |
|-----|---------------|---------------|---------------|---------------|
| 1   | $-\delta - 2\varepsilon$ | $-\delta + 2\varepsilon$ | $\delta$ | $\delta$ |
| 2   | $-\delta + 2\varepsilon$ | $-\delta - 2\varepsilon$ | $\delta$ | $\delta$ |
| 3   | $\delta$ | $\delta$ | $-\delta - 2\varepsilon$ | $-\delta + 2\varepsilon$ |
| 4   | $\delta$ | $\delta$ | $\delta$ | $-\delta - 2\varepsilon$ |
| 5   | $-\delta - 2\varepsilon$ | $\delta$ | $\delta$ | $-\delta + 2\varepsilon$ |
| 6   | $-\delta + 2\varepsilon$ | $\delta$ | $\delta$ | $\delta$ |
| 7   | $\delta$ | $-\delta + 2\varepsilon$ | $-\delta - 2\varepsilon$ | $\delta$ |
| 8   | $\delta$ | $-\delta - 2\varepsilon$ | $-\delta + 2\varepsilon$ | $\delta$ |
| 9   | $-\delta - 2\varepsilon$ | $\delta$ | $\delta$ | $-\delta - 2\varepsilon$ |
| 10  | $-\delta + 2\varepsilon$ | $\delta$ | $\delta$ | $\delta$ |
| 11  | $\delta$ | $-\delta + 2\varepsilon$ | $\delta$ | $-\delta - 2\varepsilon$ |
| 12  | $\delta$ | $-\delta - 2\varepsilon$ | $\delta$ | $-\delta + 2\varepsilon$ |

Minimisers: $1, 5, 9$  
Maximisers: $2, 8, 12$  
When $\varepsilon < \delta$: $3, 4, 7, 8, 11, 12$  
When $\varepsilon = \delta$: $I \setminus \{1, 5, 9\}$  
When $\varepsilon > \delta$: $I \setminus \{2, 8, 12\}$  

from which we conclude that $\lambda_i = 0$ for $i = 5, \ldots, 12$ and thus $e^{(1)} = \sum_{i=1}^{4} \lambda_i e^{(i)}$. Now, using $H_0$ we obtain

$$-\delta - 2\varepsilon = H_0 e^{(1)} = \sum_{i=1}^{4} \lambda_i H_0 e^{(i)}.$$

Since $\varepsilon, \delta > 0$ it is easy to see (see Table 6) that $\lambda_1 = 1$ and $\lambda_i = 0, i = 2, 3, 4$. We conclude that $e^{(1)}$ is a vertex.

In the interest of brevity in future proofs of extremality of subsets we will name only the relevant family of four-dimensional hyperplanes, for example for the above lemma we would say that this follows from $H_{33}$ and $H_0$.

Edges. Contrary to what we are used to in two and three dimensions (see Remark 6.4 below), the convex hull of every pair of vertices is an edge of $C(\mathcal{E})$:

Lemma 6.3. The set of edges of $C(\mathcal{E})$ is $\{[e, f] \mid e, f \in \mathcal{E}\}$.

Henceforth, a compatible edge is the convex hull of a pair of compatible vertices, and an incompatible edge is the convex hull of a pair of incompatible vertices.

We prove Lemma 6.3 here except for incompatible edges when $\varepsilon > \delta$. In Remark 6.10 we present a Mathematica-aided proof which is valid for $\varepsilon \neq \delta$. 
Proof. (for compatible edges and, when \( \varepsilon \leq \delta \), for incompatible edges) By symmetry it suffices to prove that the eleven edges \([e^{(1)}, e^{(i)}], i \in I \setminus \{1\}\), are extremal.

This is easy to verify for the compatible edges: For example, \(H_{33}\) and \(H_{12}\) show that \([e^{(1)}, e^{(2)}]\) is extremal. The proof for the other compatible edges (with \(e^{(1)}\) as a vertex) is similar.

We now turn to the incompatible edges, for example \([e^{(1)}, e^{(6)}]\). Let \(\mu \in [0, 1]\) and \(\lambda \in \Lambda\) such that

\[
\mu e^{(1)} + (1 - \mu)e^{(6)} = \sum_{i=1}^{12} \lambda_i e^{(i)}.
\]

Consider first the case \(\varepsilon < \delta\). Then \(H_{11}\) and \(H_2\) show that, in fact,

\[
\mu e^{(1)} + (1 - \mu)e^{(6)} = \sum_{i \in \{1, 2, 5, 6\}} \lambda_i e^{(i)}.
\]

However \(\dim \text{aff} \text{span}\{e^{(1)}, e^{(2)}, e^{(5)}, e^{(6)}\} = 3\) [8, Dimension_Calculations.nb] and thus \(C([e^{(1)}, e^{(2)}, e^{(5)}, e^{(6)}])\) is a three-dimensional tetrahedron. It follows that \(\lambda_5 = \lambda_2 = 0\) and thus \([e^{(1)}, e^{(6)}]\) is extremal.

