

Variational Models in Martensitic Phase Transformations with Applications to Steels



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BY

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Abstract

This thesis concerns the mathematical modelling of phase transformations with a special emphasis on martensitic phase transformations and their application to the modelling of steels.

In Chapter 1, we develop a framework that determines the optimal transformation strain between any two Bravais lattices and use it to give a rigorous proof of a conjecture by E.C. Bain in 1924 on the optimality of the so-called *Bain strain*.

In Chapter 2, we review the Ball-James model and related concepts. We present some simplification of existing results.

In Chapter 3, we pose a conjecture for the explicit form of the quasiconvex hull of the three tetragonal wells, known as the *three-well problem*. We present a new approach to finding inner and outer bounds.

In Chapter 4, we focus on highly compatible, so called *self-accommodating*, martensitic structures and present new results on their fine properties such as estimates on their minimum complexity and bounds on the relative proportion of each martensitic variant in them.

In Chapter 5, we investigate the contrary situation when self-accommodating microstructures do not exist. We determine, whether in this situation, it is still energetically favourable to nucleate martensite within austenite. By constructing different types of inclusions, we find that the optimal shape of an inclusion is flat and thin which is in agreement with experimental observation.

In Chapter 6, we introduce a mechanism that identifies transformation strains with orientation relationships. This mechanism allows us to develop a simpler, strain-based approach to phase transformation models in steels. One novelty of this approach is the derivation of an explicit dependence of the orientation relationships on the ratio of tetragonality of the product phase.

In Chapter 7, we establish a correspondence between common phenomenological models for steels and the Ball-James model. This correspondence is then used to develop a new theory for the $(5\ 5\ 7)$ lath transformation in low-carbon steels. Compared to existing theories, this new approach requires a significantly smaller number of input parameters. Furthermore, it predicts a microstructure morphology which differs from what is conventionally believed.

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Prologue

Every year more than 1.3 billion tonnes of steel are produced and the estimated global turnover is close to one trillion US dollars making it the second biggest industry in the world [Wor16]. The strongest and thus one of the most important forms of steel is *martensite*, named after the German metallurgist Adolf Martens (1850–1914). Most of the modern theoretical treatment of martensitic steels goes back to E.C. Bain's seminal paper 'The Nature of Martensite' [Bai24] and till the present day, the transformation strain required to transform the high temperature to the low temperature phase of martensitic steels is known as the 'Bain strain'. Unsurprisingly, the early theoretical treatment of metals concerned almost exclusively steels and one of the most important theories that emerged is known as the 'Crystallographic Theory of Martensite' (see e.g. [Wec+53; BM54]). Despite its success in predicting important features of steels such as habit plane normals, a shortcoming of the crystallographic theory is its phenomenological nature, i.e. it describes and relates the observed phenomena but is not based on first principles. This shortcoming may have been one of the reasons why Ball & James [BJ87] revisited the crystallographic theory and developed a new energetic model based on non-linear elasticity. This model, now known as the Ball-James model, turned out to be extremely successful. It was not only able to recast the original results but, due to a more fundamental understanding of the underlying mechanism, was able to help design and understand materials with outstanding properties, such as ultra-low hysteresis materials or shape-memory alloys.

The newly discovered alloys are only some of many examples that, besides steel, undergo a 'martensitic' phase transformation. A common feature of all martensitic

transformations is a stress or temperature induced change of the lattice structure. In most cases the cooling rate is extremely high, so that the atoms do not have enough time to diffuse and instead rearrange purely displacively. In honour of Bain's pioneering work, even in this more general set-up, the required strains to change the lattice structure are often still referred to as the Bain strains.

In spite of their common roots, the future development and applications of the two different theories seem to have been strictly separated ever since. Whereas the metallurgy community remained faithful to the original crystallographic theory, a significant part of the research on new materials and metallic alloys adapted the Ball-James model. A likely reason for this lack of overlap is the difference in terminology and underlying quantities. Even though, broadly speaking, both theories analyse the transformation from one phase to another, the fundamental quantities in the phenomenological are often direct observables such as the orientation relationships, whereas the Ball-James model is based on the transformation strains. In addition to its success in the prediction of phenomena in materials science, the Ball-James model also motivated a wide range of mathematical research, particularly in the multi-dimensional calculus of variations.

The starting point for much of the work contained in this thesis can be traced back to my first encounter with theories of steels at the International Conference of Martensitic Phase transformations 2014 in Bilbao, Spain. Strolling around the poster presentations I was puzzled that in martensitic steels it seemed customary to distinguish between 24 different (so called Kurdjumov-Sachs) variants. However, from a mathematical point of view, given a cubic parent phase, this could only happen if the product phase had no symmetry, i.e. is triclinic. But in fact, the product phase is either body-centred cubic or tetragonal and thus in either case, one would have at most three distinct variants and not 24.

After many discussions with material scientists, it was clear to me that even though both theories use similar terminology their meanings are often completely different.

Together with my colleague and future collaborator, K. Koumatos, we set out to bridge this gap. Whereas at the start of this process the goal was purely the understanding of the concepts used, it soon occurred to us that with a mathematical approach one may be able to go beyond the description of observed features and create a predictive theory. One of the most striking consequences of this theory was the prediction of a different, and thus controversial, microstructure morphology of low carbon steels. The results, which were presented at the European Conference of Martensitic Phase Transformation 2015, were criticised by the referee as contravening experimental evidence. However, independent experiments in early 2016 suggest that our predictions may have been correct after all. The precise form of our new theory and predictions will be the topic of the final Chapter 7 of this thesis. An important cornerstone towards this theory will be Chapter 6, which establishes the connection between the 24 Kurdjumov-Sachs variants and the transformation strains. Both chapters embody Part II which primarily concerns the modelling of steels. In contrast, Part I concerns the mathematical modelling of martensitic phase transformations in general.

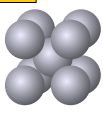
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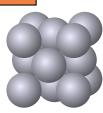
MODELLING MARTENSITIC PHASE TRANSFORMATIONS

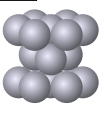
Martensitic phase transformation are a special class of solid-to-solid first order phase transformations in crystalline solids. To make this overview self-contained we will henceforth define each of these terms and clarify further common terminology. Crystalline solids are materials consisting of atoms (or groups of atoms) that are arranged periodically in all three spatial dimensions. This arrangement is then called the (crystalline) *lattice* and one distinguishes between simple and multi-lattices. In a simple lattice all lattice elements are related to each other by multiples of three (linearly independent) lattice vectors, whereas in a multi-lattice, only a fraction of the lattice elements are related to each other in this way. Typical examples of simple lattices are crystals of pure elements and typical examples of multi-lattices are *alloys*, i.e. mixtures of several elements. The smallest possible group of neighbouring atoms that can generate the entire lattice by periodicity is called the *unit cell* of the lattice. As can be seen from Table 0.1 the majority of elements has either a face-centred cubic (fcc), body-centred cubic (bcc) or hexagonal close packed (hcp) lattice structure. A material, such as iron, may have different lattice structures at different temperatures or, more generally, at some other parameter. Each possible

Tab. 0.1. Periodic table with elements highlighted that are solid and have either a body-centred cubic (bcc), face-centred cubic (fcc) or hexagonal close packed (hcp) crystal structure at room temperature (after [Wik16]).

	I	II											III	IV	V	VI	VII	VIII	
1	1 H																	2 He	
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo	
8	119 Un																		
* Lanthanides				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
** Actinides				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

bcc


fcc


hcp


lattice structure of a material is called an *allotrope* or *phase* and a change from one phase to another thus called a *phase transformation*.

A specific class of phase transformation are martensitic phase transformations. There, a high-temperature phase called *austenite* transforms into a low temperature phase called *martensite*. A defining feature is that the transformation is of first order and purely displacive. That is, when reaching a critical temperature the lattice structure changes suddenly (discontinuously) and without diffusion. Usually, the critical temperature is defined as the highest temperature at which the phase transformation from austenite to martensite first takes place and called the *martensite start temperature* (M_S). However, the transformation never completes at one single temperature but rather spans a temperature interval. The highest temperature at which all of the austenite has transformed to martensite is called the *martensite finish temperature* (M_F). Some martensitic transformations, in particular those responsible for the shape-memory effect, are *thermoelastic*, that is, upon heating they transform back to the austenite. Analogously to the martensite start and finish temperatures, the lowest temperature at which martensite transforms back into austenite is the *austenite start temperature* A_S and the lowest temperature at which

all the martensite has transformed back to austenite is known as the *austenite finish temperature* A_F . Without exception, the critical temperatures for the forward and backward transformations are not identical. The difference between the two is called the *thermal hysteresis* and can be regarded as a measure of reversibility. In particular, so-called ultra-low hysteresis materials are able to undergo a very high number of thermic cycles without changing their physical properties.

Commonly, the austenite lattice has higher symmetry than the martensite and the phase transformation is thus symmetry lowering. Because of this loss in symmetry there are several energetically equivalent transformation strains that can transform the austenite to martensite. Each possible choice is called a *martensitic variant*. Figure 0.1 illustrates this concept in the example of a thermoelastic cubic-to-tetragonal transformation. The precise form of the variants is dictated by the requirement that the parent (austenite) lattice needs to be transformed to the product (martensite) lattice. In Chapter 1, we will use this requirement to develop a framework that determines the martensitic variants based on a criterion of minimal atomic movement.

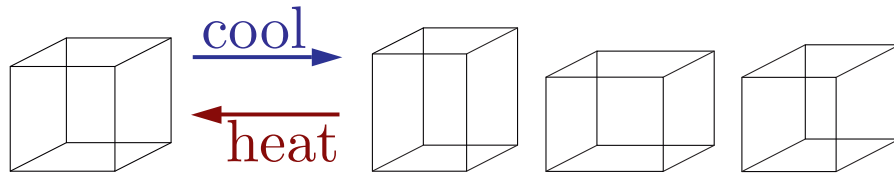


Fig. 0.1. Schematic representation of a thermoelastic, i.e. reversible, martensitic transformation. The cubic austenite (left) transforms into one of three possible tetragonal martensitic variants upon cooling. Each tetragonal variant returns to the single cubic austenite variant upon heating.

These martensitic variants will play an important rôle in the Ball-James model which will be reviewed in Chapter 2. Depending on whether the material is above or below the critical temperature θ_c , the total free energy density W will either be minimal at the austenite or any of the martensite variants. Since there is no energetic reason for a material to prefer one variant or the other, the corresponding energy functional E will turn out to be non-convex. Consequently, one cannot expect to have minimisers but only minimising sequences. On a microscopic scale, these minimising sequences

correspond to complex patterns of co-existing martensitic variants that produce a *microstructure*. On a macroscopic scale, that is by zooming out in experimental terms or by considering the relaxed energy in mathematical terms, the deformation gradients of all possible minimisers form what is known as the quasiconvex hull of the wells. The explicit determination of this hull, in the case of a cubic-to-tetragonal phase transformation, will be the topic of Chapter 3.

In some situations, the martensite can form a microstructure that is macroscopically equivalent to the austenite. This special situation is known as *self-accommodation* and plays an important rôle in the understanding of the shape memory effect. In Chapter 4, we investigate such structures in more detail. We provide bounds on the volume fraction of each contained martensitic variant and give estimates on their minimum complexity. Finally, in Chapter 5 we investigate what happens if the martensite cannot be self-accommodating. In this case, it is impossible to fit martensitic microstructures inside the austenite without introducing strain. We determine the energy cost for such inclusions and by minimising it draw conclusions on their optimal shape.¹

We finish this introduction by stating some preliminary definitions and lemmata that will be essential throughout. Additional notation will be introduced in the respective chapters.

Preliminaries: Function and Matrix Spaces

Throughout, all integrals are taken with respect to the Lebesgue measure $d\lambda$. For the measure of a set Ω we will write $|\Omega| := \lambda(\Omega)$. All functions are to be understood in the usual sense of equivalence classes and their properties are only relevant λ -almost everywhere (a.e.). In particular $\sup$ and $\inf$ are to be understood as ess sup and ess inf and if we consider continuity it will mean that there exists a continuous

¹Within the class of shapes under consideration.

representative in its equivalence class. Further, for functions, $\|\cdot\|$ without subscript, will always mean the L^2 norm and for vectors/matrices, $|\cdot|$ without subscript, will always mean the Euclidean/Frobenius norm.²

Definition 0.1. (L^p - and Sobolev spaces)

Let $1 \leq p < \infty$ and let $\Omega \subset \mathbb{R}^n$ be an open, bounded set with Lipschitz boundary. For a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ we define the norm

$$\|f\|_{p;\Omega} \equiv \|f\|_{L^p(\Omega)} := \left(\int_{\Omega} |f|^p \right)^{\frac{1}{p}}.$$

If $p = \infty$ we define

$$\|f\|_{\infty;\Omega} \equiv \sup_{x \in \Omega} |f(x)| := \inf\{\alpha > 0 : \lambda(\{x \in \Omega : |f(x)| > \alpha\}) = 0\}.$$

We say

$$f \in L^p(\Omega) \iff \|f\|_{p;\Omega} < \infty.$$

If the function $\mathbf{f} = (f_1, \dots, f_n) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is vector valued we say

$$\mathbf{f} \in L^p(\Omega) \iff \|f_i\|_{p;\Omega} < \infty$$

for every component f_i , $i = 1, \dots, n$.

Let $f \in L^p(\Omega)$ and suppose that the (weak) gradient ∇f exists with $\nabla f \in L^p(\Omega)$.

Then we say that $f \in W^{1,p}(\Omega)$. The corresponding norms are given by

$$\begin{aligned} \|f\|_{W^{1,p}(\Omega)} &\equiv \|f\|_{1,p} := \left(\|f\|_p^p + \|\nabla f\|_p^p \right)^{1/p} && \text{for } 1 \leq p < \infty, \\ \|f\|_{W^{1,\infty}(\Omega)} &\equiv \|f\|_{1,\infty} := \max\{\|f\|_{\infty}, \|\nabla f\|_{\infty}\} && \text{for } p = \infty. \end{aligned}$$

If it is clear from the context we may omit the set Ω in the notation. We further define for $1 \leq p < \infty$ the set $W_0^{1,p}$ as the closure of C_0^∞ with respect to $\|\cdot\|_{1,p}$. For $p = \infty$ we define

$$W_0^{1,\infty} := W^{1,\infty} \cap W_0^{1,1}.$$

²Both norms are in fact the same if one identifies $n \times m$ matrices with $n \cdot m$ vectors.

Definition 0.2. (Bounded Radon measures)

We define the set $C_0(\mathbb{R}^n)$ of continuous functions that vanish at infinity by

$$C_0(\mathbb{R}^n) := \{f \in C(\mathbb{R}^n, \mathbb{R}) \mid \lim_{|x| \rightarrow \infty} f(x) \rightarrow 0\}$$

together with the norm inherited from $C(\mathbb{R}^n, \mathbb{R})$, i.e. $\|f\|_\infty := \sup_{x \in \mathbb{R}^n} |f(x)|$. Its dual space is the space $\mathcal{M}(\mathbb{R}^n)$ of bounded Radon measures.

$$\mathcal{M}(\mathbb{R}^n) := (C_0(\mathbb{R}^n))^*$$

and thus the weak convergence of measures in $\{\mu_n\} \subset \mathcal{M}(\mathbb{R}^n)$ is defined by

$$\mu_n \xrightarrow{*} \mu \iff \langle \mu_n, f \rangle \longrightarrow \langle \mu, f \rangle \quad \forall f \in C_0(\mathbb{R}^n),$$

where as usual $\langle \mu, f \rangle := \int_{\mathbb{R}^n} f \, d\mu$. Let $K \subset \mathbb{R}^n$ and $y_i : \Omega \longrightarrow \mathbb{R}$. We will say that $y_i(\cdot) \longrightarrow K$ in measure iff

$$\lim_{i \rightarrow \infty} |\{x \in \Omega : \text{dist}(y_i(x), K) \geq \varepsilon\}| = 0 \text{ for all } \varepsilon > 0.$$

Definition 0.3. (The vector space of matrices over $\mathcal{R}$)

Let $\mathcal{R} \in \{\mathbb{Z}, \mathbb{R}^3\}$. By $\mathcal{R}^{3 \times 3}$ we denote the vector space of 3×3 matrices over $\mathcal{R}$. We define an inner product on $\mathcal{R}^{3 \times 3}$ by $\langle A, B \rangle = \text{Tr}(A^T B)$ and the corresponding norm by

$$|A|^2 = \text{Tr}(A^T A),$$

where $\text{Tr } A = \sum_{i=1}^3 A_{ii}$ denotes the trace and A^T the transpose of A .

Definition 0.4. (Important groups and sets of matrices)

- $\mathcal{R}_{\text{sym}}^{3 \times 3} := \{A \in \mathcal{R}^{3 \times 3} : A^T = A\}$ (Symmetric matrices).
- $\mathcal{R}_+^{3 \times 3} := \mathcal{R}^{3 \times 3} \cap \{\det > 0\}$ (Orientation preserving matrices).
- $\text{GL}(3, \mathcal{R}) := \mathcal{R}^{3 \times 3} \cap \{A \in \mathcal{R}^{3 \times 3} \text{ is invertible}\}$ (General linear group).
- $\text{GL}^+(3, \mathcal{R}) := \text{GL}(3, \mathcal{R}) \cap \mathcal{R}_+^{3 \times 3}$ (Invertible and orientation preserving matrices).

- $\text{SL}(3, \mathbb{Z}) := \text{GL}^+(3, \mathbb{Z}) = \{A \in \mathbb{Z}^{3 \times 3} : \det A = 1\}$ (Special linear group).
- $\text{SO}(3) = \{R \in \mathbb{R}^{3 \times 3} : R^T R = \mathbb{I}, \det R = 1\}$ (Group of proper rotations).

Further, we define the multiplication of a matrix F and a set of matrices $\mathcal{S}$ by $F \cdot \mathcal{S} := \{FS : S \in \mathcal{S}\}$.

Preliminaries: Crystallography

Matrix groups of particular importance in the modelling of martensitic phase-transformations are the symmetry groups of the respective phases. We denote by $\mathcal{P}_a$ and $\mathcal{P}_m$ the symmetry group of the austenite and martensite respectively. One of the most important symmetry groups is the so-called cubic Laue group $\mathcal{P}^{24}$.

Definition 0.5. (Cubic Laue group $\mathcal{P}^{24}$)

The cubic Laue Group $\mathcal{P}^{24} \subset \text{SO}(3)$ is the set of all proper rotations that map a cube, with axes parallel to the standard orthonormal coordinate frame $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, to itself. A list of all elements can be found in Appendix F.

Lemma 0.1. (Characterisation of $\mathcal{P}^{24}$, [PZ02, Ch. 3.2.1])

Let $Q = [-1, 1]^3$ be the cube of side length 2 centred at 0 and define $\mathcal{P}^{24} = \{P \in \text{SO}(3) : PQ = Q\}$. Then $|\mathcal{P}^{24}| = 24$ and $\mathcal{P}^{24} = \text{SO}(3) \cap \text{SL}(3, \mathbb{Z})$.

Proof. Suppose that $P \in \mathcal{P}^{24}$ and let $\{\mathbf{e}_i\}_{i=1,2,3}$ denote the standard basis of $\mathbb{R}^3$. By linearity, P maps the face centres of Q to face centres, i.e. for each $i = 1, 2, 3$ there exists $j \in \{1, 2, 3\}$ such that $P\mathbf{e}_i = \pm\mathbf{e}_j$. Therefore, $P_{ki} = P\mathbf{e}_i \cdot \mathbf{e}_k = \pm\delta_{kj} \in \{-1, 0, 1\}$ and thus $P \in \text{SL}(3, \mathbb{Z})$.

Conversely, if $P \in \text{SO}(3) \cap \text{SL}(3, \mathbb{Z})$, its columns form an orthonormal basis and since P has integer entries the columns have to be in the set $\{\pm\mathbf{e}_i\}_{i=1,2,3}$. Hence, P is of the form

$$P = \sum_{j=1}^3 \pm\mathbf{e}_{k_j} \otimes \mathbf{e}_j$$

and $P\mathbf{e}_i = \pm(\mathbf{e}_i \cdot \mathbf{e}_j)\mathbf{e}_{k_j}$.³ Thus, P maps face centres of Q to face centres and, by linearity, the cube to itself. Further, there are precisely six choices (3×2) for the first column $\pm\mathbf{e}_{k_1}$, four choices (2×2) for $\pm\mathbf{e}_{k_2}$ and two choices for $\pm\mathbf{e}_{k_3}$. Thus, taking into account the determinant constraint, there are 24 elements in $\mathcal{P}^{24}$. $\square$

Remark 0.1. Essentially the same proof can be used to show that $\text{SO}(n) \cap \text{SL}(n, \mathbb{Z}) = \mathcal{P}^{N_n}$, where $\mathcal{P}^{N_n}$ denotes the symmetry group of a n -dimensional cube and $N_n = 2^{n-1}n!$. As before the value of N_n arises from having $2 \times n$ choices for the first column of Q , then $2 \times (n-1)$ choices for the second column of Q , ... and the last column of Q is already fully determined by the determinant constraint.

Definition 0.6. (Crystallographic notation for normals and directions)

Let $a, b, c \in \mathbb{R}$ and $\mathcal{F} = [\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3] \in \text{GL}^+(3, \mathbb{R})$ denote the matrix with columns $\mathbf{f}_i \in S^2 = \{v \in \mathbb{R}^3 : |v| = 1\}$, so that $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ is a (positively oriented) basis of $\mathbb{R}^3$ which we call α . We define the reciprocal basis $\{\mathbf{f}_1^*, \mathbf{f}_2^*, \mathbf{f}_3^*\}$ as the columns of $\mathcal{F}^* = \mathcal{F}^{-\text{T}}$. We write $(a \ b \ c)_\alpha$ to denote a normalised vector in the reciprocal α basis, i.e.

$$(a \ b \ c)_\alpha = \frac{a\mathbf{f}_1^* + b\mathbf{f}_2^* + c\mathbf{f}_3^*}{\sqrt{a^2 + b^2 + c^2}}$$

and we write $[a \ b \ c]$ to denote a normalised vector in the α basis, i.e.

$$[a \ b \ c]_\alpha = \frac{a\mathbf{f}_1 + b\mathbf{f}_2 + c\mathbf{f}_3}{\sqrt{a^2 + b^2 + c^2}}.$$

If $\mathcal{F}$ is an orthonormal basis, $\mathcal{F}$ coincides with $\mathcal{F}^*$. Further, it is common to make the identification $-a = \bar{a}$ and as a convention, whenever there is no index, the vectors are always understood with respect to the standard Euclidean basis. In order to distinguish notations, whenever we want to refer to a regular (non-normalised) vector we write (a, b, c) .

Definition 0.7. (Crystallographic equivalence)

Given a direction $[a \ b \ c]$ we denote by $\langle a \ b \ c \rangle$ the set of crystallographically equivalent directions, i.e. $\langle a \ b \ c \rangle = \mathcal{P} \cdot [a \ b \ c]$, and by $\{a \ b \ c\}$ we denote the set of crystallograph-

³Recall that $\mathbf{a} \otimes \mathbf{b}$ denotes the 3×3 matrix with components $(\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j$.

ically equivalent normals, i.e. $\{a\,b\,c\} = \mathcal{P}.(a\,b\,c)$, where $\mathcal{P}$ denotes the symmetry group of the crystal lattice.

Optimality of General Lattice Transformations

A key quantity in the modelling of martensitic phase transformations is the knowledge of the transformation strains, i.e. of the linear transformations that map the austenite lattice to the martensite lattice. In this chapter, we develop a general framework that, based on criteria of minimal atom movement, determines the (optimal) linear transformation strain(s) between any two Bravais lattices. Apart from an existence proof of such an optimal transformation, a precise algorithm together with a GUI (Graphical User Interface) to determine these optimal transformations is provided. An important application of this theory is a rigorous proof of a conjecture by E.C. Bain in 1924 on the optimality of the so-called *Bain strain* in the face-centred cubic to body-centred cubic transformation observed in steels. Further applications include the face-centred cubic to body-centred tetragonal transition as well as the transformation between two triclinic phases of terephthalic acid. The results presented in this chapter have been published in [KM16b].

1.1 Background

In his seminal article on ‘The nature of martensite’ [Bai24] Bain proposed a mechanism that transforms the face-centred cubic (fcc) lattice to the body-centred cubic (bcc) lattice, a phase transformation most importantly manifested in low carbon steels. He writes:

“It is reasonable, also, that the atoms themselves will rearrange [...] by a method that will require least temporary motion. [...] A mode of atomic shift requiring minimum motion was conceived by the author [...]”.