Next consider the case \(\varepsilon = \delta\). Then \(H_{11}, H_{13}, H_1\) and \(H_2\) show that in fact

\[
\mu e^{(1)} + (1 - \mu)e^{(6)} = \sum_{i \in \{1, 5, 6\}} \lambda_i e^{(i)}.
\]

However \(\dim \text{aff} \text{span}\{e^{(1)}, e^{(5)}, e^{(6)}\} = 2\) [8, Dimension_Calculations.nb] and thus \(C([e^{(1)}, e^{(5)}, e^{(6)}])\) is a triangle. It follows that \(\lambda_5 = 0\) and thus \([e^{(1)}, e^{(6)}]\) is extremal.

The extremality of the other incompatible edges (with \(e^{(1)}\) as a vertex) follows from symmetry. □

Remark 6.4. In dimensions less than four the only polytopes for which the convex hull of every pair of vertices is an edge are the \(n\)-tetrahedra (line segments, triangles and tetrahedra in dimensions one, two and three, respectively). However for every \(n > 3\) and every \(d > n\), there exists an \(n\)-dimensional convex polytope with \(d\) vertices for which the convex hull of every pair of vertices is extremal. See, for example [7, Section 13], [12, Section 3] or [40, Corollary 0.8].

The facets of \(C(\mathcal{E})\). The algorithm we use to determine the facets of \(C(\mathcal{E})\) is as follows [8, Faceting.nb]. It assumes that the affine span of the set is five-dimensional, that the cardinality of the set is small and thus that computational efficiency is not a consideration.

Algorithm 6.5. 1. First we form a set of all four-dimensional tetrahedra with vertices in \(\mathcal{E}\) as follows:

(a) Pick all five-tuples from \(\mathcal{E}\):

\[
\{S \subset \mathcal{E} \mid \#S = 5\}.
\]
Discard those five-tuples whose affine span is not four dimensional:
\[ G_1 := \{ S \subset E \mid \#S = 5, \dim \text{aff span}(S) = 4 \}. \]

2. Of these tetrahedra we discard any whose convex hull is not contained in \( \partial C(E) \). We do this as follows:
(a) Let \( G_2 = G_1 \).
(b) Pick \( S \in G_2 \).
(c) Translate the origin to some \( e \in S \). (The next two steps are carried out in this co-ordinate system.)
(d) Compute a normal \( n \in S^3 \times S^2 \alpha + \beta \) to \( \text{aff span}(S) \).
(e) If \( \langle n, e \rangle \) has the same sign for all \( e \in E \setminus S \) then \( C(S) \subset \partial C(E) \). Otherwise remove \( S \) from \( G_2 \).
(f) Repeat steps (2b) to (2e) till all tetrahedra in \( G_2 \) have been tested.

We now obtain
\[ G_2 = \{ S \subset E \mid \#S = 5, \dim \text{aff span}(S) = 4, C(S) \subset \partial C(E) \}. \]

This is the set of all four-dimensional tetrahedra (with vertices in \( E \)) whose union is \( \partial C(E) \).

3. The final step is to form the facets of \( C(E) \) by judiciously taking unions of sets in \( G_2 \) as follows:
(a) Let \( G_3 = G_2 \).
(b) Pick \( S_1, S_2 \in G_3 \).
(c) If \( \dim \text{aff span}(S_1 \cup S_2) = 4 \) then \( S_1 \) and \( S_2 \) are parts of the same facet. In \( G_3 \), replace \( S_1 \) and \( S_2 \) by \( S_1 \cup S_2 \).
(d) Repeat steps (3b) and (3c) until every union of sets in \( G_3 \) increases the dimension, that is, until it is true that
\[ \forall S_1, S_2 \in G_3, \quad \dim \text{aff span}(S_1 \cup S_2) = 4 \implies S_1 = S_2. \] (6.1)

This is the set of all the facets of \( C(E) \). Note that it is a set of \( n \)-tuples where \( n \geq 5 \).

The results of a Mathematica implementation of Algorithm 6.5 are summarised in Observations 6.6, 6.7 and 6.8 below. These reveal that the facet structure depends on whether \( \varepsilon < \delta \), \( \varepsilon = \delta \) or \( \varepsilon > \delta \). All three possibilities are realisable in that there exist cubic-to-monoclinic-I phase transformations corresponding to each. (See, for example, [4, Fig. 4.3 and (4.11) on pp. 52–53] for the relationship between \( \varepsilon, \delta \) and the unit cells of the cubic and monoclinic lattices.) However, curiously, \( \varepsilon < \delta \) for all the monoclinic-I materials of which we are aware, see Table 2; we return to this point in Section 8.