Bain, 1924

The key observation that led to his famous correspondence was that *“If one regards the centers of faces as corners of a new unit, a body-centered structure is already at hand; however, it is tetragonal instead of cubic”*. He remarks that this is not surprising *“as it is the only easy method of constructing a bcc atomic structure from the fcc atomic structure”*.

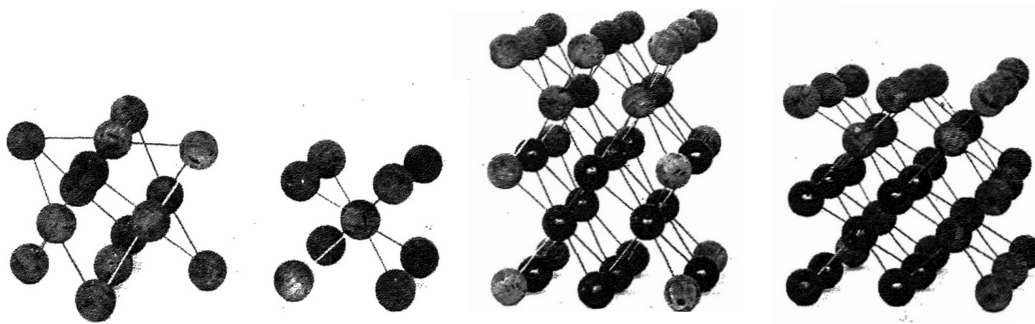


Fig. 1.1. From E.C. Bain: the small models (left) show the face-centred cubic (fcc) and body-centred cubic (bcc) unit cells; the large models (right) represent 35 atoms in an fcc and bcc arrangement respectively.

Even though now widely accepted, his mechanism, which he illustrated with a model made of cork balls and needles (see Fig. 1.1), was not without criticism from his contemporaries. In their fundamental paper Kurdjumov & Sachs [KS30] wrote [free translation from German] that “nothing certain about the mechanism of the martensite transformation is known. Bain imagines that a tetragonal unit cell within the fcc lattice transforms into a bcc unit cell through compression along one direction and expansion along the two other. However, a proof of this hypothesis is still missing”.¹ Interestingly, without being aware of it, the authors implicitly used the Bain mechanism in their derivation of the Kurdjumov-Sachs orientation relationships (see Appendix A for a step-by-step analysis of the original construction).

¹“Über den Mechanismus dieser „Martensitumwandlung“ ist bisher nichts Sicheres bekannt. Bain stellt sich vor, daß eine tetragonalkörperzentrierte Elementarzelle des Austenits durch Schrumpfung in der einen Richtung und Ausdehnung in den beiden anderen in die kubischraumzentrierte des α -Eisens übergeht. Eine Bestätigung für diese Anschauung konnte bisher nicht erbracht werden.”

In subsequent years, the determination of the transformation mechanism remained of great interest. In their paper on ‘Atomic Displacements in the Austenite-Martensite Transformation’ [JW48] Jaswon and Wheeler again acknowledged that

“Of all the possible distortions of a primitive unit cell of the face-centred cubic structure, which could generate a body-centred cubic structure of the given relative orientation, the one which actually occurs is the smallest”.

Jaswon and Wheeler, 1948

By combining it with experimental observations of the orientation relationships they devised an algorithm to derive the strain tensor. However, their approach is only applicable to cases where the orientation relationship is known a-priori.

With the years passing and a number of supporting experimental results (for a discussion see e.g. [BW72]) the Bain mechanism rose from a conjecture to a widely accepted fact. Nevertheless, almost a century after Bain first announced his correspondence a rigorous proof based on the assumption of minimal atom movement has been missing. Of course, the transformation from fcc to bcc is not the only instance where the determination of the transformation strain is of interest. The overall question remains the same: which transformation strain(s), out of all the possible deformations mapping the lattice of the parent phase to the lattice of the product phase, require(s) the least atomic movement?

To provide a definite answer to this question one first needs to quantify the notion of least atomic movement in such a way that it does not require additional input from experiments. Then one needs to establish a framework that singles out the optimal transformation among the infinite number of possible lattice transformation strains. One way to appropriately quantify least atomic movement is the criterion of smallest principal strains as suggested by Lomer [Lom55]. In his paper, Lomer compared 1600 different lattice correspondences for the β - to α -phase transition in Uranium and concluded that only one of them involved strains of less than 10%. More recently, in

[Che+16] an algorithm is proposed to determine the transformation strain based on a similar minimality criterion (see Remark 1.5) that also allows for the consideration of different sublattices.

In the present work, a criterion of least atomic movement in terms of a family of different strain measures is considered. For each such strain measure, we rigorously prove the existence of an optimal lattice transformation between *any* two Bravais lattices.² As a main application, it is shown that the Bain strain is the optimal lattice transformation from fcc to bcc with respect to three of the most commonly used strain measures.

1.2 Mathematics of Lattices

Before we turn towards the formal definition of lattices we recall some features of matrix norms.

Definition 1.1. (Matrix norms)

For a given matrix $A \in \mathbb{R}^{3 \times 3}$ we define the following norms

- *Frobenius norm:*

$$|A| = \sqrt{\text{Tr}(A^T A)} = \sqrt{\sum_{i,j=1}^3 A_{ij}^2}.$$

- *Spectral norm:*

$$|A|_2 = \sup_{|x|=1} |Ax| = \sqrt{\max_{i=1,2,3} \lambda_i(A^T A)} = \max_{i=1,2,3} \nu_i(A),$$

where for $i = 1, 2, 3$, $\nu_i(A)$ are the principal stretches/singular values of A and $\lambda_i(A^T A)$ are the eigenvalues of $A^T A$.

²In particular, no assumptions are made on the type of lattice points (e.g. atoms, molecules) or on the relation between the point groups of the two lattices.

- *Column max norm:*

$$\|A\|_{2,\infty} = \max_{i=1,2,3} |A\mathbf{e}_i| = \max_{i=1,2,3} |\mathbf{a}_i|,$$

where $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ are the columns of A .

Additionally, we will henceforth write $\text{col}[A] := \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ to denote the columns of a matrix A and then write $A = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]$.

The proofs of the following statements are elementary and can be found in standard textbooks on linear algebra (see e.g. [Gen07]).

Lemma 1.1. (*Properties of matrix norms*)

Both the Frobenius norm and the spectral norm are unitarily equivalent, that is

$$|RAS| = |A| \tag{1.1}$$

for any $R, S \in \text{SO}(3)$. Further both norms are sub-multiplicative, that is given $A, B, C \in \mathbb{R}^{3 \times 3}$ then $|ABC| \leq |A||B||C|$ and thus in particular if $|A||C| \neq 0$ then

$$|B| \geq \frac{|ABC|}{|A||C|}. \tag{1.2}$$

Further the spectral norm is compatible with the Euclidean norm on $\mathbb{R}^3$, that is

$$|Ax| \leq |A|_2 |x|. \tag{1.3}$$

We also define the following sets of matrices that will be of particular importance for the quantitative determination of optimal lattice transformations.

Definition 1.2. ($\text{SL}^k(3, \mathbb{Z})$)

For $k \in \mathbb{N}$ define

$$\text{SL}^k(3, \mathbb{Z}) := \{A \in \text{SL}(3, \mathbb{Z}) : |A_{mn}| \leq k \text{ for all } m, n \in \{1, 2, 3\}\}$$

and

$$\mathrm{SL}^{-k}(3, \mathbb{Z}) := \{A \in \mathrm{SL}(3, \mathbb{Z}) : |(A^{-1})_{mn}| \leq k \text{ for all } m, n \in \{1, 2, 3\}\}.$$

Clearly $\mathrm{SL}^j(3, \mathbb{Z}) \subset \mathrm{SL}^k(3, \mathbb{Z})$ for all $0 \leq j \leq k$ and $|\mathrm{SL}^{-k}(3, \mathbb{Z})| = |\mathrm{SL}^k(3, \mathbb{Z})|$ for all $k \in \mathbb{Z}$. For example we have $|\mathrm{SL}^1(3, \mathbb{Z})| = 3\,480$, $|\mathrm{SL}^2(3, \mathbb{Z})| = 67\,704$, $|\mathrm{SL}^3(3, \mathbb{Z})| = 640\,824$, $|\mathrm{SL}^4(3, \mathbb{Z})| = 2\,597\,208$, $|\mathrm{SL}^5(3, \mathbb{Z})| = 10\,460\,024$ and $|\mathrm{SL}^6(3, \mathbb{Z})| = 28\,940\,280$.

Next, we introduce the notion of (simple) Bravais lattices and define them in a slightly different way than commonly found in the literature (see e.g. [Bha03, Ch. 3]). This definition will turn out to simplify the forthcoming analysis.

Definition 1.3. (Bravais lattice)

Let $F = [\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3] \in \mathrm{GL}^+(3, \mathbb{R})$, where $\mathrm{col}[F] = \{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ are the columns of F . We define the *Bravais lattice* $\mathcal{L}(F)$ generated by F as the lattice generated by $\mathrm{col}[F]$, i.e.

$$\mathcal{L}(F) := \mathrm{col}[F \cdot \mathbb{Z}_+^{3 \times 3}].$$

Thus, by definition, a Bravais lattice is $\mathrm{span}_{\mathbb{Z}}\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ together with an orientation.

Henceforth, we always assume that both the parent and product lattices are (simple) Bravais lattices.

Definition 1.4. (Primitive, base-, body- and face-centred unit cells)

Let $\mathcal{L} = \mathcal{L}(F)$ be generated by $F \in \mathrm{GL}^+(3, \mathbb{R})$. We call the parallelepiped spanned by $\mathrm{col}[F]$ with one atom at each vertex a *primitive unit cell* of the lattice. We call a primitive unit cell with additional atoms in the centre of the bases a *base-centred* unit cell, we call a primitive unit cell with one additional atom in the body centre a *body-centred* (bc) unit cell and we call a primitive unit cell with additional atoms in the centre of each of the faces a *face-centred* (fc) unit cell.

Remark 1.1. For any lattice generated by a base-, body- or face-centred unit cell there is a primitive unit cell that generates the same lattice. The following table gives

the lattice vectors that generate the equivalent primitive unit cell for a given base-centred (C), body-centred (I) or face-centred (F) unit cell spanned by the vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c}) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3$. For our purposes all unit cells that generate the same lattice

Tab. 1.1. Lattice vectors of a primitive unit cell that generates the same lattice. For example, if one has a base-centred unit cell along the standard Euclidean basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, the primitive unit cell with lattice vectors $\{\frac{\mathbf{e}_1 - \mathbf{e}_2}{2}, \frac{\mathbf{e}_1 + \mathbf{e}_2}{2}, \mathbf{e}_3\}$ generates the same lattice.

primitive (P)	base-centred (C)	body-centred (I)	face-centred (F)
$\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$	$\{\frac{\mathbf{a}-\mathbf{b}}{2}, \frac{\mathbf{a}+\mathbf{b}}{2}, \mathbf{c}\}$	$\{\frac{-\mathbf{a}+\mathbf{b}+\mathbf{c}}{2}, \frac{\mathbf{a}-\mathbf{b}+\mathbf{c}}{2}, \frac{\mathbf{a}+\mathbf{b}-\mathbf{c}}{2}\}$	$\{\frac{\mathbf{b}+\mathbf{c}}{2}, \frac{\mathbf{a}+\mathbf{c}}{2}, \frac{\mathbf{a}+\mathbf{b}}{2}\}$

are equivalent and in order to keep the presentation as simple as possible we will always work with the primitive description of a lattice. However, we note that often in the literature the unit cell is chosen such that it has maximal symmetry.

For example for a face-centred cubic lattice, the unit cell would be chosen as face-centred and spanned by $\text{col}[\mathbb{I}] = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ so that it has the maximal $\mathcal{P}^{24}$ symmetry. However, if one considers primitive unit cells that span the same fcc lattice, the one with maximal symmetry is given by the last entry in Table 1.1 and thus spanned by $\text{col}[F]$, where

$$F = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

and has only 6-fold symmetry.

Lemma 1.2. (Identical lattice bases, [Bha03, Result 3.1])

Let $\mathcal{L}(F)$ be generated by $F = [\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3]$ and $\mathcal{L}(G)$ be generated by $G = [\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3]$.

Then

$$\mathcal{L}(F) = \mathcal{L}(G) \Leftrightarrow G = F\mu \Leftrightarrow \mathbf{g}_i = \sum_{j=1}^3 \mu_{ji} \mathbf{f}_j,$$

for some $\mu \in \text{SL}(3, \mathbb{Z})$. The same result holds for a face-, base- and body-centred unit cell.

Given two distinct Bravais lattices it is natural to ask how one can transform one lattice into the other. We will call this process a *lattice transformation* and we will always assume that this transformation is homogeneous (i.e. linear).

Definition 1.5. (Lattice transformation)

Given two lattices $\mathcal{L}_0 = \mathcal{L}(F)$ and $\mathcal{L}_1 = \mathcal{L}(G)$ generated by $F, G \in \text{GL}^+(3, \mathbb{R})$ we call any matrix $H \in \text{GL}^+(3, \mathbb{R})$ such that $H \cdot \mathcal{L}_0 = \mathcal{L}_1$ a *lattice transformation* from $\mathcal{L}_0$ to $\mathcal{L}_1$.

Remark 1.2. In the terminology of Ericksen (see e.g. [PZ02, p. 62ff.]), if $\mathcal{L}_0 = \mathcal{L}_1$ (i.e. $G = F\mu$), the matrices H in Definition 1.5 are precisely all the orientation preserving elements in the *global symmetry group* of F . Additionally, the matrices H that are also rotations constitute the *point group* of the lattice. We point out that, in this terminology, $\mathcal{P}^{24}$ is the point group of any cubic lattice.

We end this section by defining the atom density of the lattice $\mathcal{L}(F)$ and relating it to the determinant of F .

Definition 1.6. (Atom density)

For a given lattice $\mathcal{L}$ we define the atom density $\rho(\mathcal{L})$ by

$$\rho(\mathcal{L}) := \lim_{N \rightarrow \infty} \frac{\#\{Q_N \cap \mathcal{L}\}}{N^3},$$

where $Q_N = [0, N]^3$ is the cube with side-length N and $\#$ counts the number of elements in a discrete set. Thus $\rho(\mathcal{L})$ is the average number of atoms per unit volume.

Lemma 1.3. Let $\mathcal{L} = \mathcal{L}(F)$ be generated by $F \in \text{GL}^+(3, \mathbb{R})$ then

$$\rho(\mathcal{L}) = \frac{1}{\det F}.$$

In particular a transformation $H = GF^{-1}$ from $\mathcal{L}_0 = \mathcal{L}(F)$ to $\mathcal{L}_1 = \mathcal{L}(G)$ does not change the atom density if and only if it is volume preserving, i.e. $\det H = 1$. Further the atom density is well defined.

Proof. Denote by $\mathcal{U} \subset \mathbb{R}^3$ the unit cell spanned by $\text{col}[F]$, so that the volume of $\mathcal{U}$ is given by $|\mathcal{U}| = \det F$. Taking n distinct points $x_i \in \mathcal{L}$ we find that $|\bigcup_{i=1}^n (x_i + \mathcal{U})| = n \det F$ since all elements are disjoint (up to zero measure). Let l denote the side length of the smallest cube that contains $\mathcal{U}$. Further, as in Definition 1.6, let $Q_N = [0, N]^3$ denote a cube of side-length N and define $Q_N^\pm = [\mp 2l, N \pm 2l]^3$. Then

$$Q_N^- \subset \bigcup_{x \in \mathcal{L} \cap Q_N} (x + \mathcal{U}) \subset Q_N^+$$

and thus by taking the volumes of the sets we obtain

$$(N - 4l)^3 \leq \#\{Q_N \cap \mathcal{L}\} \det F \leq (N + 4l)^3.$$

Dividing by N^3 and taking the limit $N \rightarrow \infty$ yields the result. Since this limit exists for all sequences $N \rightarrow \infty$ the density is well defined. $\square$

1.3 Metrics and Equivalence Relations on Matrices and Lattices

Before defining an equivalence relation on matrices and lattices we recall the definitions of a (pseudo-)metric.

Definition 1.7. (Pseudometric and metric)

Let X be a vector space and $x, y, z \in X$. A map $d : X \times X \rightarrow [0, \infty)$ is a *pseudometric* if

1. $d(x, x) = 0$,
2. $d(x, y) = d(y, x)$ (*symmetry*),
3. $d(x, z) \leq d(x, y) + d(y, z)$ (*triangle inequality*).

If in addition d is positive definite, i.e. $d(x, y) = 0 \Leftrightarrow x = y$, we call d a *metric*.

Definition 1.8. (Equivalent matrices and lattices)

We define an equivalence relation $\sim$ between matrices F, G in $\text{GL}^+(3, \mathbb{R})$ by

$$F \sim G :\Leftrightarrow \exists R \in \text{SO}(3) : G = RF,$$

so that the equivalence class $[F]$ of F is given by $[F] = \{G \in \mathbb{R}_+^{3 \times 3} : F \sim G\}$. We denote the quotient space, i.e. the space of all equivalence classes, by

$$\overline{\text{GL}^+(3, \mathbb{R})} := \{[F] : F \in \text{GL}^+(3, \mathbb{R})\}.$$

Furthermore, we define an equivalence relation $\sim$ between two lattices $\mathcal{L}_0$ and $\mathcal{L}_1$ by

$$\mathcal{L}_0 \sim \mathcal{L}_1 :\Leftrightarrow \exists R \in \text{SO}(3) : \mathcal{L}_1 = R.\mathcal{L}_0.$$

We are now in a position to define a metric on the quotient spaces.

Lemma and Definition 1.9. (Induced metric)

Any pseudometric $d : \text{GL}^+(3, \mathbb{R}) \times \text{GL}^+(3, \mathbb{R}) \rightarrow [0, \infty)$ with the property

$$d(F, G) = 0 \Leftrightarrow G = T^*F \text{ for some } T^* \in \text{SO}(3) \quad (*)$$

naturally induces a metric $\bar{d}$ on $\overline{\text{GL}^+(3, \mathbb{R})}$ via

$$\bar{d}([F], [G]) = \min_{R, S \in \text{SO}(3)} d(RF, SG).$$

Proof. The quantity $\bar{d}$ is clearly well defined, so that in particular $\bar{d}([F], [G]) = \bar{d}(F, G)$ and we may henceforth drop the $[\cdot]$ in the arguments of $\bar{d}$. We first show that $\bar{d}$ is a metric on $\overline{\text{GL}^+(3, \mathbb{R})}$. Positivity and symmetry are obvious from the definition. For definiteness note that if $\min_{R, S \in \text{SO}(3)} d(RF, SG) = 0$ then by $(*)$ we

have $S^*G = T^*R^*F$ for some $R^*, S^*, T^* \in \text{SO}(3)$ and thus $F \sim G$. It remains to show the triangle inequality. We have

$$\begin{aligned}
\bar{d}(F, H) &= \min_{R, S \in \text{SO}(3)} d(RF, SH) \\
&\leq \min_{R, S} (d(RF, G) + d(G, SH)) \\
&\leq \min_{R, S'} (d(RF, S'G) + \cancel{d(G, S'G)}) + \min_{R', S} (d(SH, R'G) + \cancel{d(G, R'G)}) \\
&= \bar{d}(F, G) + \bar{d}(G, H),
\end{aligned}$$

where we have used the triangle inequality, symmetry of d and $(*)$. $\square$

Example 1.1. The family of maps $d_r : \text{GL}^+(3, \mathbb{R}) \times \text{GL}^+(3, \mathbb{R}) \rightarrow [0, \infty)$, $r \in \mathbb{R} \setminus \{0\}$ given by

$$d_r(F, G) = |(F^T F)^{r/2} - (G^T G)^{r/2}|$$

are pseudometrics such that $(*)$ holds. In particular, each of them induces a metric $\bar{d}_r$ on the quotient space $\overline{\text{GL}^+(3, \mathbb{R})}$.

Proof. Positivity is obvious. The triangle inequality follows from the corresponding property of the Frobenius norm, i.e.

$$\begin{aligned}
d_r(F, H) &= |(F^T F)^{r/2} - (H^T H)^{r/2}| \\
&\leq |(F^T F)^{r/2} - (G^T G)^{r/2}| + |(G^T G)^{r/2} - (H^T H)^{r/2}| = d_r(F, G) + d_r(G, H)
\end{aligned}$$

and the property $(*)$ follows from

$$\begin{aligned}
d_r(F, G) = 0 &\Leftrightarrow (F^T F)^{r/2} = (G^T G)^{r/2} \Leftrightarrow (FG^{-1})^T (FG^{-1}) = \mathbb{I} \\
&\Leftrightarrow FG^{-1} \in \text{SO}(3) \Leftrightarrow F = T^*G \text{ for some } T^* \in \text{SO}(3).
\end{aligned}$$

$\square$

Remark 1.3. The metric d_2 has previously been used in [Bha03, Chapter 3], where it was defined as the distance between the metric $C_F = F^T F = (\mathbf{f}_i \cdot \mathbf{f}_j)_{ij}$ of a set of

lattice vectors $\text{col}[F] = \{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ and the metric $C_G = G^T G = (\mathbf{g}_i \cdot \mathbf{g}_j)_{ij}$ of a set of lattice vectors $\text{col}[G] = \{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$. The use of the term metric in [Bha03] is not to be confused with our use of metric.

1.4 Optimal Lattice Transformations

This section embodies the main part of the chapter. We first establish what we mean by an optimal transformation from one lattice to another and then, for a family of such criteria, show the existence of optimal transformations between any two Bravais lattices.

Lemma 1.4. *Let $\mathcal{L}_0 = \mathcal{L}(F)$ and $\mathcal{L}_1 = \mathcal{L}(G)$ be generated by $F, G \in \text{GL}^+(3, \mathbb{R})$. Then all possible lattice transformations from $\mathcal{L}_0$ to $\mathcal{L}_1$ are given by $H_\mu = G\mu F^{-1}$, $\mu \in \text{SL}(3, \mathbb{Z})$. In particular, the lattices coincide if and only if there exists $\mu \in \text{SL}(3, \mathbb{Z})$ such that $G\mu F^{-1} = \mathbb{I}$ and they are equivalent, i.e. $\mathcal{L}_0 \sim \mathcal{L}_1$, if and only if there exists $\mu \in \text{SL}(3, \mathbb{Z})$ such that $G\mu F^{-1} \in \text{SO}(3)$.*

Proof. Let $H_\mu = G\mu F^{-1}$, $\mu \in \text{SL}(3, \mathbb{Z})$. Then

$$\begin{aligned} H_\mu \cdot \mathcal{L}_0 &= H_\mu \cdot \mathcal{L}(F) = H_\mu \cdot \text{col}[F \cdot \mathbb{Z}_+^{3 \times 3}] = \text{col}[H_\mu F \cdot \mathbb{Z}_+^{3 \times 3}] \\ &= \text{col}[G\mu F^{-1} F \cdot \mathbb{Z}_+^{3 \times 3}] = \text{col}[G\mu \cdot \mathbb{Z}_+^{3 \times 3}] = \text{col}[G \cdot \mathbb{Z}_+^{3 \times 3}] = \mathcal{L}_1, \end{aligned}$$

where we used that μ is invertible over $\mathbb{Z}$, so that $\mu \cdot \mathbb{Z}_+^{3 \times 3} = \mathbb{Z}_+^{3 \times 3}$. Thus H_μ is a lattice transformation from $\mathcal{L}_0$ to $\mathcal{L}_1$. For the reverse direction we know by Lemma 1.2 that $\mathcal{L}(F) = \mathcal{L}(F')$ if and only if $F' = F\mu'$, $\mu' \in \text{SL}(3, \mathbb{Z})$ and $\mathcal{L}(G) = \mathcal{L}(G')$ if and only if $G' = G\mu''$, $\mu'' \in \text{SL}(3, \mathbb{Z})$. Therefore, all possible generators for $\mathcal{L}_0$ are given by $F\mu'$, $\mu' \in \text{SL}(3, \mathbb{Z})$ and all possible generators for $\mathcal{L}_1$ are given by $G\mu''$, $\mu'' \in \text{SL}(3, \mathbb{Z})$. Thus any lattice transformation from $\mathcal{L}_0$ to $\mathcal{L}_1$ is given by

$$H_{\mu'}^{\mu''} = G\mu''\mu'^{-1}F^{-1}, \quad \mu', \mu'' \in \text{SL}(3, \mathbb{Z}).$$

But by the group property we may set $H_\mu := H_{\mu'}^{\mu''}$ with $\mu = \mu''\mu'^{-1} \in \text{SL}(3, \mathbb{Z})$. $\square$

Definition 1.10. (*d*-optimal lattice transformations)

Given two lattices $\mathcal{L}_0 = \mathcal{L}(F)$ and $\mathcal{L}_1 = \mathcal{L}(G)$ with $F, G \in \text{GL}^+(3, \mathbb{R})$ and a metric d , we call a lattice transformation $H_\mu = G\mu F^{-1}$, $\mu \in \text{SL}(3, \mathbb{Z})$ (cf. Lemma 1.4) *d*-optimal if it minimises the distance to $\mathbb{I}$ with respect to d , i.e. $H_{\min} = G\mu_{\min}F^{-1}$, where

$$\mu_{\min} = \arg \min_{\mu \in \text{SL}(3, \mathbb{Z})} d(H_\mu, \mathbb{I}). \quad (1.4)$$

If d is a pseudometric satisfying (*), we call a transformation *d*-optimal if it is optimal with respect to the induced metric $\bar{d}$ on the quotient space $\overline{\text{GL}^+(3, \mathbb{R})}$, i.e. the *d*-optimal transformation is the one that is *d*-closest to being a pure rotation and maps $\mathcal{L}_0$ to a lattice in the equivalence class $[\mathcal{L}_1] := \{\mathcal{L} : \mathcal{L} \sim \mathcal{L}_1\}$ of $\mathcal{L}_1$.