In the observations below, each group of facets is the orbit under \( S_4 \) of any facet in it [8, Facet_Symmetry.nb]. Within each group the facets are listed in lexical order. Facets that occur for both \( \varepsilon < \delta \) and \( \varepsilon > \delta \) are shown in bold face.

**Observation 6.6.** (Monoclinic-Ia martensite, \( \varepsilon < \delta \)) When \( \varepsilon < \delta \), the 25 four-dimensional facets of \( C(E) \) consist of the convex hulls of
1. 12 facets with 5 vertices each:
   \{1, 2, 3, 7, 10\}, \{1, 2, 4, 6, 11\}, \{1, 3, 4, 5, 9\}, \{1, 5, 7, 8, 9\},
   \{1, 5, 9, 11, 12\}, \{2, 3, 4, 8, 12\}, \{2, 5, 6, 8, 12\}, \{2, 8, 9, 10, 12\},
   \{3, 5, 6, 7, 10\}, \{3, 7, 10, 11, 12\}, \{4, 6, 7, 8, 11\}, \{4, 6, 9, 10, 11\};

2. 4 pairs of \(T_3\)s (see Section 7), each facet is invariant under \(r_0\):
   \{1, 2, 5, 6, 11, 12\}, \{1, 2, 7, 8, 9, 10\}, \{3, 4, 5, 6, 9, 10\}, \{3, 4, 7, 8, 11, 12\}  
   \text{(6.2)}

3. 6 pairs of pairwise compatible three-tuples:
   \{1, 2, 5, 8, 9, 12\}, \{1, 3, 5, 7, 9, 10\}, \{1, 4, 5, 6, 9, 11\},
   \{2, 3, 7, 8, 10, 12\}, \{2, 4, 6, 8, 11, 12\}, \{3, 4, 6, 7, 10, 11\};

4. 3 facets with 8 vertices each; each facet is invariant under \(r_0\):
   \{1, 2, 3, 4, 5, 6, 7, 8\}, \{1, 2, 3, 4, 9, 10, 11, 12\}, \{5, 6, 7, 8, 9, 10, 11, 12\}.  
   \text{(6.3)}

**Observation 6.7.** \((\varepsilon = \delta)\) When \(\varepsilon = \delta\), the 7 four-dimensional facets of \(\mathcal{C}(\mathcal{E})\) consist of the convex hulls of

1. 4 facets with 9 vertices each:
   \{1, 2, 3, 5, 7, 8, 9, 10, 12\}, \{1, 2, 4, 5, 6, 8, 9, 11, 12\},
   \{1, 3, 4, 5, 6, 7, 9, 10, 11\}, \{2, 3, 4, 6, 7, 8, 10, 11, 12\};  
   \text{(6.4)}

2. 3 facets with 8 vertices each; each facet is invariant under \(r_0\):
   \{1, 2, 3, 4, 5, 6, 7, 8\}, \{1, 2, 3, 4, 9, 10, 11, 12\}, \{5, 6, 7, 8, 9, 10, 11, 12\}.  
   \text{(6.3)}

**Observation 6.8.** \((\text{Monoclinic-Ib martensite, } \varepsilon > \delta)\) When \(\varepsilon > \delta\), the 33 four-dimensional facets of \(\mathcal{C}(\mathcal{E})\) consist of the convex hulls of

1. 12 facets which are the images under \(r_0\) of the five-vertex facets that occur when \(\varepsilon < \delta\):
   \{1, 2, 3, 5, 12\}, \{1, 2, 4, 8, 9\}, \{1, 3, 4, 7, 11\}, \{1, 5, 6, 7, 11\},
   \{1, 7, 9, 10, 11\}, \{2, 3, 4, 6, 10\}, \{2, 6, 7, 8, 10\}, \{2, 6, 10, 11, 12\},
   \{3, 5, 7, 8, 12\}, \{3, 5, 9, 10, 12\}, \{4, 5, 6, 8, 9\}, \{4, 8, 9, 11, 12\};

2. 12 other five vertex facets (together these are invariant under \(r_0\)):
   \{1, 3, 5, 9, 12\}, \{1, 3, 7, 10, 11\}, \{1, 4, 5, 8, 9\}, \{1, 4, 6, 7, 11\},
   \{1, 5, 7, 9, 11\}, \{2, 3, 5, 8, 12\}, \{2, 3, 6, 7, 10\}, \{2, 4, 6, 10, 11\},
   \{2, 4, 8, 9, 12\}, \{2, 6, 8, 10, 12\}, \{3, 5, 7, 10, 12\}, \{4, 6, 8, 9, 11\};
3. 6 pairs of pairwise compatible three-tuples:

\{1, 2, 5, 8, 9, 12\}, \{1, 3, 5, 7, 9, 10\}, \{1, 4, 5, 6, 9, 11\},
\{2, 3, 7, 8, 10, 12\}, \{2, 4, 6, 8, 11, 12\}, \{3, 4, 6, 7, 10, 11\};

4. 3 facets with 8 vertices each; each facet is invariant under $r_0$:

\{1, 2, 3, 4, 5, 6, 7, 8\}, \{1, 2, 3, 4, 9, 10, 11, 12\}, \{5, 6, 7, 8, 9, 10, 11, 12\}.

(6.3)

Remark 6.9. The extremality of facets that are invariant under $r_0$ can be verified as in the proof of Lemma 6.2: $H_{11}, H_{22}, H_{33}$ show that the facets in (6.3) are extremal. $H_i, i = 0, 1, 2, 3$, show that pairs of $T_3$s in (6.2) are extremal, since $\varepsilon < \delta$ implies $-\delta - 2\varepsilon < -\delta < \delta - 2\varepsilon < \delta < \delta + 2\varepsilon$.

In addition, $H_i, i = 0, 1, 2, 3$, also show that the facets in (6.4) are extremal, see Table 6. For the remaining facets extremality can be verified through a computation of normals [8, Facet_Normal.nb].

Remark 6.10. (Proof of Lemma 6.3 when $\varepsilon \neq \delta$) Observations 6.6 and 6.8 lead to a proof of Lemma 6.3 when $\varepsilon \neq \delta$: Observe that every edge is shared by at least four facets. (This is particularly easy to check for the incompatible edges. Each incompatible edge is contained in precisely one facet from each group.) It follows that every edge is extremal (see for example [2, Chapter 6] or the other references listed in Section 2.2).

Remark 6.11. We remark that this phenomenon of polytope facet structure depending on lattice parameters is not possible for the other martensites (that is, cubic-to-tetragonal, cubic-to-trigonal and cubic-to-orthorhombic) because they form $n$-tetrahedra (for $n = 2, 3, 5$, respectively) and thus their facet structure is fixed.

7. Non-Laminate Microstructures in $\mathcal{R}(E)$

In this section we use the results of the preceding sections to derive our central results about non-laminate microstructures in monoclinic-I martensite. These include $T_3$ microstructures formed by the strains in $E$ (Section 7.1) and $T_3$ microstructures formed by the nodes of these $T_3$s (Section 7.2).

7.1. (Level-1) $T_3$s and Related Microstructures

As mentioned earlier there are precisely eight 3-tuples of pairwise incompatible vertices (see Table 3):

\[ \mathcal{E}_3^{\parallel} = \{ \{e^{(1)}, e^{(6)}, e^{(12)}\}, \{e^{(1)}, e^{(8)}, e^{(10)}\}, \{e^{(2)}, e^{(5)}, e^{(11)}\}, \{e^{(2)}, e^{(7)}, e^{(9)}\}, \{e^{(3)}, e^{(6)}, e^{(9)}\}, \{e^{(3)}, e^{(8)}, e^{(11)}\}, \{e^{(4)}, e^{(5)}, e^{(10)}\}, \{e^{(4)}, e^{(7)}, e^{(12)}\} \}. \]
Since
\[ \text{sign det}(e^{(1)} - e^{(6)}) = \text{sign det}(e^{(6)} - e^{(12)}) = \text{sign det}(e^{(12)} - e^{(1)}) \neq 0 \]

and likewise for the other 3-tuples, see Table 3, we obtain by Lemma 4.3 that each of these 3-tuples forms a $T_3$. (See also Remark 5.13.)

Let $v_{i,j,k} = \{e^{(i)}, e^{(j)}, e^{(k)}\} \in \mathcal{E}_3^{3}$. We set

\[ \tau_{i,j,k} = \mathcal{R}(v_{i,j,k}), \]
\[ T := \{ \tau_{i,j,k} | v_{i,j,k} \in \mathcal{E}_3^{3} \}. \]

For $\tau \in T$ and $r \in S_4 \times C_2$, by $r \tau$ we mean the $T_3$ formed by the image under $r$ of the vertices of $\tau$. (The existence of such $T_3$s follows from $S_4 \times C_2$ being a symmetry group of $\mathcal{E}_3^{3}$ as was shown in Lemma 5.12). The symmetry relations

Fig. 5. The symmetry of the eight $T_3$s
between the $T_3$s is illustrated in Fig. 5. As we shall see (Example 7.3 below) each $\tau \in T$ is specially related to $r_0 \tau$; we refer to it as the dual of $\tau$.

Before we proceed further we note that each of these eight $T_3$s is symmetric (Definition 4.6) and has distinct nodes (Definition 4.5). Moreover, all eight $T_3$s are similar (Definition 4.8):

**Lemma 7.1.** All $T_3$s in $T$ are similar, and each is symmetric and has distinct nodes.

**Proof.** The symmetry of each $T_3$ and the similarity of all $T_3$s in $T$ follow from Remark 5.13.

Now consider the nodes of $\tau_{1,8,10}$. Suppose, on the contrary, that $e_{1,8} = e_{8,10} = e_{10,1}$. (Here we use the notation of Section 4.) Then, by symmetry, the nodes coincide with the barycentre of the $T_3$ which is $\frac{1}{3} \left( e^{(1)} + e^{(8)} + e^{(10)} \right)$. However, an elementary calculation shows that this barycentre is incompatible with $e_1, e_8$ and $e_{10}$ which is a contradiction (see Definition 4.1). Thus $\tau_{1,8,10}$ has distinct nodes and by symmetry this is true for all eight $T_3$s. $\square$

From Proposition 4.9 and symmetry it follows that the barycentre of each $v \in E^3$ is contained in $R(v)$. From Observations 6.6 and 6.7, when $\varepsilon \leq \delta$, each $T_3$ in $T$ along with its dual is contained in a facet of $C(E)$. In particular for each $\tau \in T$, the symmetrised rank-one convex hull of $\tau \cup r_0 \tau$ is contained in a facet of $C(E)$ and is thus a part of the boundary of the symmetrised rank-one convex hull of $E$:

$$R(\tau \cup r_0 \tau) \subset \partial R(E). \quad (7.1)$$

Example 7.3 below reveals that $R(\tau \cup r_0 \tau)$ is four dimensional and that each point in it can be attained by laminates of $T_3$ microstructures. In other words, $R(\tau \cup r_0 \tau)$ contains a four-dimensional set of $T_3$s. Before we show this we first construct a three-dimensional set of $T_3$s which lies in $\partial R(E)$ when $\varepsilon \leq \delta$.

**Example 7.2.** (A three-dimensional set of $T_3$s) Let $\tau \in T$. From Table 3, the elements of $E$ with which all the vertices of $\tau$ are compatible are precisely the vertices of $r_0 \tau$. Following the construction introduced in Lemma 4.10, we construct a three-dimensional set of $T_3$s from $\tau$ and (any) one vertex from $r_0 \tau$. There are three such continua of $T_3$s, one for each vertex of $r_0 \tau$. Analogously there are three such sets constructed from $r_0 \tau$ and the vertices of $\tau$.

Note that this example shows that $T_3$s exist not only in $E$ but also in $L_1(E) \setminus E$, since the vertices of almost all of the $T_3$s so constructed are themselves attained by a lamination of strains in $E$. However, in the next example the construction of $T_3$s precedes the construction of laminates.

**Example 7.3.** (A four-dimensional set of laminates of nodes of $T_3$s) From each $\tau \in T$ and its dual we construct a four-dimensional set of laminates of nodes of $T_3$s. We do this explicitly for $\tau_{1,8,10}$ and its dual $\tau_{2,7,9}$; the construction for the other pairs is similar.
First we note that each point in one of these $T_3$s is compatible with the corresponding point (that is, the point with the same barycentric coordinates) in its dual. In fact, this is true even after a cyclic permutation of the vertices: $\forall x, y, z \in \mathbb{R},$

$$xe^{(1)} + ye^{(8)} + ze^{(10)} \parallel xe^{(2)} + ye^{(9)} + ze^{(7)}, xe^{(7)} + ye^{(2)} + ze^{(9)},$$

$$xe^{(9)} + ye^{(7)} + ze^{(2)}.$$

This is immediate from the calculation [8, Pair_of_Level-1_T3s.nb]:

$$\det \left( (xe^{(1)} + ye^{(8)} + ze^{(10)}) - (xe^{(2)} + ye^{(9)} + ze^{(7)}) \right)$$

$$= \det \left( (xe^{(1)} + ye^{(8)} + ze^{(10)}) - (xe^{(7)} + ye^{(2)} + ze^{(9)}) \right)$$

$$= \det \left( (xe^{(1)} + ye^{(8)} + ze^{(10)}) - (xe^{(9)} + ye^{(7)} + ze^{(2)}) \right)$$

$$= 0.$$

Thus, in particular, each node of $\tau_{1,8,10}$ is compatible with every node of $\tau_{2,7,9}$ (and vice versa). Since the nodes of a $T_3$ are pair-wise compatible it follows that these six nodes (that is in the notation of Section 4, $e_{1,8}, e_{8,10}, e_{10,1}, e_{2,9}, e_{9,7}$ and $e_{7,2}$) are pair-wise compatible (see Fig. 6, note that the figure is schematic; in fact $\tau$ and $r_0\tau$ share the same barycenter). We conclude that:

$$\mathcal{C}([e_{1,8}, e_{8,10}, e_{10,1}, e_{2,9}, e_{9,7}, e_{7,2}]) \subset \mathcal{R}([e_1, e_2, e_7, e_8, e_9, e_{10}]).$$