Example 1.2. For the pseudometrics d_r from Example 1.1 the explicit expressions for the distance in (1.4) read

$$d_r(H, \mathbb{I}) = |(H^T H)^{r/2} - \mathbb{I}| = \left(\sum_{i=1}^3 (\nu_i^r - 1)^2 \right)^{1/2}, \quad (1.5)$$

where ν_i , $i = 1, 2, 3$ are the principal stretches/singular values of H . The quantities $(H^T H)^{r/2} - \mathbb{I}$ are clearly measures of principal strain and are known as the Doyle-Ericksen strain tensors (see [DE56, p. 65]). For $r = 1$, it is simple to verify that

$$d_1(H, \mathbb{I}) = \text{dist}(H, \text{SO}(3)) = \min_{R \in \text{SO}(3)} |H - R|.$$

Remark 1.4. For a general metric d as in Definition 1.10, the optimal transformation $H_{\min}$ between $\mathcal{L}(F)$ and $\mathcal{L}(G)$ is unchanged under actions of the point groups of both lattices, i.e.

$$H_{\min} = G \arg \min_{\mu \in \text{SL}(3, \mathbb{Z})} d(G\mu F^{-1}, \mathbb{I}) F^{-1} = (PG) \arg \min_{\mu \in \text{SL}(3, \mathbb{Z})} d((PG)\mu(QF)^{-1}, \mathbb{I})(QF)^{-1}$$

for any P in the point group of $\mathcal{L}(G)$ and Q in the point group of $\mathcal{L}(F)$. If one considers pseudometrics satisfying (*) the notion of optimality is not only invariant

under actions of the respective point groups but also under rigid body rotations of the product lattice. Thus Definition 1.10 returns an equivalence class $[H_{\min}] \in \overline{\text{GL}^+(3, \mathbb{R})}$ of d -optimal transformations. By the polar decomposition theorem we may, and henceforth always will, pick the symmetric representative

$$\bar{H}_{\min} := \sqrt{H_{\min}^T H_{\min}} \in \mathbb{R}_{\text{sym}}^{3 \times 3},$$

i.e. the pure *stretch component* of the transformation $H_{\min}$. Note that in general the set of minimising equivalence classes $\{[H_{\min}] : H_{\min} \text{ is } d\text{-optimal}\}$ may contain more than one element. In such a case, different regions of the parent lattice may transform according to any of these optimal strains, giving rise to e.g. twinning (cf. Chapter 2).

The pseudometrics d_r are additionally invariant under rotations from the right, i.e. $d_r(H, \mathbb{I}) = d_r(HS, \mathbb{I})$ for all $S \in \text{SO}(3)$. For any such pseudometric, a rigid body rotation R of the parent lattice $\mathcal{L}_0$ results in an optimal transformation with stretch component $R\bar{H}_{\min}R^T$, where $\bar{H}_{\min}$ is the stretch component of the optimal transformation from $\mathcal{L}_0$ to $[\mathcal{L}_1]$. Note that $R\bar{H}_{\min}R^T$ is simply $\bar{H}_{\min}$ expressed in a different basis and in particular, even though the coordinate representation is different, the underlying transformation mechanism is unchanged.

Our main theorem says that a d_r -optimal lattice transformation always exists and the following lemma will be the crucial tool in the proof.

Key Lemma 1.5. *Let H be a lattice transformation from $\mathcal{L}_0 = \mathcal{L}(F)$ to $\mathcal{L}_1 = \mathcal{L}(G)$ and consider a lattice vector $\mathbf{f} \in \mathcal{L}_0$ that is transformed by H to $\mathbf{g} = H\mathbf{f}$. Then*

$$\nu_{\max}(H) \geq |\mathbf{g}|/|\mathbf{f}| \geq \nu_{\min}(H),$$

where $\nu_{\min}(H)$, $\nu_{\max}(H)$ denote, respectively, the smallest and largest principal stretches/singular values of H . In particular for any $s > 0$,

$$d_s(H, \mathbb{I}) = \left(\sum_{i=1}^3 (\nu_i^s - 1)^2 \right)^{1/2} \geq \max_i \frac{|H\mathbf{f}_i|^s}{|\mathbf{f}_i|^s} - 1, \quad (1.6)$$

$$d_{-s}(H, \mathbb{I}) = \left(\sum_{i=1}^3 (\nu_i^{-s} - 1)^2 \right)^{1/2} \geq \max_i \frac{|H^{-1}\mathbf{g}_i|^s}{|\mathbf{g}_i|^s} - 1, \quad (1.7)$$

where $\text{col}[F] = \{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ and $\text{col}[G] = \{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$.

Proof. Consider the singular value decomposition of $H = UDV$, where $D = \text{diag}(\nu_1, \nu_2, \nu_3)$ and $U, V \in \text{SO}(3)$. Then

$$|\mathbf{g}| = |UDV\mathbf{f}| = |DV\mathbf{f}| \leq \max_i \nu_i(H) |V\mathbf{f}| = \nu_{\max}(H) |\mathbf{f}|$$

and analogously for the lower bound. □

Theorem 1.1. *Given two lattices $\mathcal{L}_0 = \mathcal{L}(F)$ and $\mathcal{L}_1 = \mathcal{L}(G)$ generated by $F, G \in \text{GL}^+(3, \mathbb{R})$ respectively, there exists a d_r -optimal lattice transformation $H_{\mu_{\min}} = G\mu_{\min}F^{-1}$, for any $r \in \mathbb{R} \setminus \{0\}$. For $s > 0$ all optimal changes of basis are contained in the finite compact sets*

$$d_s : \left\{ \mu \in \text{SL}(3, \mathbb{Z}) : \|\mu\|_{2,\infty}^s \leq \frac{\|F\|_{2,\infty}^s}{\nu_{\min}^s(G)} (m_s^0 + 1) \right\}, \quad (1.8)$$

$$d_{-s} : \left\{ \mu \in \text{SL}(3, \mathbb{Z}) : \|\mu^{-1}\|_{2,\infty}^s \leq \frac{\|G\|_{2,\infty}^s}{\nu_{\min}^s(F)} (m_{-s}^0 + 1) \right\}, \quad (1.9)$$

where $\nu_{\min}(A)$ denotes the smallest principal stretch/singular value of A and

$$m_r^0 := d_r(H_{\mathbb{I}}, \mathbb{I}) = d_r(GF^{-1}, \mathbb{I}).$$

Proof. As the minimisation is over the discrete set $\text{SL}(3, \mathbb{Z})$ it suffices to show that the minimum is attained in a (compact) finite subset of $\text{SL}(3, \mathbb{Z})$ given by (1.8) and

(1.9). Let $H_\mu = G\mu F^{-1}$, $\mu \in \text{SL}(3, \mathbb{Z})$ be a lattice transformation from $\mathcal{L}_0 = \mathcal{L}(F)$ to $\mathcal{L}_1 = \mathcal{L}(G)$. Then, letting $\{\mathbf{e}_i\}_{i=1,2,3}$ denote the standard basis vectors of $\mathbb{R}^{3 \times 3}$,

$$H_\mu \mathbf{f}_i = G\mu F^{-1} F \mathbf{e}_i = G\mu \mathbf{e}_i \text{ and } H_\mu^{-1} \mathbf{g}_i = F\mu^{-1} G^{-1} G \mathbf{e}_i = F\mu^{-1} \mathbf{e}_i$$

and thus, by using the Key Lemma 1.5 and (1.3), we obtain

$$\begin{aligned} d_s(H_\mu, \mathbb{I}) &\geq \max_i \frac{|G\mu \mathbf{e}_i|^s}{|\mathbf{f}_i|^s} - 1 \geq \frac{\|\mu\|_{2,\infty}^s}{|G^{-1}|_2^s \|F\|_{2,\infty}^s} - 1 = \frac{\nu_{\min}^s(G) \|\mu\|_{2,\infty}^s}{\|F\|_{2,\infty}^s} - 1, \\ d_{-s}(H_\mu, \mathbb{I}) &\geq \max_i \frac{|F\mu^{-1} \mathbf{e}_i|^s}{|\mathbf{g}_i|^s} - 1 \geq \frac{\|\mu^{-1}\|_{2,\infty}^s}{|F^{-1}|_2^s \|G\|_{2,\infty}^s} - 1 = \frac{\nu_{\min}^s(F) \|\mu^{-1}\|_{2,\infty}^s}{\|G\|_{2,\infty}^s} - 1, \end{aligned}$$

where in the equality we have used that $\{\nu_i(A^{-1})\}_{i=1,2,3} = \{(\nu_i(A))^{-1}\}_{i=1,2,3}$. Thus $d_r(H_\mu, \mathbb{I}) > d_r(H_\mathbb{I}, \mathbb{I})$ for all μ in the complement of the respective sets given by (1.8) and (1.9) and therefore H_μ cannot be d_r -optimal. $\square$

Remark 1.5. The distance $d_1(H, \mathbb{I})$ seems to be the most natural candidate to determine the transformation requiring least atomic movement. The quantities $\nu_i - 1$ measure precisely the displacement along the principal axes and thus their use is in line with the criterion of smallest principal strains as in e.g. [Bha01], [BW72] and [Lom55].

The distance $d_2(H, \mathbb{I})$ seems natural from a mathematical perspective as the tensor $H^T H$ corresponds to the flat metric induced by the deformation H . Even though motivated through different norms, the quantity $d_2(H, \mathbb{I})$ has also been used in [BJ92, Theorem 2.4] (see also [Eri80] and [Pit84]) to define the Ericksen-Pitteri neighbourhood of a lattice generating matrix. Since the notation is different we will outline the correspondence. In the notation of [BJ92] the measure of the distance between a lattice generating matrix $G = [\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3] \in \text{GL}^+(3, \mathbb{R})$ and $F = [\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3] \in \text{GL}^+(3, \mathbb{R})$ is given by $\|\mathbf{f}_i \cdot \mathbf{f}_j - \mathbf{g}_i \cdot \mathbf{g}_j\|$, where $\|M_{ij}\|^2 = |M_{ij} \mathbf{g}^i \otimes \mathbf{g}^j|^2$ and the $\mathbf{g}^i$'s are the reciprocal lattice vectors, i.e. $\mathbf{g}^i \cdot \mathbf{g}_j = \delta_{ij}$. Now define $H = \sum_i \mathbf{f}_i \otimes \mathbf{g}^i$ then

$$d_2(H, \mathbb{I}) = |H^T H - \mathbb{I}|^2 = |\mathbf{f}_i \cdot \mathbf{f}_j \mathbf{g}^i \otimes \mathbf{g}^j - \mathbf{g}_i \cdot \mathbf{g}_j \mathbf{g}^i \otimes \mathbf{g}^j| = \|\mathbf{f}_i \cdot \mathbf{f}_j - \mathbf{g}_i \cdot \mathbf{g}_j\|,$$

where we used that $\sum_i \mathbf{g}_i \otimes \mathbf{g}^i = \mathbb{I}$. By definition we have $\mathbf{g}_i = G\mathbf{e}_i$ and thus $\mathbf{g}^i = G^{-T}\mathbf{e}_i$ and $\mathbf{f}_i = F\mathbf{e}_i$. Thus

$$\|\mathbf{f}_i \cdot \mathbf{f}_j - \mathbf{g}_i \cdot \mathbf{g}_j\| = |G^{-T}F^T F G^{-1} - \mathbb{I}| = |G^{-T}(C_F - C_G)G^{-1}|,$$

where we used that $H = \sum_i \mathbf{f}_i \otimes \mathbf{g}^i = \sum_i F\mathbf{e}_i \otimes \mathbf{e}_i G^{-1} = FG^{-1}$.³ Finally, the distance $d_{-2}(H, \mathbb{I})$ has recently been used in [Che+16] in order to avoid singular behaviour when considering sublattices.

Below we illustrate the differences of d_1 , d_2 and d_{-2} through a simple but instructive one-dimensional example.

Example 1.3. (A comparison of different optimality conditions)

We consider two atoms A, B that are originally at unit distance, i.e. $|A - B| = 1$ and then move the atom B to its deformed position B' . Thus H is simply a scalar quantity given by $H = |A - B'|/|A - B| = |A - B'|$. It can be seen from Table 1.2 that d_1

Tab. 1.2. A comparison between three optimality conditions in a simple one-dimensional example. Two atoms, A and B , are originally at unit distance and then atom B is moved to its deformed position B' . The table shows the values of the deformation distances resulting from this deformation for $r = 1, 2, -2$. The last column expresses the relationship between a contraction y and an expansion x such that the respective deformation distances coincide.

	$B' - B = 0.5,$	$B' - B = -0.5,$	deformation y such that
r	$H = A - B' = 1.5$	$H = A - B' = 0.5$	$d_r(y, \mathbb{I}) = d_r(x, \mathbb{I})$
1	$d_1(H, \mathbb{I}) = 0.5$	$d_1(H, \mathbb{I}) = 0.5$	$y = 2 - x$
2	$d_2(H, \mathbb{I}) = 1.25$	$d_2(H, \mathbb{I}) = 0.75$	$y = \sqrt{2 - x^2}$
-2	$d_{-2}(H, \mathbb{I}) = 0.5$	$d_{-2}(H, \mathbb{I}) = 3$	$y = \frac{1}{\sqrt{2 - x^2}}$

depends only on the distance between B and B' ; an expansion by 100% has the same d_1 distance to $\mathbb{I}$ as a contraction to 0, i.e. moving A onto B . The metric d_2 penalises expansions more than contractions; e.g. an expansion by $\approx 141\%$ has the same d_2 distance to 1 as a contraction to 0. The metric d_{-2} penalises contractions significantly more than expansions; e.g. an expansion by ∞ has the same d_{-2} distance to $\mathbb{I}$ as a contraction to $\approx 70\%$, i.e. reducing the distance between A and B by $\approx 30\%$.

³We note that in [BJ92] the notation for F and G is reversed, i.e. H maps from G to F .

A Remark on the Computation of the Optimal Transformation

Theorem 1.1 provides the necessary compactness result to reduce the original minimisation problem over the infinite set $\text{SL}(3, \mathbb{Z})$ to a finite subset given by (1.8) and (1.9) respectively. To this end, it is worth noting that the smaller the deformation distance $m_r^0 = d_r(GF^{-1}, \mathbb{I})$ of the initial lattice basis the smaller the radius of the ball in $\text{SL}(3, \mathbb{Z})$ that contains the optimal μ . However, in specific cases, where better estimates are available, it might be advantageous to start with an initial lattice basis that is not optimal.

Nevertheless, in order to explicitly determine the optimal transformations one still needs to compare the distances $d_r(H_\mu, \mathbb{I})$ for all elements contained in the finite sets given by (1.8) and (1.9) respectively. This can easily be carried out with any modern computer algebra program and possible implementations can be found in Appendix B.

In order to ensure that the solution of this finite minimisation problem is correct one needs to verify that the difference Δ between the minimal and the second to minimal deformation distance is large compared to possible rounding errors (if any). The computations in Sections 1.4 and 1.4 for the Bain strain from fcc to bcc/bct are exact and thus without rounding errors. In Section 1.4 regarding the optimal transformation in terephthalic acid we find that $\Delta > 0.015$ which is large compared to machine precision.

The Bain Strain in fcc-to-bcc

Having established the general theory of optimal lattice transformations we apply these results to prove the optimality of the Bain strain with respect to the three

different lattice metrics d_r , $r = -2, 1, 2$, from Example 1.3. In these cases we rigorously prove the optimality of the Bain strain first proposed in [Bai24].

Theorem 1.2. (*Bain Optimality*)

In a transformation from an fcc to a bcc lattice with no change in atom density, there are three distinct equivalence classes of d_r -optimal lattice transformations for $r = 1, 2, -2$. The stretch components are given by

$$\bar{H}_{\min} \in \{\text{diag}(2^{-1/3}, 2^{1/6}, 2^{1/6}), \text{diag}(2^{1/6}, 2^{-1/3}, 2^{1/6}), \text{diag}(2^{1/6}, 2^{1/6}, 2^{-1/3})\},$$

i.e. the three Bain strains are the d_r -optimal lattice transformations in a volume preserving fcc-to-bcc transformation for $r = 1, 2, -2$. The respective minimal metric distances are

$$\begin{aligned} m_{\min,1} &= d_1(H_{\min}, \mathbb{I}) = \sqrt{(2^{-1/3} - 1)^2 + 2(2^{1/6} - 1)^2} \approx 0.269, \\ m_{\min,2} &= d_2(H_{\min}, \mathbb{I}) = \sqrt{(2^{-2/3} - 1)^2 + 2(2^{1/3} - 1)^2} \approx 0.522, \\ m_{\min,-2} &= d_{-2}(H_{\min}, \mathbb{I}) = \sqrt{(2^{2/3} - 1)^2 + 2(2^{-1/3} - 1)^2} \approx 0.656. \end{aligned}$$

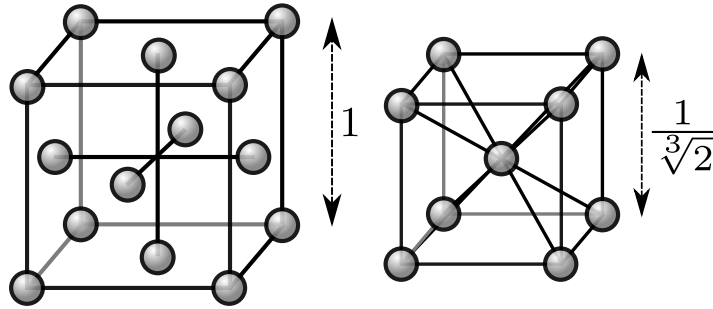


Fig. 1.2. Face-centred (left) and body-centred cubic unit cells (right) with equal atom density.

Proof. Let $\mathcal{L}_0$ denote the fcc lattice, where the fcc unit cell has unit volume and let $\mathcal{L}_1$ denote the bcc lattice with the same atom density (see Fig. 1.2). Then $\mathcal{L}_0 = \mathcal{L}(F)$ and $\mathcal{L}_1 = \mathcal{L}(B)$, where

$$F = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} = [\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3], \quad B = \frac{2^{-1/3}}{2} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} = [\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3] \quad (1.10)$$

and, in particular, $\det F = \det B = 4^{-1}$. Let $H_\mu = B\mu F^{-1}$, $\mu \in \text{SL}(3, \mathbb{Z})$ denote the lattice transformation from $\mathcal{L}_0$ to $\mathcal{L}_1$ (cf. Lemma 1.4). By definition H_μ is optimal if μ satisfies (1.4). We first show the optimality with respect to d_1 and d_2 . We may find an upper bound on the minimum by only considering $\mu \in \text{SL}^1(3, \mathbb{Z})$ (cf. Definition 1.2). Testing all elements in $\text{SL}^1(3, \mathbb{Z})$ we find exactly 72 such μ 's and all corresponding deformations are (volume preserving) Bain strains. To complete the proof we employ our key Lemma 1.5 to show that any $\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^1(3, \mathbb{Z})$ cannot be optimal with respect to either d_1 or d_2 . Let $\mu \in \mathbb{Z}^{3 \times 3}$ be given by

$$\mu = \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_1 & \beta_2 & \beta_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}. \quad (1.11)$$

Then $\mathbf{b}_{\mu,i} = H_\mu \mathbf{f}_i = B\mu \mathbf{e}_i = \alpha_i \mathbf{b}_1 + \beta_i \mathbf{b}_2 + \gamma_i \mathbf{b}_3$ and after dropping the index i we obtain

$$|\mathbf{b}_\mu|^2 = (\alpha^2 + \beta^2 + \gamma^2)|\mathbf{b}_1|^2 + 2(\alpha\beta + \beta\gamma + \alpha\gamma)\langle \mathbf{b}_1, \mathbf{b}_2 \rangle, \quad (1.12)$$

where we have used that $|\mathbf{b}_i| = |\mathbf{b}_j|$ and $\langle \mathbf{b}_i, \mathbf{b}_j \rangle = \langle \mathbf{b}_k, \mathbf{b}_l \rangle$ for all $i \neq j$ and $k \neq l$. We compute $|\mathbf{f}_i| = 2^{-1/2}$, $|\mathbf{b}_i|^2 = 3 \cdot 2^{-8/3}$ and $\langle \mathbf{b}_i, \mathbf{b}_j \rangle = -2^{-8/3}$. By (1.6) we estimate

$$d_1(H_\mu, \mathbb{I}) \geq \frac{2^{-4/3} (\rho(\alpha, \beta, \gamma))^{1/2}}{2^{-1/2}} - 1, \quad (1.13)$$

$$d_2(H_\mu, \mathbb{I}) \geq \frac{2^{-8/3} \rho(\alpha, \beta, \gamma)}{2^{-1}} - 1 \quad (1.14)$$

where $\rho(\alpha, \beta, \gamma) := \alpha^2 + \beta^2 + \gamma^2 + (\alpha - \beta)^2 + (\beta - \gamma)^2 + (\alpha - \gamma)^2$. If $\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^1(3, \mathbb{Z})$ then $\rho(\alpha, \beta, \gamma) \geq 8$ and thus

$$d_1(H_\mu, \mathbb{I}) \geq 2^{2/3} - 1 > 0.5 \gg m_{\min,1} \text{ and } d_2(H_\mu, \mathbb{I}) \geq 2^{4/3} - 1 > 1.5 \gg m_{\min,2}.$$

To show d_{-2} -optimality we consider $H_\mu = B(F\mu^{-1})^{-1}$ and use the ansatz (1.11) for μ^{-1} instead of μ . We compute

$$|F\mu^{-1} \mathbf{e}_i|^2 = \frac{1}{4} \left((\alpha + \beta)^2 + (\beta + \gamma)^2 + (\alpha + \gamma)^2 \right)$$

and we note that $\mathbf{b}_i = H_\mu F \mu^{-1} \mathbf{e}_i$. Thus by (1.7) we can estimate

$$d_{-2}(H_\mu, \mathbb{I}) \geq \frac{\frac{1}{4}\sigma(\alpha, \beta, \gamma)}{3 \cdot 2^{-8/3}} - 1 = 2 \cdot 2^{2/3} - 1 > 2.17 \gg m_{\min, -2}, \quad (1.15)$$

where $\sigma(\alpha, \beta, \gamma) := (\alpha + \beta)^2 + (\beta + \gamma)^2 + (\alpha + \gamma)^2$ and we have used that $\sigma(\alpha, \beta, \gamma) \geq 6$ for $\mu^{-1} \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^1(3, \mathbb{Z})$. Therefore the d_{-2} -optimal μ is contained in $\text{SL}^{-1}(3, \mathbb{Z})$. $\square$

Corollary 1.3. *The three Bain strains remain the d_r -optimal lattice transformations, $r = 1, 2, -2$, from fcc to bcc if the volume changes by λ^3 , provided that $\lambda > 0.84$ for $r = 1$, $\lambda > 0.64$ for $r = 2$ and $\lambda < 1.19$ for $r = -2$. The stretch components of the three optimal equivalence classes are given by*

$$\bar{H}_{\min}^\lambda \in \{\lambda \text{diag}(2^{-1/3}, 2^{1/6}, 2^{1/6}), \lambda \text{diag}(2^{1/6}, 2^{-1/3}, 2^{1/6}), \lambda \text{diag}(2^{1/6}, 2^{1/6}, 2^{-1/3})\}.$$

The minimal metric distances are given by

$$\begin{aligned} m_{\min, 1}^\lambda &= d_1(H_{\min}^\lambda, \mathbb{I}) = \sqrt{(2^{-1/3}\lambda - 1)^2 + 2(2^{1/6}\lambda - 1)^2}, \\ m_{\min, 2}^\lambda &= d_2(H_{\min}^\lambda, \mathbb{I}) = \sqrt{(2^{-2/3}\lambda^2 - 1)^2 + 2(2^{1/3}\lambda^2 - 1)^2}, \\ m_{\min, -2}^\lambda &= d_{-2}(H_{\min}^\lambda, \mathbb{I}) = \sqrt{(2^{2/3}\lambda^{-2} - 1)^2 + 2(2^{-1/3}\lambda^{-2} - 1)^2}. \end{aligned}$$

Proof. Replace $\mu \rightarrow \lambda\mu$ in (1.11) in the proof of Theorem 1.2. Then (1.13), (1.14) and (1.15) respectively read

$$\begin{aligned} d_1(H_\mu^\lambda, \mathbb{I}) &\geq \frac{2^{-4/3}(\lambda^2 \rho(\alpha, \beta, \gamma))^{1/2}}{2^{-1/2}} - 1 \geq \frac{2^{1/6}}{2} \lambda \cdot \inf_{\mathcal{S}} \rho^{1/2} - 1, \\ d_2(H_\mu^\lambda, \mathbb{I}) &\geq \frac{2^{-8/3} \lambda^2 \rho(\alpha, \beta, \gamma)}{2^{-1}} - 1 \geq 2^{-2/3} \lambda^2 \cdot \inf_{\mathcal{S}} \rho - 1, \\ d_{-2}(H_\mu^\lambda, \mathbb{I}) &\geq \frac{\frac{1}{4}\sigma(\alpha, \beta, \gamma)}{3 \cdot 2^{-8/3} \lambda^2} - 1 \geq \frac{2^{2/3}}{3 \lambda^2} \cdot \inf_{\mathcal{S}} \sigma - 1. \end{aligned}$$

If as above $\mathcal{S} = \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^1(3, \mathbb{Z})$ then $\inf_{\mathcal{S}} \rho = 8$ and thus $d_1(H_\mu^\lambda, \mathbb{I}) \geq m_{\min, 1}^\lambda$ for $\lambda > 0.84$ and $d_2(H_\mu^\lambda, \mathbb{I}) \geq m_{\min, 2}^\lambda$ for $\lambda > 0.64$ and $\inf_{\mathcal{S}} \sigma = 6$ so that $d_{-2}(H_\mu^\lambda, \mathbb{I}) \geq m_{\min, -2}^\lambda$ for $\lambda < 1.19$. $\square$

The following Remark concerns the relationship between the 72 minimising states.