Each point in this convex hull is attained by a lamination of the nodes of $\tau_{1,8,10}$ and $\tau_{2,7,9}$. A simple Mathematica verification [8, Dimension.nb] shows that this convex hull is four-dimensional. (Thus the maximum depth of lamination required is also four, see proof of Theorem 2.11.)

Note that when $\varepsilon \leq \delta$, from (7.1),

$$\mathcal{C}([e_{1,8}, e_{8,10}, e_{10,1}, e_{2,9}, e_{9,7}, e_{7,2}]) \subset \partial \mathcal{R}(\mathcal{E}). \quad (7.2)$$
7.2. Level-2 $T_3$s and Related Microstructures

Next, we construct new $T_3$s from the nodes of the $T_3$s in $\mathcal{T}$. We refer to the former $T_3$s as Level-1 $T_3$s and to the new $T_3$s as Level-2 $T_3$s. Level-2 $T_3$s allow us to construct a five-dimensional set of $T_3$s, see Construction 7.5 below.

**Construction 7.4.** Let $\tau \in \mathcal{T}$ and let $\tau_1, \tau_2, \tau_3 \in \mathcal{T}$ be chosen such that, in Fig. 5, the line joining $\tau$ and $\tau_i$ is an edge of the cube for $i = 1, 2, 3$ (thus $\tau_i = r_{j1}^\pm \tau$ for some $j = 1, 2, 3$). Note that the set $\{\tau_1, \tau_2, \tau_3\}$ is invariant under any element of $S_4$ that leaves $\{\tau, r_0\tau\}$ invariant (these are rotations of $\frac{2\pi}{3}$ through the major diagonal formed by $\tau$ and $r_0\tau$). Let $r$ be an element of this group (that is, one of two such rotations). Now let $n_1$ be a node of $\tau_1$. Then $n_1, rn_1, r^2n_1$ form a symmetric $T_3$ with distinct nodes. Similarly for $n_2, rn_2, r^2n_2$ and $n_3, rn_3, r^2n_3$. This is illustrated in Fig. 7.

**Proof.** We show that $n_1, rn_1, r^2n_1$ form a $T_3$ explicitly for $\tau = \tau_{3,8,11}, \tau_1 = \tau_{1,8,10}, \tau_2 = \tau_{2,5,11}$ and $\tau_3 = \tau_{3,6,9}$; the result for the other 3-tuples follows by symmetry.

Since $n_1 \in \tau_{1,8,10}$, it has the barycentric representation $xe^{(1)} + y e^{(8)} + ze^{(10)}$ for some $x, y, z \in [0,1]$ with $x + y + z = 1$. Then, as can be easily checked (Table 5),
\{r n_1, r^2 n_1\} = \{x e^{(5)} + y e^{(11)} + z e^{(2)}, x e^{(9)} + y e^{(3)} + z e^{(6)}\}.

(Nota the order of the vertices.) It can be verified [8, Level-2_T3s.nb] that
\[
\det\left(\left(\langle x e^{(1)} + y e^{(8)} + z e^{(10)}\rangle - \langle x e^{(5)} + y e^{(11)} + z e^{(2)}\rangle\right)\right)
= \det\left(\left(\langle x e^{(5)} + y e^{(11)} + z e^{(2)}\rangle - \langle x e^{(9)} + y e^{(3)} + z e^{(6)}\rangle\right)\right)
= \det\left(\left(\langle x e^{(9)} + y e^{(3)} + z e^{(6)}\rangle - \langle x e^{(1)} + y e^{(8)} + z e^{(10)}\rangle\right)\right)
\neq 0.
\]

Thus, by Lemma 4.3, Remark 4.7 and (5.3), \(n_1, r n_1, r^2 n_1\) form a symmetric \(T_3\). (From Remark 4.7 it would have sufficed to check that one of the determinants above is non-zero.) To show that the nodes of this \(T_3\) are distinct it suffices to check that the barycentre of the \(T_3\) is incompatible with (one of) its nodes (see proof of Lemma 7.1). From [8, Level-2_T3s.nb]:
\[
\left\langle x e^{(1)} + y e^{(8)} + z e^{(10)}, x e^{(5)} + y e^{(11)} + z e^{(2)}, x e^{(9)} + y e^{(3)} + z e^{(6)}\right\rangle
\frac{1}{3}\left(\langle x e^{(1)} + y e^{(8)} + z e^{(10)}\rangle + \langle x e^{(5)} + y e^{(11)} + z e^{(2)}\rangle + \langle x e^{(9)} + y e^{(3)} + z e^{(6)}\rangle\right).
\]

Which completes the proof. \(\Box\)

Since there are eight choices of \(\tau\) and three choices of \(n_1\) for each choice of \(\tau\), by this construction we obtain 24 \(T_3\)s.

Finally, Example 7.3 and Construction 7.4 can be combined to construct a five-dimensional set of \(T_3\)s whose vertices are themselves laminates of nodes of (level-1) \(T_3\)s.

**Construction 7.5.** Let \(\tau \in \mathcal{T}\) and let \(\tau_1, \tau_2, \tau_3 \in \mathcal{T}\) and \(r \in S_4\) be as in Construction 7.4 above. Let \(n_{1,i}\) and \(n'_{1,i}, i = 1, 2, 3\) be the nodes of \(\tau_1\) and its dual, respectively. Pick \(\mu_i, \mu'_i \in [0, 1]\) such that \(\sum_{i=1}^{3} \mu_i + \sum_{i=1}^{3} \mu'_i = 1\) and let
\[
p_1 = \sum_{i=1}^{3} \mu_i n_{1,i} + \sum_{i=1}^{3} \mu'_i n'_{1,i}.
\]

Note that \(p_1\) is an element of the four-dimensional set constructed in Example 7.3 and thus can be attained by a lamination of \(n_{1,i}, n'_{1,i}, i = 1, 2, 3\). We assert that \(p_1, r p_1, r^2 p_1\) form a symmetric \(T_3\). The union of the \(T_3\)s as \(p_1\) varies yields a five-dimensional set. When \(\varepsilon \leq \delta\) from (7.2), this set intersects the boundary of the symmetrised rank-one convex hull of \(E\).

**Proof.** A Mathematica calculation [8, Level-2_T3s.nb] shows this explicitly for \(\tau_1 = \tau_{1,8,10}, \tau_2 = \tau_{2,5,11}\) and \(\tau_3 = \tau_{3,6,9}\) (that is, \(\tau = \tau_{3,8,11}\)), the construction for the other 3-tuples is similar.
To see that the set of $T_3$s constructed here is five-dimensional, it suffices to note that $p_1$ is picked from a four-dimensional set which, not being closed under $r$, does not contain the $T_3$s formed by $p_1, rp_1, r^2p_1$. It follows that the union of the $T_3$s (as $p_1$ varies) constructed here is a five-dimensional set.

It is natural at this point to ask whether the nodes of level-2 $T_3$s form level-3 $T_3$ and, more generally, whether the nodes of level-$n$ $T_3$s from level-$(n + 1)$ $T_3$s. We postpone these questions to [9] and instead conclude by considering some implications of the results presented here.

8. Conclusions

8.1. Mathematical Comments

While we have, in the later half of this paper, focused on monoclinic-I martensite, it is clear that our general strategy can, in principle, be applied to any finite set in $S_c^{3 \times 3}$; indeed in [9] we apply it also to monoclinic-II martensite. Here we briefly comment on the two main components of our strategy, namely an understanding of the algebraic structure of symmetrised rank-one convex cones, and an understanding of the polytope structure of the given set.

The algebraic structure of symmetrised rank-one convex cones. While we have a complete understanding of symmetrised rank-one convexity in two-dimensions (Sections 3 and 4, and [10]), the algebraic structure of symmetrised rank-one convex cones is not yet sufficiently well understood in higher dimensions. A key missing ingredient is a characterisation, in terms of canonical forms, of real cubic polynomials in several variables. This problem in invariant theory seems unsolved for three and more variables. The fruitfulness of our approach in two-dimensions suggests that it might be valuable to more fully explore the algebraic aspects of symmetrised rank-one convexity.

When $\varepsilon < \delta$ we demonstrate the existence of $T_3$s that attain points on the boundary of $C(E)$, more precisely, that attain points on the four-dimensional facets of $C(E)$. Though (as a Mathematica calculation [8, Facet-T3Pair.nb] shows) the $T_3$s do not belong to the three-dimensional facets (of the four-dimensional facets) of $C(E)$, we suspect that the symmetrised rank-one convex hull of monoclinic-I martensite is strictly larger than the lamination hull. If so, the question arises as to how much larger it is. In terms of dimensions a perturbation argument shows that $R(E) \setminus L(E)$ would be at least two-dimensional. In fact we suspect that it is five-dimensional.