Remark 1.6. (Relations between the minimal deformations for fcc-to-bcc)

Let $\mathcal{L}(F)$ and $\mathcal{L}(B)$ be the fcc and bcc lattices respectively. Let μ_0 be one of the optimal changes of lattice basis and $H_i = B\mu_i F^{-1}$, $i = 0, \dots, 71$ denote the 72 optimal lattice deformations associated to the optimal changes of basis $\mu_i \in \text{SL}(3, \mathbb{Z})$ given by Theorem 1.2. Then all optimal H_i 's and corresponding μ_i 's are given by

$$H_{PQ} = PH_0Q = B\mu_{PQ}F^{-1}, \quad P, Q \in \mathcal{P}^{24},$$

where $\mu_{PQ} = B^{-1}PB\mu_0F^{-1}QF \in \text{SL}(3, \mathbb{Z})$. We note that the latter equation holds since $\mathcal{P}^{24}$ is the point group of both cubic lattices and thus $B^{-1}PB$ and $F^{-1}QF$ are contained in $\text{SL}(3, \mathbb{Z})$. Since there are only three equivalence classes of optimal lattice transformations, the 72 optimal changes of lattice basis split into three sets of 24 μ_{PQ} 's such that the 24 corresponding H_{PQ} 's lie in the same equivalence class.

Stability of the Bain strain

Theorem 1.2 showed that the Bain strain is optimal in an fcc-to-bcc phase transformation. In this section, we restrict our attention to $r = 1, 2$ and show that the Bain strain remains optimal for a range of lattice parameters in an fcc-to-bct phase transformation. This type of transformation is found in steels with higher carbon content. The strategy of the proof is to treat the bct phase as a perturbation of the bcc phase. To this end, for B as in (1.10), let the bct lattice be generated by

$$B_{AC} = \text{diag}(A, A, C)B = 2^{-4/3} \begin{pmatrix} -A & A & A \\ A & -A & A \\ C & C & -C \end{pmatrix}, \quad (1.16)$$

so that C denotes the elongation (or shortening) of the bcc cell in the z -direction and A the elongation (or shortening) in the x - and y -direction. We note that, since $\mathcal{P}^{24} = \text{SL}(3, \mathbb{Z}) \cap \text{SO}(3)$, the lattice $\mathcal{L}(B_{AC})$ is equivalent to the lattices $\mathcal{L}(\text{diag}(A, C, A)B)$ and $\mathcal{L}(\text{diag}(C, A, A)B)$. Further we define $m_i^{0,AC} = d_i(\text{diag}(2^{1/6}A, 2^{1/6}A, 2^{-1/3}C), \mathbb{I})$.

The following proposition provides the most important ingredient.

Proposition 1.1. (*The first excited state*)

In a volume preserving transformation from an fcc to a bcc lattice the second to minimal deformation distances are given by

$$m_1^1 := \min_{\substack{\mu \in \text{SL}(3, \mathbb{Z}) \\ \mu \neq \mu_{\min}}} d_1(H_\mu, \mathbb{I}) \approx 0.70 \quad \text{and} \quad m_2^1 := \min_{\substack{\mu \in \text{SL}(3, \mathbb{Z}) \\ \mu \neq \mu_{\min}}} d_2(H_\mu, \mathbb{I}) \approx 1.64.$$

In particular, all H_μ with $\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^2(3, \mathbb{Z})$ have distance strictly larger than m_r^1 , $r = 1, 2$. We call any deformation H_μ and the corresponding change of basis μ that has deformation distance m_r^1 , $r = 1, 2$ an excited state.

Proof. The proof follows along the same lines as the proof of Theorem 1.2. Firstly, we show with the help of a computer that the second to minimal deformation distance within $\text{SL}^2(3, \mathbb{Z})$ is given by the above and secondly, by (1.13) and (1.14) respectively applied on $\text{SL}(3, \mathbb{Z}) \setminus \text{SL}^2(3, \mathbb{Z})$, we know that there cannot be any excited states in $\text{SL}(3, \mathbb{Z}) \setminus \text{SL}^2(3, \mathbb{Z})$. $\square$

Corollary 1.2. (*The first excited state' with volume change*)

In a transformation from an fcc to a bcc lattice with volume change λ^3 the second to minimal deformation distances are given by

$$m_1^{1,\lambda} := \min_{\substack{\mu \in \text{SL}(3, \mathbb{Z}) \\ \mu \neq \mu_{\min}}} d_1(H_\mu^\lambda, \mathbb{I}) = 2^{-3/2} \sqrt{25 \cdot 2^{1/3} \lambda^2 - 4 \cdot 2^{2/3} (4 + \sqrt{17}) \lambda + 24},$$

$$m_2^{1,\lambda} := \min_{\substack{\mu \in \text{SL}(3, \mathbb{Z}) \\ \mu \neq \mu_{\min}}} d_2(H_\mu^\lambda, \mathbb{I}) = 2^{-3} \sqrt{305 \cdot 2^{2/3} \lambda^4 - 400 \cdot 2^{1/3} \lambda^2 + 192}.$$

In particular all H_μ^λ with $\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^2(3, \mathbb{Z})$ have distance strictly larger than $m_r^{1,\lambda}$, $r = 1, 2$.

Theorem 1.4. *The Bain strain is a d_1 - and d_2 -optimal lattice transformation from an fcc to a bct lattice with lattice parameters A, C in the range*

$$\{(A, C) : C \geq A > 0.75 \text{ and } m_1^1 - 3^{3/2}|B_{AC} - B| \geq m_1^{0,AC}\} \quad \text{for } r = 1,$$

$$\{(A, C) : C \geq A > 0.75 \text{ and } m_2^1 - 27|B_{AC}^T B_{AC} - B^T B| \geq m_2^{0,AC}\} \quad \text{for } r = 2,$$

(cf. Figure 1.3). For $C > A$ the stretch components of the optimal lattice transformations are given by $\bar{H}_{\min}^{AC}$ in the set

$$\left\{ \begin{pmatrix} 2^{1/6}A & 0 & 0 \\ 0 & 2^{1/6}A & 0 \\ 0 & 0 & 2^{-1/3}C \end{pmatrix}, \begin{pmatrix} 2^{1/6}A & 0 & 0 \\ 0 & 2^{-1/3}C & 0 \\ 0 & 0 & 2^{1/6}A \end{pmatrix}, \begin{pmatrix} 2^{-1/3}C & 0 & 0 \\ 0 & 2^{1/6}A & 0 \\ 0 & 0 & 2^{1/6}A \end{pmatrix} \right\}.$$

The respective minimal metric distances are

$$m_{\min,1}^{AC} = d_1(H_{\min}^{AC}, \mathbb{I}) = \left(2 \left(2^{1/6}A - 1 \right)^2 + \left(2^{-1/3}C - 1 \right)^2 \right)^{1/2} = m_1^{0,AC}, \quad (1.17)$$

$$m_{\min,2}^{AC} = d_2(H_{\min}^{AC}, \mathbb{I}) = \left(2 \left(\left(2^{1/6}A \right)^2 - 1 \right)^2 + \left(\left(2^{-1/3}C \right)^2 - 1 \right)^2 \right)^{1/2} = m_2^{0,AC} \quad (1.18)$$

and are achieved by exactly 24 distinct $\mu \in \text{SL}(3, \mathbb{Z})$. The case $C = A$ corresponds to an fcc-to-bcc transformation with volume change λ^3 with $\lambda = A = C$ and we refer to Corollary 1.3.

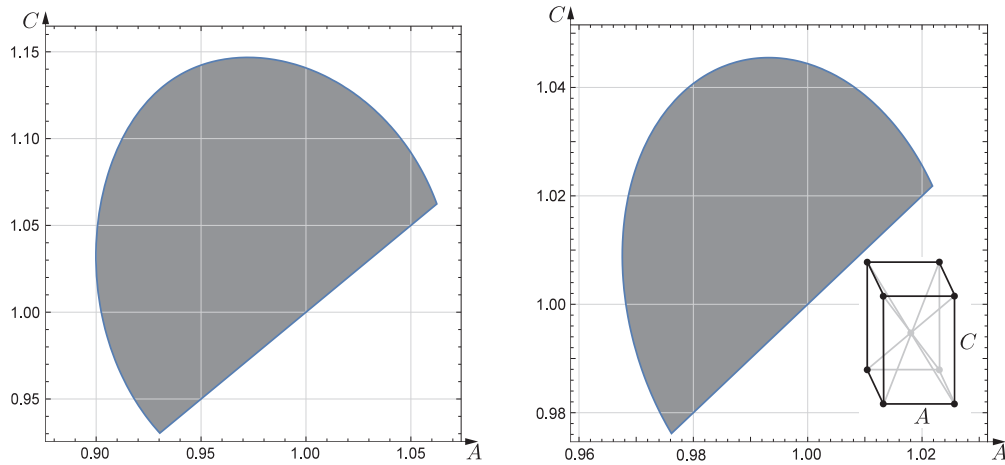


Fig. 1.3. The range of A, C where the Bain strain remains d_1 -optimal (left) and d_2 -optimal (right).

Example 1.4. $A = C = 1$ recovers Theorem 1.2. $C > A$ corresponds to the usual fcc-to-bct transformation for steels with higher carbon content. $C = \sqrt{2}A = 2^{1/3}$ is the bct lattice that is contained in the fcc lattice, i.e. $d(\mathcal{L}_0, \mathcal{L}_1) = 0$.

Proof (of Theorem 1.4). We will show that precisely 24 of the 72 μ 's that were optimal in the fcc-to-bcc transition remain optimal. Let us start from one of those optimal transformations from fcc to bcc given by e.g.

$$\mu_0 = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

We know that $H_{\mu_0}^{\text{AC}} = B_{\text{AC}}\mu_0 F^{-1}$ is optimal for $A = C = 1$, where B_{AC} is given by (1.16). The deformation distance is $d_r(H_{\mu_0}^{\text{AC}}, \mathbb{I}) = m_{\min, r}^{\text{AC}}$ with $m_{\min, r}^{\text{AC}}$ given by (1.17) and (1.18) respectively. Further there exist 24 different μ 's and corresponding H_{μ}^{AC} 's that have the same distance. This follows as in Remark 1.6 with the only difference that the point group of the bct lattice only has 8 elements. Then, due to the invariance of d_1 and d_2 under multiplication from the left or right by any rotation, the 24 matrices H_{μ}^{AC} trivially have the same distance to $\mathbb{I}$ and one may easily verify that these H_{μ}^{AC} 's are equally split into the three equivalence classes as in the statement of the Theorem.

The remaining 48 μ 's that were optimal for fcc-to-bcc lead to a larger deformation distance. One of these non-optimal lattices is generated by

$$\tilde{B}_{\text{AC}} = 2^{-4/3} \begin{pmatrix} -A & A & 0 \\ A & A & 0 \\ -C & -C & -2C \end{pmatrix}$$

with

$$\begin{aligned} \left(d_1(\tilde{B}_{AC}F^{-1}, \mathbb{I})\right)^2 - \left(m_{\min,1}^{AC}\right)^2 &= 2^{-5/3} (C - A) \left(2^{1/6} A^2 + 2^{1/6} C^2 - 4 + 2^{3/2}\right) > 0 \\ \Leftrightarrow C > A \text{ and } A^2 + C^2 > \frac{2^{5/6}}{2 - \sqrt{2}} &\Leftrightarrow C > A > 0.75 \end{aligned} \quad (1.19)$$

and

$$\begin{aligned} \left(d_2(\tilde{B}_{AC}F^{-1}, \mathbb{I})\right)^2 - \left(m_{\min,2}^{AC}\right)^2 &= 2^{-4/3} (C - A) (A + C) \left(3 A^2 + 3 C^2 - 2 \cdot 2^{2/3}\right) > 0 \\ \Leftrightarrow C > A \text{ and } A^2 + C^2 > \frac{2^{8/3}}{3} &\Leftrightarrow C > A > 0.75 \end{aligned} \quad (1.20)$$

which holds true for all $C > A$ in the range under consideration. The remaining 47 non-optimal deformations H_μ^{AC} are all $\mathcal{P}^{24}$ related and thus have the same distance; in particular larger than $m_{\min,r}^{AC}$.

To show the minimality of the 24 H_μ^{AC} 's, we make use of our result on the first excited state to compare their distance to $\mathbb{I}$ against all the remaining μ 's that were non-optimal in the fcc-to-bcc transition. In particular, we need to show that

$$m_{\min,i}^{AC} < \min_{\mu \neq \mu_{\min}} d_r(H_\mu^{AC}, \mathbb{I}), \quad r = 1, 2,$$

where $H_\mu^{AC} = B_{AC}\mu F^{-1}$ and $\mu_{\min}$ is any of the 72 minimising μ 's from Theorem 1.2. Let us set $H_\mu := H_\mu^{11}$ and, using the properties of d_r (cf. Example 1.1), estimate

$$\begin{aligned} \min_{\mu \neq \mu_{\min}} d_r(H_\mu^{AC}, \mathbb{I}) &\geq \min_{\mu \neq \mu_{\min}} \left(d_r(H_\mu, \mathbb{I}) - d_r(H_\mu^{AC}, H_\mu)\right) \\ &\geq m_r^1 - \max_{\mu \neq \mu_{\min}} d_r(H_\mu^{AC}, H_\mu), \end{aligned} \quad (1.21)$$

where m_r^1 denotes the first excited state (cf. Proposition 1.1). We obtain

$$\begin{aligned} d_1(H_\mu^{AC}, H_\mu) &\leq |H_\mu^{AC} - H_\mu| \leq |B_{AC} - B| |\mu F^{-1}|, \\ d_2(H_\mu^{AC}, H_\mu) &\leq |H_\mu^{AC\top} H_\mu^{AC} - H_\mu^\top H_\mu| \leq |B_{AC}^\top B_{AC} - B^\top B| |\mu F^{-1}|^2 \end{aligned}$$

and with the help of a computer we calculate $\max_{\mu \in \text{SL}^1(3, \mathbb{Z})} |\mu F^{-1}| = 3^{3/2}$. Thus a sufficient condition that the Bain strain is d_1 -optimal within $\text{SL}^1(3, \mathbb{Z})$ is that $0.75 < A \leq C$ satisfy

$$m_1^1 - 3^{3/2} |B_{\text{AC}} - B| \geq m_{\min, 1}^{\text{AC}}$$

yielding the area drawn in Figure 1.3 (left). To exclude any $\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^1(3, \mathbb{Z})$ we replace $\mathbf{b}$ by $\mathbf{b}_{\text{AC}} = \text{diag}(A, A, C)\mathbf{b}$ in (1.12) in the proof of Theorem 1.2 and estimate $|b_{\text{AC}}| \geq A|b|$. Concluding as in (1.13) we arrive at

$$\min_{\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^1(3, \mathbb{Z})} d_1(H_\mu^{\text{AC}}, \mathbb{I}) \geq 2^{2/3} A - 1, \quad (1.22)$$

which needs to be larger than $m_{\min, 1}^{\text{AC}}$. This holds true e.g. for $A \in [0.85, 1.7]$ and $C \in [A, 1.7]$. The proof of the d_2 -optimality proceeds analogously. To obtain d_2 -optimality within $\text{SL}^1(3, \mathbb{Z})$ we need to satisfy

$$m_2^1 - 27 |B_{\text{AC}}^{\text{T}} B_{\text{AC}} - B^{\text{T}} B| \geq m_{\min, 2}^{\text{AC}}$$

for all $0.75 < A \leq C$ which yields the area drawn in Figure 1.3 (right). To exclude all elements in the complement of $\text{SL}^1(3, \mathbb{Z})$ we have to ensure that $2^{4/3} A - 1 > m_{\min, 2}^{\text{AC}}$ which holds true e.g. for $A \in [0.75, 1.5]$ and $C \in [A, 1.5]$. $\square$

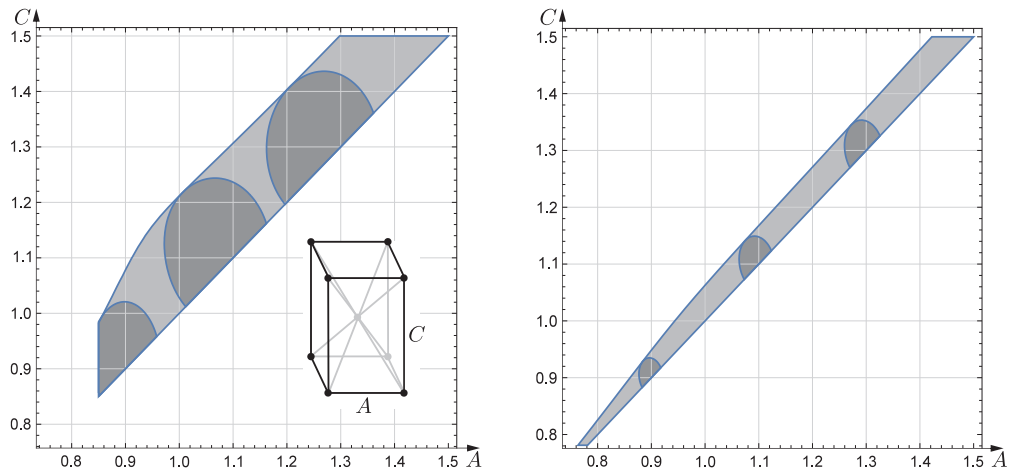


Fig. 1.4. Extended d_1 -optimality (left) and d_2 -optimality (right) range for A and C . The dark shaded regions are obtained by a perturbation argument about the fixed optimal transformations $H_{\min}^{\lambda_0}$, $\lambda_0 = 0.9, 1.1, 1.3$. The light shaded regions are obtained by a perturbation argument about the (A, C) -dependent optimal transformation $H_{\min}^{\lambda(A, C)}$ with $\lambda(A, C) = 0.995\sqrt{AC}$.

Remark 1.7. By employing Corollary 1.3 and Corollary 1.2 we may extend the range of optimal parameters A and C in Theorem 1.4 (cf. Figure 1.3) by shifting the reference point from $A = C = 1$ to $A = C = \lambda$. This enables us to show that the Bain strain remains the d_1 - and d_2 -optimal lattice deformation from fcc to bct in a much larger range of lattice parameters $C \geq A$. The shaded regions in Figure 1.4 show the values of A, C such that the deformation $H_{\min}^{\text{AC}}$ remains d_1 - and d_2 -optimal.

Proof. The main idea of the proof is to consider the element $H_\mu^\lambda = \lambda H_\mu$ which is optimal in an fcc-to-bcc transformation with volume change (cf. Corollary 1.3) and ‘closest’ to H_μ^{AC} . Thus in (1.21) we write

$$\min_{\mu \neq \mu_{\min}} d_r(H_\mu^{\text{AC}}, \mathbb{I}) \geq \min_{\mu \neq \mu_{\min}} \left(d_r(H_\mu^\lambda, \mathbb{I}) - d_r(H_\mu^\lambda, H_\mu^{\text{AC}}) \right)$$

and for d_1 we estimate

$$\min_{\mu \neq \mu_{\min}} d_1(H_\mu^{\text{AC}}, \mathbb{I}) \geq m_1^{1,\lambda} - \max_{\mu \neq \mu_{\min}} |\lambda H_\mu - H_\mu^{\text{AC}}| \geq m_1^{1,\lambda} - \lambda \max_{\mu \neq \mu_{\min}} |\mu F^{-1}| |B - B_{\frac{A}{\lambda} \frac{C}{\lambda}}|.$$

To obtain the d_1 -optimality in $\text{SL}^1(3, \mathbb{Z})$, we again use $\max_{\mu \in \text{SL}^1(3, \mathbb{Z})} |\mu F^{-1}| = 3^{3/2}$ so that $m_1^{1,\lambda} - \lambda 3^{3/2} |B - B_{\frac{A}{\lambda} \frac{C}{\lambda}}| \geq m_{\min,1}^{\text{AC}}$. Condition (1.22) regarding d_1 -optimality outside $\text{SL}^1(3, \mathbb{Z})$ remains unchanged. Both conditions combined yield the area shown in Figure 1.4 (left). Analogously in order to show d_2 -optimality we estimate

$$\begin{aligned} \min_{\mu \neq \mu_{\min}} d_2(H_\mu^{\text{AC}}, \mathbb{I}) &\geq m_2^{1,\lambda} - \max_{\mu \neq \mu_{\min}} |\lambda^2 H_\mu^{\text{T}} H_\mu - H_\mu^{\text{AC T}} H_\mu^{\text{AC}}| \\ &\geq m_2^{1,\lambda} - \lambda^2 \max_{\mu \neq \mu_{\min}} |\mu F^{-1}|^2 \left| B^{\text{T}} B - B_{\frac{A}{\lambda} \frac{C}{\lambda}}^{\text{T}} B_{\frac{A}{\lambda} \frac{C}{\lambda}} \right| \end{aligned}$$

and again use $\max_{\mu \in \text{SL}^1(3, \mathbb{Z})} |\mu F^{-1}| = 3^{3/2}$ to show d_2 -optimality within $\text{SL}^1(3, \mathbb{Z})$. The condition to be d_2 -optimal outside $\text{SL}^1(3, \mathbb{Z})$ remains unchanged. Both conditions combined yield the area shown in Figure 1.4 (right). $\square$

Remark 1.8. The previous estimates can be iterated, i.e. instead of picking the H_μ^λ that is closest to H_μ^{AC} one may pick any $H_\mu^{\text{AC}'}$ that is in the range indicated in Figure 1.4 that is closest to H_μ^{AC} .