Convex polytopes. Since the convex hull of any finite set is a convex polytope, it is natural that an attempt to determine the semi-convex hull of a finite sets takes advantage of the structure of the convex polytopes they generate. This seems not to have been considered in the literature except for Theorem 2.11. Lemma 6.3 and Remark 6.4 demonstrate the counter-intuitive behaviour of high-dimensional polytopes, and thus the usefulness of knowledge of the theory of convex polytopes.

Moreover, when, as in the example of monoclinic-I martensite considered here, the faceting structure of the polytope depends on the material parameters, it might
Table 7. $\lambda$ and $(\alpha - \beta)\delta + \varepsilon^2 - \delta^2$ for the $T_3$s in $T$ for NiTi, CuZr and TiNiCu [8, Lambda.nb]

| Material  | $\lambda$ | $(\alpha - \beta)\delta + \varepsilon^2 - \delta^2$ |
|-----------|-----------|-------------------------------------------------|
| NiTi      | 0.6830    | 0.0024                                          |
| TiNiCu    | 0.6683    | 0.0021                                          |
| CuZr      | 0.0396    | -0.0015                                         |

be expected that qualitative features of the semi-convex hulls and envelopes depend on the material parameters as well. If so, this heightens the possible utility of these polytopes for evaluating semi-convex hulls and envelopes.

8.2. Implications for Mechanics

Two kinds of monoclinic-I martensite. Curiously, all cubic-to-monoclinic-I materials that we are aware of are monoclinic-Ia martensites (that is, those for which $\varepsilon < \delta$), see Table 2. It is natural to ask whether monoclinic-I martensite recovers more strains (modulo appropriate normalisation of the lattice parameters) as $\varepsilon - \delta$ approaches zero (with $\varepsilon = \delta$ being the ideal), and whether monoclinic-Ib martensites (that is, those for which $\varepsilon > \delta$) would demonstrate greater shape memory effect.

Monoclinic-II martensite. We have reason to believe that there are multiple kinds of monoclinic-II martensite as well. We hope to settle this question in [9].

As can be easily verified (for example [4]), the compatibility relations between the twelve transformation strains of monoclinic-II martensite are identical to those between the twelve transformation strains of monoclinic-I martensite. Then, with the help of Lemma 4.3, exactly as for monoclinic-I martensite, eight $T_3$s can be formed from these strains. This positively answers the question raised in [6, p. 863] as to whether $T_3$s can be formed from the twelve transformation strains of monoclinic-II martensite. Indeed, Lemma 4.3 presents an elementary test by which this question can be answered for any three-tuple of strains that have the same trace.

Special parameters. Throughout this paper, including in the (non-numerical) Mathematica computations, we have assumed the lattice parameters to be generic, except that we considered the case $\varepsilon = \delta$. We did identify one special case, $(\alpha - \beta)\delta + \varepsilon^2 - \delta^2 = 0$, in which all twelve strains of monoclinic-I martensite are pair-wise compatible.

The question arises as to whether a material recovers more strains as $(\alpha - \beta)\delta + \varepsilon^2 - \delta^2$ approaches zero. We suggest another parameter of importance, $\lambda := \lambda_{12} = \lambda_{23} = \lambda_{31}$ (Definition 4.6) which, however, appears to be related to $(\alpha - \beta)\delta + \varepsilon^2 - \delta^2$ for the three materials considered in Table 7.

Our reasoning is that as $\lambda$ becomes close to either 0 or 1, the nodes of a $T_3$ become closer to its vertices and the energetic penalty for a $T_3$ microstructure being approximated by a finite-rank laminate becomes smaller. Indeed, instead of constructing a finite-rank laminate from the three nodes of a $T_3$, it suffices to move only one of the vertices to a node.

As Table 7 shows $\lambda = 0.0396$ for CuZr. We hypothesise that for this material the symmetrised lamination convex hull is very close to the convex hull, and thus
the convex hull is a very good approximation to all its semi-convex hulls. The same would apply to the (semi-)convex envelopes of the corresponding energy density, as well. A similar reasoning might explain the remarkable closeness between the symmetrised lamination convex hull and the convex hull for CuAlNi (a monoclinic-II martensite) observed in [13].

Microstructure corresponding to $T_3s$. For monoclin-I martensite with $\varepsilon < \delta$ we have shown that there exists a five-dimensional set of $T_3s$ which reaches the boundary of $C(\mathcal{E})$. This raises the question as to whether the microstructures experimentally observed for strains in this set are laminate approximations to $T_3$ microstructures. We wonder, too, if experimental observations of such microstructures would provide insight into mechanisms governing microstructure formation (dynamics) and the role of surface energy.

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