If $C \leq A$, following the proof of Theorem 1.4, one finds that the optimal strain becomes

$$\bar{H}_{\min} = \begin{pmatrix} 2^{1/6} \frac{A+C}{2} & \pm 2^{1/6} \frac{A-C}{2} & 0 \\ \pm 2^{1/6} \frac{A-C}{2} & 2^{1/6} \frac{A+C}{2} & 0 \\ 0 & 0 & 2^{-1/3} A \end{pmatrix} + \text{its } \mathcal{P}^{24} \text{ conjugates}$$

at least if A and C are in the regions specified in the statement of Theorem 1.4 with $C \geq A$ replaced by $A \geq C$.

Terephthalic Acid

Terephthalic acid is a material that has two triclinic phases (Type I and II) which are very different from each other (cf. [BJ15, p.46 ff.]). Thus any lattice transformation necessarily requires large principal stretches and, unlike in the Bain setting, it is not clear what a good candidate for the optimal transformation would be. However, with the help of the proposed framework the d_r -optimal lattice transformation can easily be determined. The only required input parameters are the lattice parameters of the two triclinic unit cells (cf. [BB67, p.388 Table 2]) listed in Table 1.3.

Tab. 1.3. Lattice parameters of the triclinic unit cells of terephthalic acid.

Form	a/A°	b/A°	c/A°	$\alpha/^\circ$	$\beta/^\circ$	$\gamma/^\circ$
I	7.730	6.443	3.749	92.75	109.15	95.95
II	7.452	6.856	5.020	116.6	119.2	96.5

To apply our analysis we first ought to convert the triclinic to the primitive description.

Lemma 1.6. (Conversion from triclinic to primitive unit cell)

The triclinic unit cell with lattice parameters a, b, c and α, β, γ generates up to an overall rotation the same lattice as

$$F = \begin{pmatrix} a & b \cos(\gamma) & c \cos(\beta) \\ 0 & b \sin(\gamma) & c \sin^{-1} \gamma (\cos(\alpha) - \cos(\beta) \cos(\gamma)) \\ 0 & 0 & c (\sin^2 \beta - \sin^{-2} \gamma (\cos(\alpha) - \cos(\beta) \cos(\gamma))^2)^{1/2} \end{pmatrix}$$

Proof. Let $\text{col}[F] = \{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$. It is easy to verify that $|\mathbf{f}_1| = a$, $|\mathbf{f}_2| = b$, $|\mathbf{f}_3| = c$ and that $\angle(\mathbf{f}_1, \mathbf{f}_2) = \gamma$, $\angle(\mathbf{f}_1, \mathbf{f}_3) = \beta$, $\angle(\mathbf{f}_2, \mathbf{f}_3) = \alpha$. $\square$

Example 1.5. (Primitive cells of terephthalic acid)

Application of Lemma 1.6 to the lattice parameters in Table 1.3 leads to

$$F_I = \begin{pmatrix} 7.730 & -0.668 & -1.230 \\ 0 & 6.408 & -0.309 \\ 0 & 0 & 3.528 \end{pmatrix} \text{ and } F_{II} = \begin{pmatrix} 7.452 & -0.776 & -2.449 \\ 0 & 6.812 & -2.541 \\ 0 & 0 & 3.570 \end{pmatrix} \quad (1.23)$$

(all measures in $\text{\AA}^\circ$)

Theorem 1.5. (Optimal lattice transformations in terephthalic acid)

The unique equivalence class of d_1 - and d_2 -optimal transformations between terephthalic acid Form I and terephthalic acid Form II has a stretch component given by

$$\bar{H}_{\min} = \begin{pmatrix} 0.820 & -0.125 & -0.072 \\ -0.125 & 0.994 & -0.146 \\ -0.072 & -0.146 & 1.329 \end{pmatrix} \quad (1.24)$$

with principal stretches $\nu_1 = 0.725$, $\nu_2 = 1.033$ and $\nu_3 = 1.385$. The minimal distances are given by $m_{\min,1} = d_1(\bar{H}_{\min}, \mathbb{I}) = 0.474$ and $m_{\min,2} = d_2(\bar{H}_{\min}, \mathbb{I}) = 1.035$.

Proof. We apply Theorem 1.1 with $F = F_I$ and $G = F_{II}$. We calculate $\|F_I\|_{2,\infty} = |F_I \mathbf{e}_1| = 7.730 < 7.8$, $\nu_{\min}(F_{II}) = 3.076 > 3$, $m_1^0 = 0.529 < 0.55$ and $m_2^0 = 1.197 <$

1.2. Further we note that if $\mu \in \text{SL}(3, \mathbb{Z}) \setminus \text{SL}^{k-1}(3, \mathbb{Z})$ then $\|\mu\|_{2,\infty} \geq \sqrt{k^2 + 1}$. Therefore by (1.8) any d_1 -optimal μ satisfies

$$\|\mu\|_{2,\infty} \leq \frac{\|F\|_{2,\infty}}{\nu_{\min}(G)}(m_1^0 + 1) < \frac{7.8}{3}(0.55 + 1) = 4.03 < \sqrt{4^2 + 1}$$

and is thus contained in $\text{SL}^3(3, \mathbb{Z})$ and by (1.8) any d_2 -optimal μ satisfies

$$\|\mu\|_{2,\infty}^2 \leq \frac{\|F\|_{2,\infty}^2}{\nu_{\min}^2(G)}(m_2^0 + 1) < \frac{7.8^2}{3^2}(1.2 + 1) = 14.872$$

and is thus also contained in $\text{SL}^3(3, \mathbb{Z})$. With the help of a computer we check that within the set $\text{SL}^3(3, \mathbb{Z})$ the minimum is in both cases attained at

$$\mu_{\min} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & -1 \end{pmatrix}$$

with corresponding $\bar{H}_{\min} = \sqrt{H_{\mu_{\min}}^T H_{\mu_{\min}}}$ as in (1.24), $m_{\min,1} = d_1(\bar{H}_{\min}, \mathbb{I}) = 0.474$ and $m_{\min,2} = d_2(\bar{H}_{\min}, \mathbb{I}) = 1.035$. $\square$

Remark 1.9. We have shown that the d_1 - and d_2 -optimal transformations from Form I to Form II of terephthalic acid are the same. However the d_{-2} -optimal transformation is different and given by

$$\bar{H}_{\min,-2} = \begin{pmatrix} 0.852 & -0.119 & -0.018 \\ -0.119 & 0.950 & -0.197 \\ -0.018 & -0.197 & 1.346 \end{pmatrix}$$

with principal stretches $\nu_1 = 0.743$, $\nu_2 = 0.977$ and $\nu_3 = 1.429$. As expected the smallest principal stretch ν_1 is bigger than before since d_{-2} penalises contractions significantly more than expansions. To obtain the required analytical bounds one calculates $\|F_{II}\|_{2,\infty} = |F_{II}\mathbf{e}_1| = 7.452 < 7.46$, $\nu_{\min}(F_I) = 3.464 > 3.45$ and $m_{-2}^0 = 1.080 < 1.1$ to get $\|\mu^{-1}\|_{2,\infty}^2 < 10$ (cf. (1.9)) and thus the optimal μ lies in $\text{SL}^{-2}(3, \mathbb{Z})$.

Remark 1.10. Even though [Che+16; BJ15] also use the distance d_{-2} , the reported strains are different. However, this discrepancy is not a consequence of using sublattices but rather a consequence of using the lattice parameters from [BB67,

p.388 Table 1] for terephthalic acid II⁴ and the lattice parameters from [BB67, p.388 Table 2] for terephthalic acid I. In particular, using these mixed input parameters in ‘OptLat’ (cf. Appendix B) yields identical values.

⁴ $a = 9.54\text{\AA}, b = 5.34\text{\AA}, c = 5.02\text{\AA}, \alpha = 86.95^\circ, \beta = 134.65^\circ, \gamma = 94.8^\circ$

The Ball-James Model and Related Concepts

In this chapter we review the continuum model for martensitic phase transformations developed by Ball & James [BJ87]. Their model, which is based on non-linear elasticity and energy minimisation, will play a fundamental rôle in a majority of the developments in this thesis. We also review several closely linked mathematical concepts such as gradient Young measures and generalisations of convexity.

Description of the Model

Consider an open bounded connected Lipschitz domain $\Omega \subset \mathbb{R}^3$ which represents the undistorted austenite at temperature θ and an invertible map $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ which maps the reference configuration Ω to the deformed configuration $y(\Omega)$. The

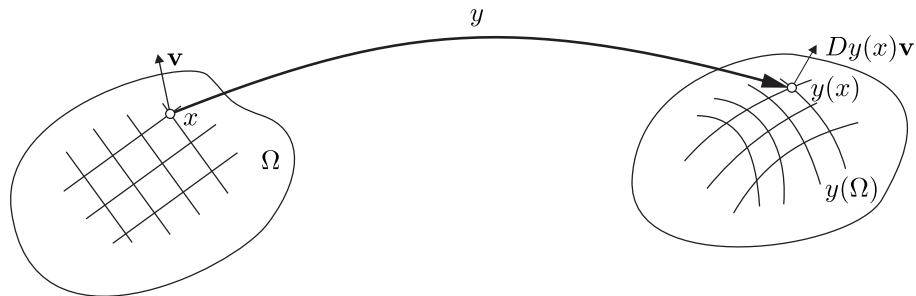


Fig. 2.1. The deformation $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ mapping the reference configuration Ω to the deformed configuration $y(\Omega)$.

main constitutive assumption is the existence of a free energy density function $W : \mathbb{R}_+^{3 \times 3} \times \Theta \rightarrow \mathbb{R}$ which depends on the local change in shape and temperature.

The behaviour of the system is determined by an energy minimisation problem of the total free energy given by

$$E(y) := \int_{\Omega} W(Dy(x), \theta) \, dx, \quad (\text{E})$$

subject to a displacement boundary condition

$$y(x)|_{\partial\Omega} = y_0(x)$$

on a suitable set of admissible functions $\mathcal{A}$. Throughout temperature is treated as a fixed parameter. From a modelling point of view the following assumptions on W are made.

Definition 2.1. (The free energy density W)

Let $W : \mathbb{R}_+^{3 \times 3} \times \Theta \rightarrow \mathbb{R}$ be continuous, $\Theta \subset \mathbb{R}$ be an interval and assume the following properties on W :

1. Frame indifference

$$W(RA, \theta) = W(A, \theta) \text{ for all } R \in \text{SO}(3), A \in \mathbb{R}_+^{3 \times 3}.$$

This encodes the fundamental axiom in continuum mechanics that the material response is invariant under the change of observer or, in other words, a rotation of the entire system does not change its energy.

2. Symmetry of the austenite

$$W(AQ, \theta) = W(A, \theta) \text{ for all } Q \in \mathcal{P}_a.$$

This encodes that the energy is invariant under a rotation that maps the austenite lattice to itself.

3. No collapse of matter

$$W(A, \theta) \rightarrow \infty \text{ as } \det A \rightarrow 0^+.$$

4. Structure of minima

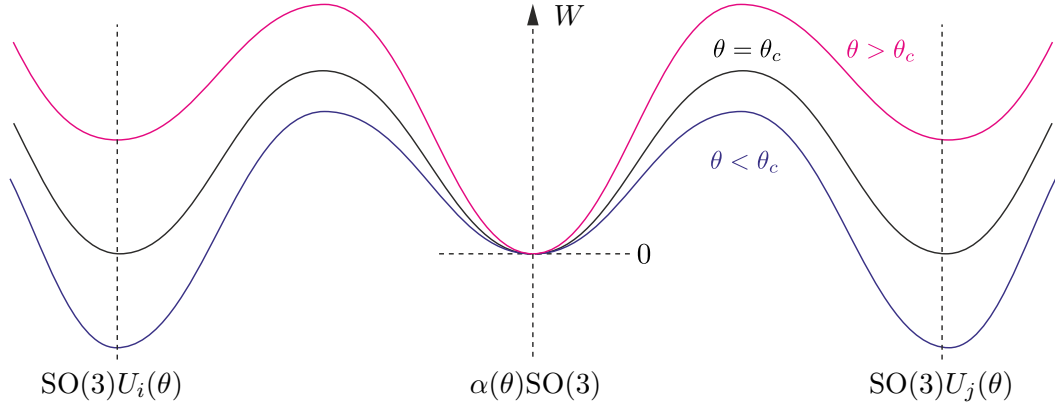


Fig. 2.2. The free energy density W below, at and above the transition temperature θ_c (normalised to $W(\alpha(\theta)\text{SO}(3)) = 0$).

We define the set $K(\theta)$ of minimising deformation gradients of W at a given temperature θ by

$$K(\theta) := \left\{ A \in \mathbb{R}_+^{3 \times 3} \mid W(A, \theta) = \min_{B \in \mathbb{R}_+^{3 \times 3}} W(B, \theta) \right\}.$$

In view of our goal to model martensitic phase transformations we require that precisely the pure austenite minimises the free energy density for $\theta > \theta_c$ and precisely the distinct variants of martensite minimise the free energy density for $\theta < \theta_c$. Therefore we assume that

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

where $\alpha(\theta)$ is a thermal expansion coefficient with $\alpha(\theta_c) = 1$ and $U_i(\theta) \in \mathbb{R}_{\text{sym}}^{3 \times 3}$ are the N (linear) transformation strains required to map the austenite lattice to the martensite lattice. To simplify computations we henceforth normalise the energy such that $W(\alpha(\theta)\text{SO}(3)) = 0$ and thus in particular $W(\text{SO}(3)U_i(\theta)) > 0$ for $\theta > \theta_c$ and $W(\text{SO}(3)U_i(\theta)) < 0$ for $\theta < \theta_c$.

By Chapter 1, we know that all martensitic variants are given by

$$R^T U_1 R, \quad R \in \mathcal{P}_a$$

and that $N = |\mathcal{P}_a| |\mathcal{P}_m|^{-1}$. In the following, the respective (globally) minimising sets will be called the *wells*. More specifically, for $\theta > \theta_c$, the set $\alpha(\theta) \text{SO}(3)$ will be called the *austenite well* and for $\theta < \theta_c$ the sets $\text{SO}(3) U_i(\theta)$, $i = 1, \dots, N$ will be called the *martensite wells*. For brevity we will often omit the temperature dependence and, since we are almost exclusively interested in the case $\theta < \theta_c$, we often refer to the sets $\text{SO}(3) U_i$ simply as the *wells*.

Example 2.1. In a cubic-to-tetragonal phase transformation $|\mathcal{P}_a| = |\mathcal{P}^{24}| = 24$, $|\mathcal{P}_m| = 8$ and the 3 martensitic variants are given by

$$U_1 = \text{diag}(\eta_1, \eta_1, \eta_2), \quad U_2 = \text{diag}(\eta_1, \eta_2, \eta_1), \quad U_3 = \text{diag}(\eta_2, \eta_1, \eta_1),$$

where $\eta_1, \eta_2 > 0$.

Remark 2.1. We note that the energy functional (E) neglects any contribution from interfacial energy. Heuristically this omission may be justified by recent experiments in [Son+13] for highly reversible materials that seem to prefer forming very complex microstructures (i.e. having many interfaces) even though simpler interfaces would be already compatible (cf. Lemma 2.2 and 2.3 for details on compatibility). Even if interfacial energy plays a more significant rôle, the zero interfacial energy limit could act as a selector for otherwise equivalent solutions.

Having established the key features of our total free energy (E) we now turn our attention to the set of admissible functions $\mathcal{A}$. From a modelling point of view, as we are dealing with elasticity rather than plasticity, we expect the deformations to not open up cracks or holes and thus require at least continuity. On the other hand we would like to allow jumps in the deformation gradients in order to allow sharp

interfaces between different variants of martensite. We therefore make the following choice

$$\mathcal{A} := \left\{ y \in W^{1,\infty}(\Omega, \mathbb{R}^3) : y|_{\partial\Omega}(x) = y_0(x) \right\}$$

and for simplicity we will always assume homogeneous boundary conditions, i.e. $y_0(x) = Fx$ for some $F \in \mathbb{R}^{3 \times 3}$. In fact, as we want to ensure invertibility of y we should additionally require that $\det Dy > 0$. But since eventually we are only interested in energy minimisers $\bar{y}$ of the total free energy (in particular $E(\bar{y}) < \infty$) we rather extend our definition of W to all of $\mathbb{R}^{3 \times 3}$ by setting

$$W(A) = \infty \text{ for all } A \text{ such that } \det A \leq 0.$$

Unfortunately, this constraint will often be difficult to incorporate and we will often turn a blind eye to it and use the original definition of W instead (cf. [Bal02, Problem 1]).

Having set up the model it is now natural to ask whether our minimisation problem (E) admits solutions satisfying the displacement boundary condition $y_0(x) = Fx$. To illustrate the difficulties that we will encounter let us assume that we are at the transformation temperature. Thus both the austenite and the martensite wells, i.e. all elements in the set $K = \text{SO}(3) \cup \text{SO}(3)U_1(\theta_c)\mathcal{P}_a$, minimise W pointwise. If solutions exist we ask how to characterise them and if they do not exist we ask whether we can expect to have approximate solutions.

Definition 2.2. (Exact and approximate solutions)

We say that $y \in W^{1,\infty}(\Omega)$ is an *exact solution* of (E) iff

$$Du \in K \text{ a.e. in } \Omega$$

and it satisfies the boundary condition $y(x) = Fx$ on $\partial\Omega$. We will say that a sequence of maps $\{y_i\}_{i=1}^\infty \subset W^{1,\infty}$ is an *approximate solution* of (E) iff

$$\lim_{i \rightarrow \infty} \text{dist}(Dy_i, K) = 0 \text{ a.e. in } \Omega$$

and each y_i satisfies the boundary condition $y_i(x) = Fx$ on $\partial\Omega$. Further we denote by $K^{\text{ex}} \subset \mathbb{R}^{3 \times 3}$ and $K^{\text{app}} \subset \mathbb{R}^{3 \times 3}$ the set of boundary conditions F that allow exact and approximate solutions, respectively.

Let us consider the most trivial case and assume that $F \in K$. Then clearly the minimum of (E) is attained and is given by $y(x) \equiv Fx$. However, it is in general not true that $K^{\text{ex}} = K$ and in particular in general $K^{\text{app}} \supsetneq K$. This corresponds to the observation that we see the co-existence of very complex patterns of different variants of martensite and austenite and not only homogeneous solutions. In order to obtain further properties of these non-trivial (approximate) solutions it is important to investigate the types of stress-free (i.e. zero energy) interfaces that can occur between the different martensite wells and thus predict the structure of the solutions that we expect to observe. The existence and non-existence of interfaces also plays a crucial rôle if we look at the austenite-martensite transition in a ‘poor man’s’ dynamical sense. That is, we consider the minimisers for a sequence of temperatures rather than an actual dynamic equation. For example, if we approach the transition temperature from above we expect to still have pure austenite but by further lowering the temperature the martensite will become energetically favourable. Our above problem then reads:

- Given $F = \mathbb{I}$, i.e. the boundary condition is the pure austenite, what martensitic structures can we expect to form?

This example will be the key problem addressed in Chapter 5.

2.1 Austenite and Martensite Interfaces

Definition 2.3. (Interfaces)

Let $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ with Ω open and connected and let Ω_A and Ω_B be two disjoint measurable sets with $|\Omega_A|, |\Omega_B| > 0$ such that $\Omega = \Omega_A \dot{\cup} \Omega_B$ and

$$Dy(x) = A \text{ for a.e. } x \in \Omega_A,$$

$$Dy(x) = B \text{ for a.e. } x \in \Omega_B,$$

for some matrices $A \neq B \in \mathbb{R}^{3 \times 3}$. Then we call $\mathcal{I} := \overline{\Omega}_A \cap \overline{\Omega}_B$ an *interface* between the two variants A and B (cf. Figure 2.3).

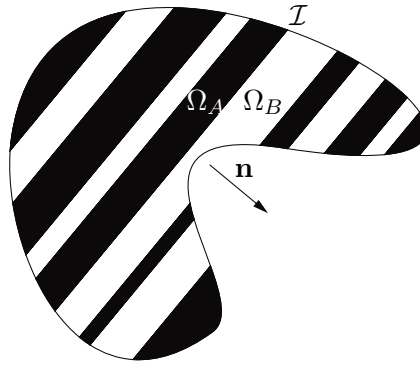


Fig. 2.3. Possible configuration of Ω_A and Ω_B defining interfaces with normal $\mathbf{n}$.

Lemma 2.1. (Properties of interfaces, [BJ87, Prop. 1])

In the notation of Definition 2.3, the matrices A and B are rank-one connected, i.e. there exist $0 \neq \mathbf{c} \in \mathbb{R}^3$, $\mathbf{n} \in S^2$ such that

$$A - B = \mathbf{c} \otimes \mathbf{n}.$$

This necessary condition, which is a consequence of the continuity of the deformation, is also called Hadamard's jump condition. Further interfaces are planar, i.e. we can write $y(x) = \mathbf{y}_0 + Bx + \rho(x)\mathbf{c}$, where $\mathbf{y}_0 \in \mathbb{R}^3$, $\mathbf{y}_0 \cdot \mathbf{c} = 0$ and $\rho \in W^{1,\infty}(\Omega, \mathbb{R})$ satisfies $D\rho(x) = 1_{\Omega_A}(x)\mathbf{n}$ a.e..

Lemma 2.2 and 2.3 will establish what types of interfaces are possible. An important ingredient will be the following proposition.

Proposition 2.1. ([BJ87, Prop. 4])

Let $C \in \mathbb{R}^{3 \times 3}$ with eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$. Then C can be written as

$$C = (\mathbb{I} + \mathbf{m} \otimes \mathbf{b})(\mathbb{I} + \mathbf{b} \otimes \mathbf{m})$$

for some $\mathbf{m}, \mathbf{b} \neq 0$ if and only if $\lambda_1 \geq 0$ and $\lambda_2 = 1$. The solutions are given by

1. If $C \neq \mathbb{I}$

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

where $\rho \neq 0$ is a constant, $\kappa, \hat{\kappa} \in \{-1, 1\}$ and $\mathbf{v}_1, \mathbf{v}_3$ are the normalised eigenvectors of C corresponding to λ_1 and λ_3 .

2. If $C = \mathbb{I}$

$$\mathbf{b} = \rho \mathbf{v}, \quad \mathbf{m} = -2\rho^{-1} \mathbf{v},$$

where $\rho \neq 0$ is a constant and $|\mathbf{v}| = 1$.

Lemma 2.2. (Possible interfaces I, [BJ87])

As before let $\text{SO}(3)$ represent the austenite well and $\text{SO}(3)U_i, i = 1, \dots, N$ the distinct martensite wells at the critical temperature θ_c . Then the following holds:

1. There are no austenite/austenite interfaces.
2. A necessary condition for austenite/martensite interfaces is that U_1 has 1 as an eigenvalue. In particular, in a cubic-to-tetragonal phase transformation, there are no austenite/martensite interfaces, unless $\eta_1 = 1$ or $\eta_2 = 1$.
3. Whenever the middle eigenvalue of $U_i U_j^{-1}$ is equal to 1 there exist martensite/martensite interfaces. In particular, martensite/martensite interfaces exist in a cubic-to-tetragonal phase transformation.

Proof. 1. Let $R, S \in \text{SO}(3)$, $R \neq S$ be in the austenite well. Then according to Proposition 2.1 we have $R - S = \mathbf{a} \otimes \mathbf{n}$, $\mathbf{a} \neq 0$ and thus after multiplication with S^T we obtain

$$R' = \mathbb{I} + \mathbf{a}' \otimes \mathbf{n}.$$

In particular R' leaves the two dimensional space $\{\mathbf{n}\}^\perp$ invariant and thus has two axes of rotation. Therefore $R' = \mathbb{I}$ and $R = S$ which is a contradiction.

2. Follows directly from Proposition 2.1.

3. The condition of compatibility reads $U_1 + \mathbf{a} \otimes \mathbf{n} = RU_j$ for some $R \in \text{SO}(3)$. After postmultiplication with U_j^{-1} the claim follows from Proposition 2.1. $\square$

The above results suggest that, generically, we cannot have a stress free interface between austenite and a single variant of martensite. However, from experiments we know that interfaces between austenite and a fine mixture of two or more variants of martensite exist even if none of the eigenvalues are equal to 1. In the next section we will introduce gradient Young measures in order to give a precise meaning of fine mixtures of phases. For now we satisfy ourselves with the following construction.

By Lemma 2.2 we can have planar interfaces between two rank-one connected variants of martensite U_1 and RU_2 and we will henceforth call two such variants *compatible* or *twin-related*. We now consider a laminate of the two compatible/twinned variants with volume fractions λ and $1 - \lambda$ respectively for a $\lambda \in (0, 1)$.

If we decrease the width of the layers and keep the volume fractions constant we obtain on average the (macroscopic) deformation gradient $\lambda U_1 + (1 - \lambda)RU_2$. We now ask whether this macroscopic deformation gradient can be rank-one connected to the austenite and thus be compatible. Figure 2.4 (after [CJ95]) shows a micrograph of finely twinned martensite that is compatible with austenite.

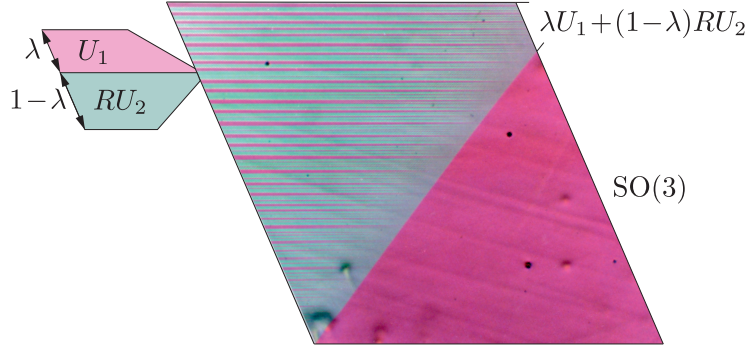


Fig. 2.4. An interface between a laminate of finely twinned martensite (left) with macroscopic deformation gradient $\lambda U_1 + (1 - \lambda)RU_2$ and austenite (right).

Lemma 2.3. (Possible interfaces II, [BJ87, Thm. 7])

Let U_1 and RU_2 , $R \in \text{SO}(3)$ be two compatible variants of martensite, i.e. $U_1 - RU_2 = \mathbf{a} \otimes \mathbf{n}$ for $\mathbf{a}, \mathbf{n} \in \mathbb{R}^3$, $\mathbf{a} \neq 0$, $|\mathbf{n}| = 1$. Then there exist austenite/twinned martensite interfaces, i.e. there exist triples $(\hat{R}, \lambda, \mathbf{b} \otimes \mathbf{m}) \in \text{SO}(3) \times (0, 1) \times \mathbb{R}^{3 \times 3}$ such that

$$U_1 + \lambda \mathbf{a} \otimes \mathbf{n} = \hat{R}^T(\mathbb{I} + \mathbf{b} \otimes \mathbf{m}) \quad (2.1)$$

holds. The solutions are given by:

1. If U_1 does not have 1 as an eigenvalue we define

$$\alpha^* := \mathbf{a} \cdot U_1(U_1^2 - \mathbb{I})^{-1}\mathbf{n}$$

and we have solutions iff

$$1 + \frac{1}{2}\alpha^* \leq 0$$

and

$$\text{Tr } U_1^2 - \det U_1^2 - 2 + \frac{1}{2\alpha^*}|\mathbf{a}|^2 \geq 0. \quad (2.2)$$

If further $1 + \frac{1}{2}\alpha^* < 0$ then strict inequality holds in (2.2) and there are exactly four distinct solutions to (2.1) of the form

$$(\hat{R}_1, \lambda^*, \mathbf{b}_1^+ \otimes \mathbf{m}_1^+), (\hat{R}_2, \lambda^*, \mathbf{b}_1^- \otimes \mathbf{m}_1^-), \\ (\hat{R}_3, \lambda^*, \mathbf{b}_2^+ \otimes \mathbf{m}_2^+), (\hat{R}_4, \lambda^*, \mathbf{b}_2^- \otimes \mathbf{m}_2^-),$$

where $\lambda^* := \frac{1}{2} \left(1 - \sqrt{1 + \frac{2}{\alpha^*}}\right) \in \left(0, \frac{1}{2}\right)$. If $1 + \frac{1}{2}\alpha^* = 0$ then $\lambda^* = \frac{1}{2}$ and there are exactly two distinct solutions if strict inequality holds in (2.2) and there is only one solution if equality holds in (2.2).

2. If U_1 does have 1 as an eigenvalue we define

$$\mu^* := \text{Tr } U_1^2 - \det U_1^2 - 2$$

and we have solutions iff $\mu^* > 0$. If $\mu^* > \frac{1}{4}|\mathbf{a}|^2$ then for each $\lambda \in (0, 1)$ there are exactly two distinct solutions

$$(\hat{R}_\lambda^+, \lambda, \mathbf{b}_\lambda^+ \otimes \mathbf{m}_\lambda^+), (\hat{R}_\lambda^-, \lambda, \mathbf{b}_\lambda^- \otimes \mathbf{m}_\lambda^-).$$

If $0 < \mu^* \leq \frac{1}{4}|\mathbf{a}|^2$ and $\bar{\lambda} := \frac{1}{2} \left(1 - \sqrt{1 - \frac{4\mu^*}{|\mathbf{a}|^2}}\right) \in \left(0, \frac{1}{2}\right]$ then for each $\lambda \in (0, \bar{\lambda}) \cup (1 - \bar{\lambda}, 1)$ there are again exactly two distinct solutions of the same form as above.

If $\lambda = \bar{\lambda}$ or $\lambda = 1 - \bar{\lambda}$ with either $\bar{\lambda} \neq \frac{1}{2}$ or $\bar{\lambda} = \frac{1}{2}$ and $\det U_0 \neq 1$ then there is only one solution

$$(\hat{R}_\lambda, \lambda, \mathbf{b}_\lambda \otimes \mathbf{m}_\lambda).$$

In all the cases above for each λ the formula for $\mathbf{b} \otimes \mathbf{m}$ is given according to Proposition 2.1 evaluated at the ordered eigenvalues of

$$C(\lambda) := (U_1 + \lambda \mathbf{a} \otimes \mathbf{n})(U_1 + \lambda \mathbf{n} \otimes \mathbf{a})$$

and the rotation $\hat{R}$ as the rotation that satisfies (2.1).

Example 2.2. (Cubic-to-tetragonal phase transformation, [BJ87, Section 5])

We now specify the situation to the cubic-to-tetragonal phase transformation with $U_1 = \text{diag}(\eta_1, \eta_1, \eta_2)$ and $\eta_1, \eta_2 \neq 1$. Then if $\lambda^* \neq \frac{1}{2}$ the conditions of the previous lemma are equivalent to

$$\{\eta_1 < 1 < \eta_2 \text{ and } \eta_1^{-2} + \eta_2^{-2} < 2\} \text{ or } \{\eta_2 < 1 < \eta_1 \text{ and } \eta_1^2 + \eta_2^2 < 2\}$$

and in this case the four distinct solutions are given by

$$\begin{aligned}\mathbf{b}_1^\pm &= \xi \left(\mp \frac{1}{2}(\delta + \tau), \pm \frac{1}{2}(\delta - \tau), -\eta_2 \right), \quad \mathbf{m}_1^\pm = \left(\mp \frac{1}{2}(\delta + \tau), \pm \frac{1}{2}(\delta - \tau), 1 \right), \\ \mathbf{b}_2^\pm &= \xi \left(\mp \frac{1}{2}(\delta - \tau), \pm \frac{1}{2}(\delta + \tau), -\eta_2 \right), \quad \mathbf{m}_2^\pm = \left(\mp \frac{1}{2}(\delta - \tau), \pm \frac{1}{2}(\delta + \tau), 1 \right),\end{aligned}$$

where¹

$$\delta^2 = \frac{\eta_2^2 + \eta_1^2 - 2}{1 - \eta_1^2}, \quad \tau^2 = \frac{2\eta_1^2\eta_2^2 - \eta_1^2 - \eta_2^2}{1 - \eta_1^2}, \quad \xi = \frac{1 - \eta_1^2}{1 + \eta_2}.$$

We note that the four solutions are related through conjugation with those elements in $\mathcal{P}^{24}$ that leave the $(3, 3)$ -component invariant.

An Alternative Derivation of λ^*

We present an alternative derivation to determine the correct volume fractions to form an interface between twinned martensite and austenite in a cubic-to-tetragonal phase transformation. Not only for this derivation, but throughout the rest of this thesis, an important tool will be *Mallard's law* (see e.g. [Bha03, Result 5.2]).

Lemma 2.4. (*Mallard's law*)

Let $(A, \mathbf{e}) \in \mathbb{R}^{3 \times 3} \times S^2$ and $B \in \mathbb{R}^{3 \times 3}$ be such that $B = PAP$, where $P = -\mathbb{I} + 2\mathbf{e} \otimes \mathbf{e}$ is a 180° rotation about the unit vector $\mathbf{e}$. Then the equation $QB = A + \mathbf{a} \otimes \mathbf{n}$ admits two solutions given by

$$\mathbf{a} = 2 \left(\frac{A^{-T}\mathbf{e}}{|A^{-T}\mathbf{e}|^2} - A\mathbf{e} \right), \quad \mathbf{n} = \mathbf{e}, \quad (\text{I})$$

$$\mathbf{a} = \frac{2N}{|A\mathbf{e}|^2} A\mathbf{e}, \quad \mathbf{n} = \frac{1}{N} \left(|A\mathbf{e}|^2 \mathbf{e} - A^T A \mathbf{e} \right). \quad (\text{II})$$

In each case, $Q = (A + \mathbf{a} \otimes \mathbf{n})B^{-1}$.

Remark 2.2. (Types of twins)

Twins described by the first solution in Mallard's law are commonly referred to as

¹We note that there is a typo in [BJ87, Eq. 5.69]. It should be $\beta = \eta_2(\eta_1^2 - 1)(1 + \eta_2)^{-1}$ instead of $\beta = \eta_2(\eta_1^2 - 1)(1 - \eta_2)^{-1}$.

Type I twins and the corresponding lattices are related by a 180° rotation about the twin plane $\frac{A^{-T}\mathbf{n}}{|A^{-T}\mathbf{n}|}$. Twins described by the second solution are known as *Type II* twins and the lattices are related by a 180° rotation about the shearing direction $\frac{\mathbf{a}}{|\mathbf{a}|}$. It may happen, and it does so in a cubic-to-tetragonal transformation, that there are two rotations by 180° relating A and B . In this case, there are seemingly four solutions from Mallard's law, however, Proposition 2.1 says that there cannot be more than two. Indeed, the Type I solution using one 180° rotation is the same as the Type II solution using the other 180° rotation and vice versa. In particular, the lattices on either side of the interface are related by both a 180° rotation about the twin plane and a 180° rotation about the shearing direction. Solutions of this type are referred to as *compound* twins.

Proof. See the proof of Lemma 7.3. □

Remark 2.3. In both cases, $A + \mathbf{a} \otimes \mathbf{n} = A(\mathbb{I} + A^{-1}\mathbf{a} \otimes \mathbf{n})$ can be written as a simple shear $\mathbb{I} + A^{-1}\mathbf{a} \otimes \mathbf{n}$ followed by A . In particular, $A^{-1}\mathbf{a} \perp \mathbf{n}$, $\mathbf{a} \perp A^{-T}\mathbf{n}$, $\mathbf{a} \perp \text{cof } A\mathbf{n}$ and $\text{cof } A^T\mathbf{a} \perp \mathbf{n}$.

Proof. The second part is an obvious consequence of the properties of the inner product between two vectors $\langle \mathbf{a}, \mathbf{b} \rangle := \mathbf{a}^T \mathbf{b}$ and the relation $\text{cof } A = \det A A^{-T}$. We show the last of the equivalent relations. For the first solution we calculate

$$\langle \text{cof } A^T \mathbf{a}, \mathbf{e} \rangle = 2(\det A \frac{\langle \text{cof } A^T A \mathbf{e}, \mathbf{e} \rangle}{|\text{cof } A \mathbf{e}|^2} - \det A \langle \mathbf{e}, \mathbf{e} \rangle) = \det A (|\mathbf{e}|^2 - |\mathbf{e}|^2) = 0$$

and for the second solution we simply observe that $\text{cof } A^T \mathbf{a} \propto \mathbf{e}$ and

$$\langle \mathbf{e}, \mathbf{n} \rangle \propto |A\mathbf{e}|^2 - \langle A\mathbf{e}, A\mathbf{e} \rangle = 0.$$

□

With Mallard's law (Lemma 2.4) at hand we are able to derive the necessary volume fractions in the twinned martensite more efficiently.

Theorem 2.1. *A simple laminate between the wells U_1 and U_2 that can form an interface with austenite is given by*

$$L(\lambda_i) = U_1 + 2\lambda_i \left(\frac{U_1^{-1} \mathbf{n}_k}{|U_1^{-1} \mathbf{n}_k|^2} - U_1 \mathbf{n}_k \right) \otimes \mathbf{n}_k, \quad (2.3)$$

where $i, k \in \{1, 2\}$, $\mathbf{n}_k \in \{[1 \ 1 \ 0], [1 \ \bar{1} \ 0]\}$ and

$$\lambda_i = \frac{1}{2} \pm \frac{1}{2} \frac{1}{\eta_2^2 - \eta_1^2} \sqrt{(2 - \eta_2^2 - \eta_1^2)(\eta_1^2 - 2\eta_1^2\eta_2^2 + \eta_2^2)}. \quad (2.4)$$

In particular an interface exists iff $(2 - \eta_2^2 - \eta_1^2)(\eta_1^2 - 2\eta_1^2\eta_2^2 + \eta_2^2) \geq 0$. Further the solutions for the two different $\mathbf{n}_k$'s are related by conjugation with $R[180^\circ, \mathbf{e}_1]$.

Proof. By Mallard's law (Lemma 2.4) we know that all simple laminates are given by (2.3). For $\mathbf{n} = [1 \ 1 \ 0]$ we have

$$L(\lambda) = \begin{pmatrix} \eta_2 - \frac{\lambda(-\eta_1^2 + \eta_2^2)\eta_2}{\eta_1^2 + \eta_2^2} & -\frac{\lambda(-\eta_1^2 + \eta_2^2)\eta_2}{\eta_1^2 + \eta_2^2} & 0 \\ \frac{\lambda(-\eta_1^2 + \eta_2^2)\eta_1}{\eta_1^2 + \eta_2^2} & \eta_1 + \frac{\lambda(-\eta_1^2 + \eta_2^2)\eta_1}{\eta_1^2 + \eta_2^2} & 0 \\ 0 & 0 & \eta_1 \end{pmatrix}.$$

In order to have an interface with austenite we require that the middle singular value of $L(\lambda)$ is equal to 1. By the block diagonal structure of $L(\lambda)$ we know that one singular value is η_1 and we may only consider the reduced 2×2 matrix $\tilde{L}(\lambda) := L(\lambda)|_{2 \times 2}$. Let λ_1, λ_2 denote the eigenvalues of $\tilde{L}^T \tilde{L}(\lambda)$ then $\lambda_1 = 1$ or $\lambda_2 = 1$ is equivalent to

$$(\lambda_1 - 1)(\lambda_2 - 1) = 0 \Leftrightarrow \lambda_1 + \lambda_2 = 1 + \lambda_1 \lambda_2 \Leftrightarrow |\tilde{L}(\lambda)|^2 = 1 + \det^2 \tilde{L}(\lambda) = 1 + \eta_1^2 \eta_2^2,$$

which is quadratic in λ and can be solved easily. The calculation for $\mathbf{n} = [1 \ \bar{1} \ 0]$ is exactly the same by the observation that the laminates are related by a rotation $R[180^\circ, \mathbf{e}_1]$ and thus in particular have the same norm $|\tilde{L}(\lambda)|$. $\square$

Remark 2.4. In terms of the full matrix $L(\lambda) \in \mathbb{R}^{3 \times 3}$ the condition reads

$$|L(\lambda)|^2 = 1 + \eta_1^2 + \eta_1^2 \eta_2^2$$

And for a general matrix $A \in \mathbb{R}^{3 \times 3}$ with $\lambda_i = \lambda_i(A^T A)$ denoting the eigenvalues of $A^T A$ we can derive analogously

$$0 = (\lambda_1 - 1)(\lambda_2 - 1)(\lambda_3 - 1) = \det^2 A - |\operatorname{cof} A|^2 - |A|^2 - 1$$

and thus $|A|^2 = 1 - \det^2 A + |\operatorname{cof} A|^2 = 1 - \eta_1^4 \eta_2^2 + |\operatorname{cof} A|^2$.

2.2 Quasiconvexity and Gradient Young Measures

In this section, based on [BJ92], [Bal89], [KP91] and [Mül99], we briefly review the closely related concepts of quasiconvexity and gradient Young measures. Both concepts will shed light on the question of existence and properties of minimisers/minimising sequences for the minimisation problem (E).

Generalisations of Convexity

Definition 2.4. (Notions of convexity)

A function $f : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ is said to be

- *convex* iff

$$f(\lambda A + (1 - \lambda)B) \leq \lambda f(A) + (1 - \lambda)f(B) \text{ for all } A, B \in \mathbb{R}^{3 \times 3}, \lambda \in (0, 1).$$

- *polyconvex* iff there exists a convex $g : \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \times \mathbb{R} \rightarrow \mathbb{R}$ such that

$$f(A) = g(A, \operatorname{cof} A, \det A) \text{ for all } A \in \mathbb{R}^{3 \times 3}.$$

- *quasiconvex* iff for some bounded set $\Omega \subset \mathbb{R}^3$ with $|\partial\Omega| = 0$ we have

$$f(A) \leq \frac{1}{|\Omega|} \int_{\Omega} f(A + D\varphi(x)) \, dx \text{ for all } \varphi \in W_0^{1,\infty}(\Omega, \mathbb{R}^3).$$

- *rank-one convex* iff for all $A, B \in \mathbb{R}^{3 \times 3}$ with $\operatorname{rank}(A - B) = 1$ we have

$$f(\lambda A + (1 - \lambda)B) \leq \lambda f(A) + (1 - \lambda)f(B) \text{ for all } \lambda \in (0, 1).$$

Remark 2.5. The following implications hold

$$f \text{ convex} \Rightarrow f \text{ polyconvex} \Rightarrow f \text{ quasiconvex} \Rightarrow \text{rank-one convex}.$$

The definitions of *convex*, *polyconvex* and *rank-one convex* can be extended to $f : \mathbb{R}^{3 \times 3} \rightarrow \overline{\mathbb{R}} = \mathbb{R} \cup \infty$ without change and we still have

$$f \text{ convex} \Rightarrow f \text{ polyconvex} \Rightarrow \text{rank-one convex}.$$

Remark 2.6. Quasiconvexity is sometimes defined such that the above property holds for all $\Omega \subset \mathbb{R}^3$ bounded with $|\partial\Omega| = 0$. However, using Vitali's covering theorem it can be shown that whenever it holds for one such set it holds for any.

Further, if the condition of quasiconvexity holds with equality, i.e. $\int_{\Omega} f(A) \, dx = \int_{\Omega} f(A + D\varphi(x)) \, dx$ for all $\varphi \in W_0^{1,\infty}(\Omega, \mathbb{R}^3)$, we call f *quasi-affine*. In particular, the value of the integral depends only on the boundary condition and thus f is a (smooth) *Null-Lagrangian*, i.e. the Euler-Lagrange equations $\operatorname{div} D_A f(Du) = 0$ hold for all smooth functions u . Alternatively, one can define quasi-affine by requiring that the condition of quasiconvexity holds for both f and $-f$, and in the same way we can also define rank-one affine and poly-affine. It can be shown that all these notions coincide (see e.g. [Dac07, Thm 5.20]).

The Importance of Quasiconvexity

Having defined these generalisations of convexity, we show that quasiconvexity plays a fundamental rôle in the multidimensional calculus of variations. We also demonstrate how it is conceptually significantly more challenging than usual convexity. Before doing so, we briefly recall the direct method in the calculus of variations.

Theorem 2.2. *(The direct method in the calculus of variations)*

Let $I : \mathcal{V} \rightarrow \mathbb{R} \cup \{\infty\}$ be a functional on some function space $\mathcal{V}$. Assume that I is bounded from below, i.e. $\inf I > -\infty$, so that there exists a minimising sequence $\{u_n\}_n$ with $I(u_n) \rightarrow \inf I$. Then if

1. $\{u_n\}_n$ admits a converging subsequence $\{u_{n_k}\}_k \subset \{u_n\}_n$, converging to u_0 with respect to some topology τ on V and
2. I is sequentially lower semi-continuous with respect to τ

the functional has a minimiser given by u_0 , i.e. $I(u_0) = \inf\{I(u) : u \in \mathcal{V}\}$.

Throughout this thesis we will focus on the case $\mathcal{V} = W^{1,\infty}(\Omega)$ endowed with the weak-* topology, i.e.

$$u_n \xrightarrow{*} u \text{ in } W^{1,\infty}(\Omega, \mathbb{R}) \iff \begin{cases} u_n \xrightarrow{*} u \text{ in } L^\infty(\Omega, \mathbb{R}), \\ Du_n \xrightarrow{*} Du \text{ in } L^\infty(\Omega, \mathbb{R}^{3 \times 3}), \end{cases}$$

where $v_n \xrightarrow{*} v$ in $L^\infty(\Omega)$ iff $\int_\Omega v_n w \, dx \rightarrow \int_\Omega v w \, dx$ for all $v \in L^1(\Omega)$. Since $L^1(\Omega)$ is separable we can apply the Banach–Alaoglu theorem and, whenever our energy function (E) is bounded, Condition 1 in Theorem 2.2 is satisfied. It thus remains to investigate Condition 2.

In one-dimension, it is well known (see e.g. [Dac07, Th. 3.13]), that for functionals of the form (E), a necessary and sufficient condition for weak* sequential lower semi-

continuity is convexity of the integrand. The next theorem which is essentially due to [Mor52], with later refinements by [Mey65; AF84; Mar85], shows that in higher dimensions the correct condition on the integrand is quasiconvexity instead.

Theorem 2.3. *Let Ω be a bounded Lipschitz domain in $\mathbb{R}^n$ and $f : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ be continuous such that $|f(A)| \rightarrow \infty$ as $|A| \rightarrow \infty$. Then the functional $E(u) := \int_{\Omega} f(Du) dx$ is weakly* sequentially lower semicontinuous (w^*slsc) on $W^{1,\infty}(\Omega, \mathbb{R}^3)$ if and only if f is quasiconvex.*

Thus, quasiconvexity provides use with a key ingredient towards applying the direct method of calculus of variations in higher dimensions. We are lead to the following question:

- Is our free energy density W quasiconvex?

We will be able to provide a rigorous and elegant answer to this question with the help of gradient Young measures (see Remark 2.11). For now, we satisfy ourselves with the following illustration. Assume that $\theta < \theta_c$ and consider two compatible martensitic variants U_1 and $RU_2 = U_1 + \mathbf{c} \otimes \mathbf{n}$ and a unit cube Ω that is cut in half by the interface plane (cf. Figure 2.5) and whose faces are aligned with $\mathbf{n}$. Now let the boundary condition be $y(x) = \frac{1}{2}(U_1 + RU_2)x = U_1x + \frac{1}{2}\langle x, \mathbf{n} \rangle \mathbf{c} =: Ax$ with $A \notin K = \bigcup_i \text{SO}(3)U_i$ and assume without loss of generality that $W(U_1) = -\tau < 0$. Define the function $\varphi \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ by

$$\varphi(x) = \begin{cases} \frac{1}{2}\langle x, \mathbf{n} \rangle \mathbf{c} + \frac{1}{4}\mathbf{c}, & \langle x, \mathbf{n} \rangle \leq 0, \\ -\frac{1}{2}\langle x, \mathbf{n} \rangle \mathbf{c} + \frac{1}{4}\mathbf{c}, & \langle x, \mathbf{n} \rangle > 0, \end{cases}$$

so that it vanishes on the faces parallel to the interface. Now suppose that in the definition of quasiconvexity (cf. Definition 2.4) it suffices that φ vanishes at the parallel interfaces and is thus admissible in the definition of quasiconvexity. Noting that for $\langle x, \mathbf{n} \rangle \leq 0$ we have $A + D\varphi(x) = U_1 + \frac{1}{2}\mathbf{c} \otimes \mathbf{n} + \frac{1}{2}\mathbf{c} \otimes \mathbf{n} = RU_2$ and similarly for $\langle x, \mathbf{n} \rangle > 0$ we have $A + D\varphi(x) = U_1$, we conclude that the right-hand side in the

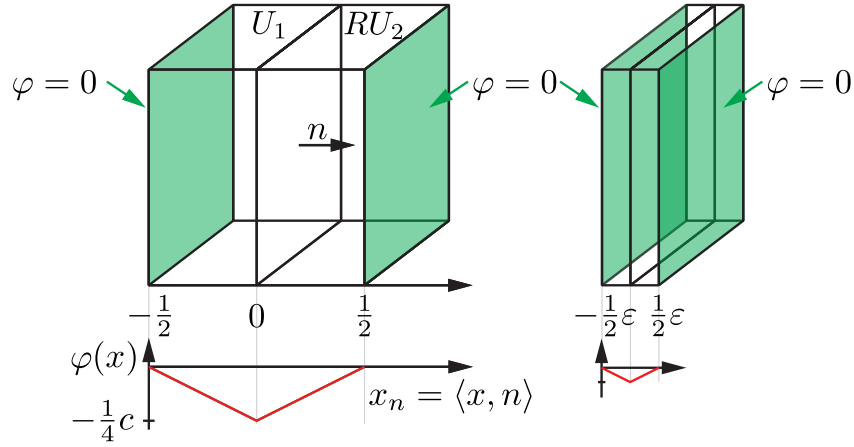


Fig. 2.5. A cube Ω with faces parallel to the interface plane between two compatible martensitic variants U_1 and $RU_2 = U_1 + c \otimes n$. The boundary condition is given by $y(x) = \frac{1}{2}(U_1 + RU_2)x$. The function $\varphi \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ vanishes at all boundary planes with normal n . On the left side of the interface plane, the deformation gradient is given by $A + D\varphi(x) = U_1$ and on the right side by $A + D\varphi(x) = RU_2$. By scaling the width of this construction by ε the situation of $\varphi \in W_0^{1,\infty}(\Omega, \mathbb{R}^3)$ is approached and the condition of quasiconvexity (cf. Definition 2.4) is violated.

definition of quasiconvexity equals $-\tau$, whereas the left-hand side is strictly bigger than $-\tau$ and thus W is not quasiconvex.

Of course, this argument relies on the (false) assumption that, in the definition of quasiconvexity, it suffices for φ to vanish at the faces with normal n . In fact, since the construction of φ is essentially one-dimensional it can never vanish at the other faces of the cube Ω . However, if one takes a thin slice of this cube (cf. Figure 2.5 (right)) and repeats the same construction, most of its boundary has normal n and thus we approximate the situation of vanishing boundary conditions. Looking at this as a limiting process and gluing the thin slices back together to get back the original cube is the motivation for the introduction of gradient Young measures in this setting.

Having established that W is *not* quasiconvex and thus by Theorem 2.3 that the functional (E) is not w^* slsc we conclude that the minimum is generally not attained. Given the absence of minimisers it is natural look at the relaxed problem

$$\bar{E}(y) = \int_{\Omega} W^{\text{qc}}(Dy) \longrightarrow \min .$$

Here, W^{qc} denotes the quasiconvex envelope of W , i.e. the largest quasiconvex function below W

$$W^{\text{qc}}(A) := \sup\{f(A) \mid f \leq W, f \text{ quasiconvex}\} \quad \text{for all } A \in \mathbb{R}^{3 \times 3}.$$

Unfortunately, only very few explicit examples or families of exclusively quasiconvex functions are known. One of the reasons for this scarcity is the absence of a local characterisation.

Theorem 2.4. (*Non-locality of quasiconvexity, [Kri99]*)

Let $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ with $m \geq 3, n \geq 2$. Then there is no local condition (i.e. a condition involving f and any number of derivatives of f at a point $A \in \mathbb{R}^{m \times n}$) that is equivalent to quasiconvexity.

The proof relies on a famous example by [Šve92] of a function in $\mathbb{R}^{3 \times 2}$ that is rank-one convex and locally quasiconvex but *not* quasiconvex. Using this example, Kristensen constructs a smooth function which is quasiconvex in the neighbourhood of any point $A \in \mathbb{R}^{m \times n}$ but is not quasiconvex itself. The same statement holds for polyconvexity instead of quasiconvexity even for $m \geq 2$.

As a results, it is usually only possible to find upper and lower bounds on W^{qc} . We have seen that polyconvexity is a notion that is weaker than convexity and stronger than quasiconvexity and rank-one convexity a notion that is weaker than quasiconvexity. Thus, by defining the polyconvex envelope W^{pc} and the rank-one convex envelope W^{rc} analogously, we are able to sandwich W^{qc} .

Another way of avoiding some of these difficulties is to employ the following (equivalent) variational definition of W^{qc} .

Definition 2.5. (The quasiconvexification of W , [Dac07, Thm. 6.9])

Let W be our free energy density. Then for $A \in \mathbb{R}^{3 \times 3}$ we define

$$W^{\text{qc}}(A) := \frac{1}{|\Omega|} \inf_{\phi \in W_0^{1,\infty}(\Omega)} \int_{\Omega} W(A + D\phi(x)) \, dx,$$

where $\Omega \subset \mathbb{R}^3$, $|\partial\Omega| = 0$ is any bounded set. In particular W^{qc} is independent of the choice of Ω .

We also define the corresponding relaxation for sets called the convex (c), polyconvex (pc), quasiconvex (qc), rank-one convex (rc) hull respectively.

Definition 2.6. (Generalised convex hulls)

Let $K \subset \mathbb{R}^{3 \times 3}$ be compact and $\alpha \in \{\text{qc}, \text{pc}, \text{rc}, \text{c}\}$. We define the α -convex hull of K by

$$K^\alpha := \{F \in \mathbb{R}^{3 \times 3} : f(F) \leq \max_{G \in K} f(G) \text{ for all } f : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R} \text{ } \alpha\text{-convex} \}.$$

If $K^\alpha = K$ we call the set K α -convex.

Remark 2.7. K^α is the set of matrices that cannot be separated from K by α -convex functions in the sense that for any $F \notin K^\alpha$ there exists an α -convex function f such that $f(F) > f(G)$ for all $G \in K$.

Further, in the case of rank-one convexity one can also define a hull by a pointwise condition rather than by sublevel sets.

Definition 2.7. (The lamination convex hull K^{lc})

Let $K^{(0)} := K$ and define

$$K^{\text{lc}} = \bigcup_{i=1}^{\infty} K^{(i)},$$

where $K^{(i+1)} := K^{(i)} \cup \{\lambda A + (1 - \lambda)B : A, B \in K^{(i)}, \text{rank } A - B = 1, \lambda \in [0, 1]\}$.

That is, the lamination convex hull is obtained by successively adding rank-one segments.

Remark 2.8. It is obvious that $K^{\text{lc}} \subset K^{\text{rc}}$. However, due to the existence of so-called T_N configurations (see e.g. [Szé04] and also [Mül99, Sec 2.5] for an overview), the two hulls generally do not coincide. We further note that some authors call K^{lc} the rank-one convex hull (see e.g. [Dac07, Thm. 7.17]).

Remark 2.9. The following inclusions hold

$$K^{\text{lc}} \subset K^{\text{rc}} \subset K^{\text{qc}} \subset K^{\text{pc}} \subset K^{\text{c}}$$

and furthermore, the quasiconvex hull K^{qc} of the martensite wells provides an (abstract) answer to our original question of what (affine) boundary conditions allow approximate solutions. We have²

$$K^{\text{app}} = K^{\text{qc}}.$$

In particular, K^{qc} tells us what minimisers we can expect to see on a macroscopic scale and is thus an important piece in the understanding of martensitic phase transformations.

Gradient Young Measures

Next we introduce Young measures to describe the macroscopic behaviour of minimising sequences more efficiently. The main application will lie in the classification of highly oscillating sequences of deformation gradients $\{Dy_i(x)\}$ that only converge weakly^(*) and in the characterisation of the limiting value $\lim_{i \rightarrow \infty} W(Dy_i(x))$ near $x \in \Omega$.

Theorem 2.5. (*Fundamental theorem for Young measures, [Bal89]*)

Let $\Omega \subset \mathbb{R}^n$ be measurable, $K \subset \mathbb{R}^n$ closed and $y_i : \Omega \rightarrow \mathbb{R}^n$ a sequence of measurable functions s.t. $y_i(\cdot) \rightarrow K$ in measure. Then there exists a subsequence $\{y_{i_k}\}_k \subset \{y_i\}_i$

²See [Mül99, Thm 4.10].

and a family of positive measures $\{\nu_x\}_{x \in \Omega} \subset \mathcal{M}(\mathbb{R}^n)$ depending measurably on x such that

1. $\|\nu_x\|_{\mathcal{M}(\mathbb{R}^n)} := \int_{\mathbb{R}^n} d\nu_x \leq 1$ for a.e. $x \in \Omega$,
2. $\text{supp } \nu_x \subset K$ for a.e. $x \in \Omega$,
3. $f(y_{i_k}) \xrightarrow{*} \bar{f}$ in $L^\infty(\Omega)$ for all $f \in C_0(\mathbb{R}^n)$, where for a.e. $x \in \Omega$ we defined

$$\bar{f}(x) := \langle \nu_x, f \rangle = \int_{\mathbb{R}^n} f(\lambda) d\nu_x(\lambda).$$

If further $\{y_{i_k}\}_k$ satisfies

$$\lim_{M \rightarrow \infty} \sup_k |\{x \in \Omega \cap U_R(0) : |y_{i_k}(x)| \geq M\}| = 0 \text{ for all } R > 0,$$

then

$$\|\nu_x\|_{\mathcal{M}(\mathbb{R}^n)} = 1 \text{ for a.e. } x \in \Omega,$$

i.e. ν_x is a probability measure for a.e. $x \in \Omega$ and for any measurable set $A \subset \Omega$ and for any $f \in C(\mathbb{R}^n)$ s.t. $\{f(y_{i_k})\}_i$ is sequentially weakly relatively compact in $L^1(A)$ we have

$$f(y_{i_k}) \rightharpoonup \bar{f} = \int_{\mathbb{R}^n} f(\lambda) d\nu_x(\lambda) \text{ in } L^1(A).$$

The above conclusion shows in particular that $\langle \nu_x, f \rangle = \int_{\mathbb{R}^n} f(\lambda) d\nu_x(\lambda)$ is well defined (since a priori $\langle \nu_x, f \rangle$ is only well defined for $f \in C_0(\mathbb{R}^n, \mathbb{R})$) and that $\langle \nu_x, f \rangle \in L^1(A)$.

We may interpret Young measures at x_0 as the probability of finding a certain value in the sequence $\{y_i(x)\}_i$ for $x \in B_r(x_0)$ in the limit $i \rightarrow \infty$ and then $r \rightarrow 0$.

Lemma 2.5. [Bal89] Let $\{y_i\}_{i=1}^\infty$ with $y_i : \Omega \rightarrow \mathbb{R}^n$ for all $i = 1, 2, \dots$ generate the Young measure $\{\nu_x\}_{x \in \Omega} \subset \mathcal{M}(\mathbb{R}^n)$ then for $\mathcal{B} \subset \mathbb{R}^n$ we have

$$\nu_{x_0}(\mathcal{B}) = \lim_{r \rightarrow 0} \lim_{i \rightarrow \infty} \frac{|\{x \in B_r(x_0) : y_i(x) \in \mathcal{B}\}|}{|B_r(x_0)|}$$

and in particular if $y_i \rightarrow y$ strongly in L^p then $\nu_x = \delta_{y(x)}$.

We now apply this theory in the context of solid phase transformations and thus we ought to characterise Young measures that arise from a sequence of gradients.

Definition 2.8. (Gradient Young measure)

Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary and let $\nu : \Omega \rightarrow \mathcal{M}(\mathbb{R}^{n \times n})$ be weakly* measurable. Then ν is called a *gradient Young measure* iff there exists a sequence $\{y_i\}_i$ with $y_i : \Omega \rightarrow \mathbb{R}^n$ s.t.

$$y_i \xrightarrow{*} y \text{ in } W^{1,\infty}(\Omega, \mathbb{R}^n)$$

and for all $\varphi \in C_0(\mathbb{R}^{3 \times 3})$ we have

$$\varphi(Dy_i(x)) \xrightarrow{*} \bar{\varphi}(x) = \int_{\mathbb{R}^{3 \times 3}} \varphi(A) d\nu_x(A) \text{ in } L^\infty(\Omega).$$

If $\nu \equiv \nu_x$ does not depend on x we will call ν a *homogeneous gradient Young measure*.

Remark 2.10. If $K = \text{supp } \nu_x \subset \mathbb{R}^{3 \times 3}$ is compact we can choose $\varphi \in C_0(\mathbb{R}^{3 \times 3})$ such that $\varphi(x)|_K = x$ and in particular since id is a minor and thus weakly continuous we have

$$Dy(x) = \int_K A d\nu_x(A) \text{ a.e. in } \Omega.$$

A similar property holds for any minor (cf. [Mor66]).

In our context, the main importance of gradient Young measures is their ability to associate a rigorous mathematical concept to the idea of a very fine mixture of phases (cf. Figure 2.5).

Definition 2.9. (Simple laminate)

We call the gradient Young measure (GYM) given by $\nu_x \equiv \lambda \delta_A + (1 - \lambda) \delta_B$ with $\text{rank}(A - B) = 1$, $A, B \in \mathbb{R}^{3 \times 3}$, $\lambda \in [0, 1]$ a *simple laminate* with volume fraction λ for the variant A and $(1 - \lambda)$ for the variant B . The centre of mass $\bar{\nu} = \langle \nu, id \rangle = \lambda A + (1 - \lambda)B$ is called the *average* or *macroscopic deformation gradient* of the laminate. See Figure 2.6 for an illustration.

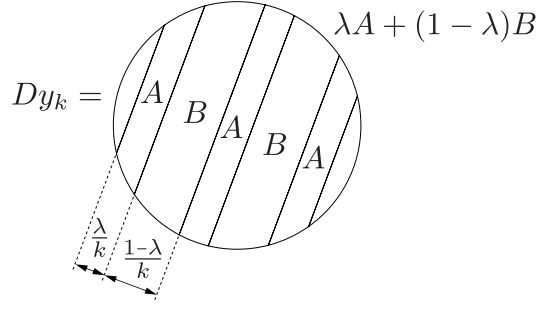


Fig. 2.6. A sequence $\{Dy_k\}_k$ of two compatible gradients, A and B , that converges to the gradient Young measure $\lambda\delta_A + (1-\lambda)\delta_B$ as $k \rightarrow \infty$. The macroscopic deformation gradient is $\lambda A + (1-\lambda)B$.

Remark 2.11. Definition 2.9 allows us to show the failure of quasiconvexity of our free energy W density more elegantly. To this end assume that $\theta < \theta_c$ and $W(U_i) = -\tau < 0$. Now consider the sequence $\{y_i\}_i$ that generates the homogeneous GYM $\nu = \lambda\delta_{U_1} + (1-\lambda)\delta_{RU_2}$ with centre of mass $F = \bar{\nu} = \lambda U_1 + (1-\lambda)RU_2$. Then on the one hand

$$\lim_{i \rightarrow \infty} \int_{\Omega} W(Dy_i(x)) \, dx = |\Omega| \int_{\text{supp } \nu} W(A) \, d\nu(A) = -|\Omega|\tau.$$

But on the other hand $F \notin \bigcup_i \text{SO}(3)U_i$ and thus $W(F) > -\tau$ (cf. Definition 2.1 (4)). Therefore, W cannot be quasiconvex.

The following theorem from [KP91] provides a characterisation of gradient Young measures (GYM) and establishes its relation to quasiconvexity.

Theorem 2.6. (Characterisation of GYM, [KP91])

Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary. Then a weakly*-measurable map $\nu : \Omega \rightarrow \mathcal{M}(\mathbb{R}^{n \times n})$ is a GYM iff $\nu_x \geq 0$ a.e. and there exists a compact set $K \subset \mathbb{R}^{3 \times 3}$ and $y \in W^{1,\infty}(\Omega, \mathbb{R}^n)$ s.t.

1. $\text{supp } \nu_x \subset K$ for a.e. $x \in \Omega$,
2. $\langle \nu_x, id \rangle = Dy(x)$ for a.e. $x \in \Omega$,
3. $\langle \nu_x, f \rangle \geq f(\langle \nu_x, id \rangle)$ for all quasiconvex $f : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and a.e. $x \in \Omega$.

Thus, roughly speaking, GYM are measures that satisfy Young's inequality for quasi-convex functions. We summarise the results in the following definition

Definition 2.10. For $K \subset \mathbb{R}^{3 \times 3}$ compact we set

$$\begin{aligned} \mathcal{M}^{\text{qc}}(K) := & \{\nu \in \mathcal{M}(\mathbb{R}^{3 \times 3}) \mid \nu \geq 0, \text{supp } \nu \subset K, \\ & \langle \nu, f \rangle \geq f(\langle \nu, id \rangle) \text{ for all } f : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R} \text{ quasiconvex}\} \end{aligned}$$

as the set of *homogeneous GYM supported on K* .

With this definition at hand we have yet another way of abstractly characterising the set of approximate solutions. We have³

$$K^{\text{app}} = K^{\text{qc}} = \{\langle \nu, id \rangle : \nu \in \mathcal{M}^{\text{qc}}(K)\}.$$

Therefore the centres of masses of homogeneous GYMs supported on K characterise the quasiconvex hull of K and thus the set of admissible boundary conditions for having minimising sequences (=approximate solutions) for the energy minimisation problem (E).

³See [Mül99, Thm 4.10].

The Three-Well Problem

In the previous chapter we have seen that for $\theta < \theta_c$ the quasiconvex hull of the martensite wells characterises all macroscopically energy minimising deformation gradients. In particular, the explicit determination of K^{qc} can help to determine what macroscopic deformations should be observable experimentally. The importance of this problem has been emphasised in [Bal02, Problem 16]. So far, the explicit determination of K^{qc} for crystalline materials in three space dimensions has only been successful in a few specific cases such as the two well-problem [BJ92] and the case of smectic C liquid crystals [Ada+07].¹ In particular, it is an open problem to find the quasiconvex hull for the three tetragonal wells in a cubic-to-tetragonal phase transformation. This problem is known as the *three-well problem*.

The goal of this chapter is to develop new methods and obtain bounds on the three-well problem. The overall method is going to be similar to previous approaches. That is, one first makes an educated guess for the outer bound K^{pc} and then shows that it coincides with the inner bound K^{lc} , which is obtained by a careful construction of laminates. A novelty in the present approach is the heavy exploitation of the inherent symmetry and a very efficient choice of laminates to construct the inner bounds. In particular, this careful choice seems to be advantageous over previous approaches by e.g. [Pei13].

We start with the exploitation of the symmetry. Commonly, particularly in the cases we are interested in, the set K is invariant under group operations. This invariance can be used to simplify the determination of generalised convex hulls.

¹For related work on isotropic materials see also [DD02; Dac07].

Lemma 3.1. (Invariance properties of α -convex hulls)

Let K be invariant under a group action G , i.e. $K = GK$ and $\alpha \in \{\text{qc}, \text{pc}, \text{rc}, \text{c}\}$. Then the α -convex hull is the sublevel set of all α -convex functions that are invariant under G .

$$K^\alpha = \{A : \phi(A) \leq \max_{B \in K} \phi(B) \text{ for all } \phi \text{ } \alpha\text{-convex and invariant under } G\} =: K^*.$$

Proof. The direction $K^\alpha \subset K^*$ is trivial. Thus it remains to show that $K^\alpha \supset K^*$. We show that $A \notin K^\alpha$ implies $A \notin K^*$. Let $A \notin K^\alpha$. Thus there exists an α -convex ϕ_0 which is not invariant under G such that

$$\phi_0(A) > \max_{B \in K} \phi_0(B).$$

We now define the G invariant function $\Phi(F)$ by

$$\Phi(F) := \max_{g \in G} \phi_0(gF),$$

which is α -convex as the supremum over α -convex functions. We obtain

$$\Phi(A) \geq \phi_0(A) > \max_{B \in K} \phi_0(B) = \max_{B \in K} \max_{g \in G} \phi_0(gB) = \max_{B \in K} \Phi(B)$$

and thus $A \notin K^*$. □

For completeness we also state the analogous result for the α -convex envelope of functions.

Lemma 3.2. (Invariance properties for α -convex envelopes)

Let $f : \mathbb{R}^{3 \times 3} \supset \Omega \rightarrow \mathbb{R}$ be invariant under the group G , i.p. $G\Omega = \Omega$ and $\alpha \in \{\text{qc}, \text{pc}, \text{rc}, \text{c}\}$. Then

$$f^\alpha(A) = \sup\{g(A) : g \leq f \text{ on } \Omega, g \text{ is } \alpha\text{-convex and } G \text{ invariant}\} =: f^*(A)$$

for all $A \in \mathbb{R}^{3 \times 3}$.

Proof. Recall that

$$f^\alpha(A) = \sup\{g(A) : g(B) \leq f(B) \text{ for all } B \in \Omega, g \text{ is } \alpha\text{-convex}\}$$

for all $A \in \mathbb{R}^{3 \times 3}$ and thus $f^\alpha \geq f^*$. Therefore it remains to show that $f^\alpha \leq f^*$. Let us assume the contrary, i.e. that there exists $A \in \mathbb{R}^{3 \times 3}$ and $g_0 \leq f$ α -convex, g_0 not G invariant such that

$$f(A) \geq g_0(A) > g(A)$$

for all g α -convex, G invariant with $g \leq f$. Now we define

$$G_0(A) := \max_{g \in G} g_0(gA),$$

which is α -convex as the supremum over α -convex functions. Then since $g_0 \leq f$ we have $g_0(gA) \leq f(gA) = f(A)$ for all $g \in G$ and thus

$$G_0(A) \leq f(A).$$

On the other hand by the definition of G_0 and by assumption we have

$$G_0(A) \geq g_0(A) > g(A),$$

for all g α -convex and G -invariant. But $G_0(A)$ is α -convex and G invariant. A contradiction. $\square$

3.1 Outer bounds on K^{qc} : The Polyconvex Hull

From now on we will focus on the three-well problem and without loss of generality we set $U_1 = \text{diag}(\eta_2, \eta_1, \eta_1)$. Having Lemma 3.1 in mind we are looking for frame indifferent polyconvex functions whose sublevel sets contain the wells. In order to achieve optimal bounds we should require that *good* polyconvex functions are constant on the wells, i.e. they do not depend on the choice of U_i corresponding

to invariance under postmultiplication with $P \in \mathcal{P}^{24}$. The following ‘elementary’ functions

$$\begin{aligned} p_1(A) &= |AP\mathbf{e}_1|^2, \\ p_2(A) &= |AP(\mathbf{e}_1 + \mathbf{e}_2)|^2, \\ p_3(A) &= |AP(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2, \\ q_i(A) &= p_i(\text{cof } A), \quad i = 1, 2, 3 \end{aligned}$$

are polyconvex for all $P \in \mathcal{P}^{24}$. Further, all sums of the above elementary polyconvex functions are polyconvex. The following polyconvex functions are good:

$$\mathcal{G} := \{p_3, q_3, f_1(A) := |A\mathbf{e}_1|^2 + |\text{cof } A\mathbf{e}_1|^2, f_2(A) := |A(\mathbf{e}_1 + \mathbf{e}_2)|^2 + |\text{cof } A(\mathbf{e}_1 - \mathbf{e}_2)|^2\}$$

Conjecture 3.1. (*The three-well problem*)

Let $K = \text{SO}(3)U_1\mathcal{P}^{24}$ with $U_1 = \text{diag}(\eta_2, \eta_1, \eta_1)$, then

$$K^{\text{qc}} = K^{\text{pc}} = K^{\text{lc}} = K^* := \{A : g(AP) \leq g(U_1) \forall g \in \mathcal{G} \text{ and } \forall P \in \mathcal{P}^{24}\} \cap \det^{-1}(\det U_1).$$

We note that since $K^{\text{pc}} = \bigcap \{f^{-1}(\{0\}) : f \text{ is polyconvex and } f|_K \equiv 0\}$ we always have $K^{\text{pc}} \subset K^*$. Further, by Remark 2.9 we know that $K^{\text{lc}} \subset K^{\text{qc}} \subset K^{\text{pc}}$ and thus we can prove the above conjecture by showing that any element in K^* can be attained by an element in K^{lc} .

However, instead of matching every element in K^* with elements in K^{lc} , it suffices to exhaust the relative² boundary ∂K^* with elements in K^{lc} . This is because, given any interior point $A \in K^*/\partial K^*$ and defining $A(t) := A + t\mathbf{a} \otimes \mathbf{n}$ for some rank-one matrix $\mathbf{a} \otimes \mathbf{n}$, we have $A(t^-) \in \partial K^*$ for some $t^- < 0$ and $A(t^+) \in \partial K^*$ for some $t^+ > 0$. That is, we can achieve $A = A(0) = \frac{t^+}{t^+ - t^-} A(t^-) + \frac{-t^-}{t^+ - t^-} A(t^+)$ as a laminate between $A(t^-)$ and $A(t^+)$ (cf. Lemma 3.5 for further details).

²Relative to the determinant constraint.

In order to determine the minimum number of required laminations we perform a quick dimensional check. By frame indifference, i.e. the left invariance of K by $\text{SO}(3)$, we may assume without loss of generality that any element in $A \in K^*$ is in upper triangular form, i.e.

$$A = \begin{pmatrix} a & d & e \\ 0 & b & f \\ 0 & 0 & c \end{pmatrix}.$$

By the determinant constraint $c = \det U_1 / (ab)$. Furthermore, since we are only interested in elements on the relative boundary of K^* , A needs to satisfy $g(A) = g(U_1)$ for some $g \in \mathcal{G}$. Therefore, ∂K^* is essentially four dimensional.

Thus, since K^{lc} inherits the frame indifference from K , it suffices to construct elements $F \in \text{SO}(3)\mathcal{M}$, where $\mathcal{M} \subset K^{\text{lc}}$ is an essentially four dimensional set that satisfies the same boundary condition, i.e.

$$g(M) = g(U_1) \text{ for all } M \in \mathcal{M}.$$

3.2 Inner Bounds on K^{qc} : The Lamination Convex Hull

By our previous considerations, we need to find a sufficiently large class (at least four dimensional) of elements in K^{lc} . The easiest way of obtaining these elements is the construction of higher order laminates. We will start with classifying all first order laminates.

Lemma 3.3. $(K^{(1)})$

The first order lamination convex hull $K^{(1)}$ coincides with the set of simple laminates between two wells. That is

$$K^{(1)} = \text{SO}(3) \left\{ F \in \mathbb{R}^{3 \times 3} : F = U_1 + \lambda \mathbf{a} \otimes \mathbf{n}, \lambda \in [0, 1] \right\} \mathcal{P}^{24},$$

where $\mathbf{a} = \sqrt{2} \frac{\eta_2^2 - \eta_1^2}{\eta_2^2 + \eta_1^2} (-\eta_2, \eta_1, 0)$ and $\mathbf{n} = \frac{1}{\sqrt{2}} (1, 1, 0)$. The values of $\mathbf{a}$ and $\mathbf{n}$ are precisely given by the first solution of Mallard's law (Lemma 2.4).

Proof. By Lemma 2.2, there are no rank-one connections between a well and itself and all rank one connections between the wells are given by Mallard's law. Further, it suffices to only take the first solution of Mallard's law. This can be seen by e.g. considering U_1 and conjugating with $P_{14} = R[180^\circ, \mathbf{e}_2]$, so that $P_{14}U_1P_{14} = U_1$, $P_{14}U_2P_{14} = U_2$ and $P_{14}\mathbf{n} = \frac{1}{\sqrt{2}}(-1, 1, 0)$ and thus we have obtained the second solution. $\square$

The Two-Well Problem Revisited

Besides providing improved bounds for the three-well problem, our approach also provides a straightforward method to prove the two-well problem.³ Let us first recall the original result:

Lemma 3.4. *(The two-well problem, [BJ87])*

Let $K_i = \text{SO}(3)U_j \cup \text{SO}(3)U_k$, $(i, j, k) \in \mathcal{S}_3$. Then the quasiconvex hull K_i^{qc} coincides with both the lamination convex and the polyconvex hull. It is given by

$$K_i^{\text{rc}} = K_i^{\text{qc}} = K_i^{\text{pc}} = \{F : \det F = \eta_1^2 \eta_2, F^T F \mathbf{e}_i = \eta_1^2 \mathbf{e}_i, |F(\mathbf{e}_j \pm \mathbf{e}_k)|^2 \leq \eta_1^2 + \eta_2^2\}.$$

Further, each element in K_i^{qc} can be achieved by at most a second order laminate.

Lemma 3.5. *(The two-well problem revisited)*

Let $U_1 = \text{diag}(\eta_2, \eta_1)$, $U_2 = \text{diag}(\eta_1, \eta_2)$ and $K = \text{SO}(2)U_1 \cup \text{SO}(2)U_2$. Then

$$K^{\text{qc}} = \left\{ F \in \mathbb{R}^{2 \times 2} : |F(\mathbf{e}_1 \pm \mathbf{e}_2)|^2 \leq \eta_1^2 + \eta_2^2, \det F = \eta_1 \eta_2 \right\} =: \tilde{K}$$

³This methods is similar to the one in [Ada+07, Lemma 4.1].

Proof. Let us first define the boundary functions

$$f_1(F) = |F(\mathbf{e}_1 + \mathbf{e}_2)|^2, \quad f_2(F) = |F(\mathbf{e}_1 - \mathbf{e}_2)|^2 = f_1(FQ)$$

of the polyconvex hull, where

$$Q = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Further, the rotation $P = P_6 = R[180^\circ, [1 \bar{1} 0]]$ relates the two diagonal wells, i.e. $U_2 = PU_1P^T$, and thus by By Mallard's law (Lemma 2.4) the first solution of the twinning equation is given by

$$S = 2 \left(\frac{\sqrt{2}\eta_1^2\eta_2^2}{\eta_1^2 + \eta_2^2} \begin{pmatrix} 1 & -1 \\ \eta_2 & \eta_1 \end{pmatrix} - \frac{1}{\sqrt{2}}(\eta_2, -\eta_1) \right) \otimes \frac{1}{\sqrt{2}}(1, -1) = \frac{\eta_2^2 - \eta_1^2}{\eta_1^2 + \eta_2^2} \begin{pmatrix} -\eta_2 & \eta_2 \\ -\eta_1 & \eta_1 \end{pmatrix}$$

and thus we have found the following elements in $K^{\text{rc}} \subset K^{\text{qc}}$

$$F_\lambda = U_1 + \lambda S = \frac{\eta_2^2 - \eta_1^2}{\eta_1^2 + \eta_2^2} \begin{pmatrix} \eta_2 \frac{\eta_1^2 + \eta_2^2}{\eta_2^2 - \eta_1^2} - \lambda\eta_2 & \lambda\eta_2 \\ -\lambda\eta_1 & \eta_1 \frac{\eta_1^2 + \eta_2^2}{\eta_2^2 - \eta_1^2} + \lambda\eta_1 \end{pmatrix}.$$

An upper triangularisation yields

$$F_\lambda = \begin{pmatrix} a & d \\ 0 & b \end{pmatrix}$$

with

$$\begin{aligned} a &= \sqrt{\frac{(\lambda(\eta_2^2 - \eta_1^2) + \eta_2^2)^2 + \eta_1^2\eta_2^2}{\eta_1^2 + \eta_2^2}}, \\ d &= \frac{\lambda(1 - \lambda)(\eta_2^2 - \eta_1^2)^2}{(\eta_1^2 + \eta_2^2)a}, \\ b &= \frac{\eta_1\eta_2}{a}, \end{aligned}$$

and we clearly have $F_0 = U_1$ and $F_1 = U_2$. Further, since $\mathbf{e}_1 - \mathbf{e}_2 \perp \mathbf{e}_1 + \mathbf{e}_2$ we have $f_1(F_\lambda) = |F_\lambda(\mathbf{e}_1 + \mathbf{e}_2)|^2 = \eta_1^2 + \eta_2^2$ for all $\lambda \in [0, 1]$ and thus the simple laminate is on the boundary of $\tilde{K}$.

We now want to show the reverse direction. That is, given any matrix G on the relative boundary of $\tilde{K}$, i.e. without loss of generality $f_1(G) = \eta_1^2 + \eta_2^2$, there exist $R \in \text{SO}(2), \lambda \in [0, 1]$ such that $G = RF_\lambda$. By the $\text{SO}(2)$ invariance we can assume that G is in upper triangular form with positive diagonal elements, i.e.

$$G = \begin{pmatrix} a & d \\ 0 & b \end{pmatrix}. \quad (3.1)$$

Further, since we want to satisfy f_1 with equality we can assume that $d \geq 0$. We also note that $a, b \in [\eta_1, \eta_2]$. This is because by assumption

$$a^2 + b^2 = a^2 + \frac{\eta_1^2 \eta_2^2}{a^2} \leq \eta_1^2 + \eta_2^2$$

and $a \mapsto a^2 + \frac{\eta_1^2 \eta_2^2}{a^2}$ is a convex function of a and achieves its maximum at the points $a = \eta_1, \eta_2$. We claim that a completely characterises G . By the determinant constraint b is given by

$$b = \frac{\eta_1 \eta_2}{a}$$

and from $f_1(G) = \eta_1^2 + \eta_2^2$ we obtain

$$(a + d)^2 + \frac{\eta_1^2 \eta_2^2}{a^2} = \eta_1^2 + \eta_2^2$$

and the only non-negative solution is

$$d = \frac{1}{a}(-a^2 + \sqrt{a^2(\eta_1^2 + \eta_2^2) - \eta_1^2 \eta_2^2}) \geq 0.$$

with $d = 0$ iff $a \in \{\eta_1, \eta_2\}$. Thus, up to rotations, all matrices that fulfil the inequality with equality only depend on one parameter a and we have shown that we can achieve all such matrices by simple laminates. Thus we have constructed the entire one-parameter family that gives equality for f_1 . The case of equality in the second equation follows analogously by symmetry considerations (postmultiplication with Q gives the solution that fulfils the second inequality with strict equality).

It remains to show the attainment result for any matrix G in the interior of $\tilde{K}$. To this end, let G be upper triangular as in (3.1) and define

$$G(t) := G + t\mathbf{e}_1 \otimes \mathbf{e}_2 = \begin{pmatrix} a & d+t \\ 0 & b \end{pmatrix}.$$

Next, we note that $\det G(t) = \det G$ and set

$$t^+ := \inf\{t : f_1(G(t)) = \eta_1^2 + \eta_2^2\}, \quad t^- := \sup\{t : f_2(G(t)) = \eta_1^2 + \eta_2^2\}$$

so that $G(t^\pm) \in K^{\text{lc}}$. We claim that $t^+ > 0$ and $t^- < 0$. To show this, recall that we can always assume $a > 0, b > 0$ and that on the boundary

$$f_i(G) = (a \pm d)^2 + b^2 = \begin{cases} a^2 + 2ad + d^2 + b^2 \rightarrow \max & \text{for } i = 1, \\ a^2 - 2ad + d^2 + b^2 \rightarrow \max & \text{for } i = 2. \end{cases}$$

In particular, $f_1(G)$ can only be maximal for $d > 0$ and $f_2(G)$ can only be maximal for $d < 0$. Therefore, $t^+ > 0$ and $t^- < 0$ as claimed and thus by setting $\lambda^* = \frac{-t^-}{t^+ - t^-} \in (0, 1)$ we arrive at

$$G = \lambda^* G(t^+) + (1 - \lambda^*) G(t^-) \in K^{\text{lc}}.$$

□

Remark 3.1. If one wants to consider the full 3×3 matrices U_1, U_2 , one just needs to add the polyconvex restrictions

$$|A\mathbf{e}_3|^2 \leq \eta_1^2 \text{ and } |\text{cof } A\mathbf{e}_3|^2 \leq \eta_1^2 \eta_2^2$$

yielding $A^T A\mathbf{e}_3 = \eta_1^2 \mathbf{e}_3$. Clearly, this restriction is satisfied by all laminates between U_1 and U_2 .

Higher Order Laminates

In the following we would like to characterise second and third order laminates. As the computations get more complex we state some auxiliary results first.

In the previous case of simple laminates, Mallard's law (Lemma 2.4) provided us with the existence and the explicit form of the rank-one connection between two wells. However, in general, we ought to determine manually whether two matrices can be (up to a rotation) rank-one connected. The following lemma is due to Ericksen [Eri91].

Lemma 3.6. *Let $A, B \in \text{GL}^+(3, \mathbb{R})$, $\det A = \det B$ and $B \notin \text{SO}(3)A$. Then*

$$\text{rank}(A - RB) = 1 \text{ for some } R \in \text{SO}(3) \iff \det(A^T A - B^T B) = 0.$$

Proof. For $\Rightarrow$ we write $B = A + \mathbf{b} \otimes \mathbf{m}$ and we note that $\text{rank}(B^T B - A^T A) \leq 2$. For $\Leftarrow$ we note that, by pre- and post-multiplication with B^{-T} and B^{-1} respectively, we may assume that $B = \mathbb{I}$ and further we may assume that $A^T A$ is diagonal with $\det A = 1$. We conclude that $\lambda_i(A^T A) = 1$ for some $i \in \{1, 2, 3\}$. If $\lambda_1 = \lambda_2 = \lambda_3 = 1$, then $A^T A = \mathbb{I}$ and thus $B \in \text{SO}(3)A$. Otherwise, since $1 = \det A = \lambda_1 \lambda_2 \lambda_3$, A can only have exactly one eigenvalue that is equal to 1 and it has to be the middle eigenvalue. Thus by [BJ87] it is rank-one connected to $\mathbb{I}$. $\square$

Lemma 3.7. *(Properties of cof and $\det$)*

1. *Let $A \in \mathbb{R}^{3 \times 3}$ then $\text{rank } A \leq 1$ iff $\text{cof } A = 0$.*
2. *Let $A, B \in \mathbb{R}^{3 \times 3}$ then $\text{cof } A = A^{2T} - A^T \text{Tr } A + \frac{1}{2} \mathbb{I} (\text{Tr}^2 A - \text{Tr } A^2)$ and*

$$\begin{aligned} \text{cof}(A \pm B) = & \text{cof } A + \text{cof } B \pm B^T A^T \pm A^T B^T \mp B^T \text{Tr } A \mp A^T \text{Tr } B \\ & \pm \mathbb{I} \text{Tr } A \text{Tr } B \mp \mathbb{I} \text{Tr } B^T A^T. \end{aligned}$$

3. *Let $A \in \mathbb{R}^{3 \times 3}$ then $\text{rank } A \leq 2$ iff $\det A = 0$.*

4. Let $A, B \in \mathbb{R}^{3 \times 3}$ then $6 \det A = \text{Tr}^3 A - 3 \text{Tr} A \text{Tr} A^2 + 2 \text{Tr} A^3$ and

$$\begin{aligned} 2 \det(A + B) = & 2 \det A + 2 \det B + \text{Tr} A \text{Tr}^2 B + \text{Tr} B \text{Tr}^2 A \\ & - \text{Tr} A \text{Tr} B^2 - \text{Tr} B \text{Tr} A^2 \\ & + 2 \text{Tr} A^2 B + 2 \text{Tr} A B^2 \\ & - 2 \text{Tr} A \text{Tr} AB - 2 \text{Tr} B \text{Tr} AB. \end{aligned}$$

5. Let $A, B \in \mathbb{R}^{3 \times 3}$ then

$$\det(A \pm B) = \det A \pm \det B + \text{Tr}(A \text{ cof } B^T) \pm \text{Tr}(B \text{ cof } A^T).$$

Proof. Since cof and $\det$ are multiplicative and a rotation does not change the rank of the matrix we may assume without loss of generality that A is diagonal. The proof of 1. and 3. are then trivial. For 2. we note that by the Cayley-Hamilton theorem any matrix $A \in \mathbb{R}^{3 \times 3}$ is a zero of its characteristic polynomial given by

$$p(\lambda) = \lambda^3 - \lambda^2 \text{Tr} A + \lambda(\text{Tr} \text{ cof } A) - \mathbb{I} \det A. \quad (3.2)$$

Multiplication of $p(A)$ by $\text{cof } A^T$ yields

$$\det A \left(A^2 - A \text{Tr} A + \mathbb{I} \text{Tr} \text{ cof } A - \text{cof } A^T \right) = 0$$

and thus $A^2 - A \text{Tr} A + \mathbb{I} \text{Tr} \text{ cof } A - \text{cof } A^T = 0$. Taking Tr yields

$$\text{Tr} \text{ cof } A = \frac{1}{2} \left(\text{Tr}^2 A - \text{Tr} A^2 \right)$$

and thus

$$\text{cof } A = A^{2T} - A^T \text{Tr} A + \frac{1}{2} \mathbb{I} \left(\text{Tr}^2 A - \text{Tr} A^2 \right).$$

Inserting $A + B$ as an argument in cof gives the result. For 4. we take the Tr of $p(A)$ (cf. (3.2)) and use the result on $\text{Tr} \text{ cof } A$ to obtain the formula for $\det A$. Finally, 5. can be obtained with the help of the previously derived expressions. $\square$

Lemma 3.7 shows that $\det$ and cof are not well behaved under addition and, in order to keep our calculations as simple as possible, we should use a multiplicative structure as often as possible. The following auxiliary lemma is trivial but will be used repeatedly and thus stated here.

Lemma 3.8. *(Properties of shears)*

Let $\mathcal{S} = \mathbb{I} + x \otimes y$ be a simple shear, i.e. $x \perp y$, then

$$\det \mathcal{S} = 1, \quad \mathcal{S}^{-\text{T}} = \text{cof } \mathcal{S} = \mathbb{I} - y \otimes x, \quad \mathcal{S}^{-1} = \mathbb{I} - x \otimes y, \quad \text{Tr } \mathcal{S} = 3.$$

Second Order Laminates

By solving the two-well problem, we have already found a special class of second order laminates. Namely those that gave rise to all elements in the quasiconvex hull of the two wells. We now set out to characterise *all* second order laminates and thus determine $K^{(2)}$. We start with the following negative result.

Lemma 3.9. *(Absence of rank-one connections between a laminate and the third well)*

There exists no rank-one connection between $K_3^{\text{qc}} \setminus (\text{SO}(3)U_1 \cup \text{SO}(3)U_2)$ and $\text{SO}(3)U_3$.

Proof. Let

$$A = R \begin{pmatrix} a & b & 0 \\ 0 & c & 0 \\ 0 & 0 & \eta_1 \end{pmatrix} \in K_3^{\text{qc}} \setminus (\text{SO}(3)U_1 \cup \text{SO}(3)U_2)$$

and without loss generality $b > 0$ (if $b = 0$ the matrix A would be on $\text{SO}(3)U_1 \cup \text{SO}(3)U_2$). By the result on the two-well problem we have $(a + b)^2 + c^2 \leq \eta_1^2 + \eta_2^2$ and further we have $ac = \eta_1\eta_2$ by the determinant constraint. Now if there exists a rank-one connection between A and $\text{SO}(3)U_3$ then $\det(A^{\text{T}}A - U_3^2) = 0$. We calculate

$$\begin{aligned} 0 &= \det(A^{\text{T}}A - U_3^2) \propto (a^2 - \eta_1^2)(b^2 + c^2 - \eta_1^2) - a^2b^2 \\ &= \eta_1^4 + a^2c^2 - \eta_1^2(a^2 + c^2) - \eta_1^2b^2 \propto \eta_1^2 + \eta_2^2 - (a^2 + c^2 + b^2) \end{aligned}$$

and thus $\eta_1^2 + \eta_2^2 = a^2 + c^2 + b^2 = (a+b)^2 + c^2 - 2ab \leq \eta_1^2 + \eta_2^2 - 2ab$, so that $2ab \leq 0$ and thus $b = 0$. A contradiction. $\square$

Lemma 3.10. $(K^{(2)})$

All possible second order laminates are either laminates between two simple laminates with equal volume fractions or laminates between a well and a simple laminate. The shearing vectors and normals are given by Mallard's law (Lemma 2.4) applied to the 'simple laminate wells'. I.e.

$$K^{(2)} = \bigcup_{i=1}^3 K_i^{\text{qc}} \cup \text{SO}(3) \left\{ F \in \mathbb{R}^{3 \times 3} : F = U_1 + \lambda \mathbf{a} \otimes \mathbf{n} + \nu \mathbf{c} \otimes \mathbf{k}, (\nu, \lambda) \in [0, 1]^2 \right\} \mathcal{P}^{24},$$

where $\mathbf{a} = \sqrt{2} \frac{\eta_1^2 - \eta_2^2}{\eta_1^2 + \eta_2^2} (\eta_2, \eta_1, 0)$ and $\mathbf{n} = \frac{1}{\sqrt{2}} (1, -1, 0)$ and either $\mathbf{k} = \frac{1}{\sqrt{2}} (0, 1, -1)$ or

$$\mathbf{k} \propto (0, 1, -1) - 2 \frac{(U + \lambda \mathbf{a} \otimes \mathbf{n})^T (U + \lambda \mathbf{a} \otimes \mathbf{n}) (0, 1, -1)}{|(U + \lambda \mathbf{a} \otimes \mathbf{n}) (0, 1, -1)|^2}$$

and the corresponding vectors $\mathbf{c}$ are given according to Mallard's law (Lemma 2.4).

Proof. It only remains to investigate second order laminates that involve all three wells. To this end let M'_1 denote the simple laminate between $U = U_1$ and U_2 with normal $\mathbf{n} = (1 \ 1 \ 0)$ and M'_2 denote the simple laminate between $U = U_1$ and U_3 with normal $\mathbf{m} = (1 \ 0 \ 1)$, i.e.

$$M'_1 = U + \lambda \mathbf{a} \otimes \mathbf{n} = (\mathbb{I} + \lambda \mathbf{a} \otimes U^{-1} \mathbf{n}) =: (\mathbb{I} + a \otimes n)U,$$

$$M'_2 = U + \mu \mathbf{b} \otimes \mathbf{m} = (\mathbb{I} + \mu \mathbf{b} \otimes U^{-1} \mathbf{m}) =: (\mathbb{I} + b \otimes m)U,$$

where, to simplify notation, we have set $a = \lambda \mathbf{a}$, $b = \mu \mathbf{b}$, $n = U^{-1} \mathbf{n}$ and $m = U^{-1} \mathbf{m}$. In particular, with this choice $a \perp n$ and $b \perp m$. To find the values λ, μ such that these two simple laminates are rank-one connected we ought to solve $\det(M_2'^T M_2' - M_1'^T M_1') = 0$ (cf. Lemma 3.6). By multiplicativity of the determinant

we may ignore the common factor U and consider $M_i := M'_i U^{-1}$ instead of M'_i . Thus we only need to solve

$$\det(M_2^T M_2 - M_1^T M_1) = \det\left((\mathbb{I} + b \otimes m)^T (\mathbb{I} + b \otimes m) - (\mathbb{I} + a \otimes n)^T (\mathbb{I} + a \otimes n)\right) = 0.$$

Since $(\mathbb{I} + a \otimes n)$ is a simple shear, by Lemma 3.8, we have $\text{cof}(\mathbb{I} + a \otimes n) = \mathbb{I} - n \otimes a$ and thus by noting that $\det M_i = 1$, we obtain

$$\begin{aligned} \det(M_2^T M_2 - M_1^T M_1) &= \det M_2^T M_2 - \det M_1^T M_1 \\ &\quad + \text{Tr } M_2^T M_2 \text{cof}(M_1^T M_1) - \text{Tr } M_1^T M_1 \text{cof}(M_2^T M_2) \\ &= \text{Tr } M_2^T M_2 \text{cof}(M_1^T M_1) - \text{Tr } M_1^T M_1 \text{cof}(M_2^T M_2) \\ &=: \text{Tr } T_2 - \text{Tr } T_1 \end{aligned}$$

by the determinant expansion formula (cf. Lemma 3.7). By symmetry, it suffices to carry out the calculation for one of the Tr terms T_i . We have

$$\begin{aligned} M_1^T M_1 &= \mathbb{I} + (a \otimes n + n \otimes a) + |a|^2 n \otimes n =: \mathbb{I} + 2(a \otimes n)^s + a^2 n \otimes n \\ \text{cof}(M_2^T M_2) &= \mathbb{I} - (b \otimes m + m \otimes b) + b \otimes b =: \mathbb{I} - 2(b \otimes m)^s + b \otimes b, \end{aligned}$$

where we have defined the symmetrisation map $(A)^s := \frac{1}{2}(A + A^T)$ and set $a^2 := |a|^2$.

We thus obtain

$$\begin{aligned} T_1 &= \mathbb{I} + \cancel{2(a \otimes n)^s} - \cancel{2(b \otimes n)^s} + \cancel{a^2 n \otimes n + b \otimes b} + a^2 n \otimes n b \otimes b \\ &\quad - \cancel{4(a \otimes n)^s (b \otimes m)^s} - 2a^2 n \otimes n (b \otimes m)^s - 2b \otimes b (a \otimes n)^s \\ &= a^2 n \otimes n b \otimes b - 2a^2 n \otimes n (b \otimes m)^s - 2b \otimes b (a \otimes n)^s, \end{aligned}$$

where we have used that $a \perp n$ and $b \perp m$ to perform the cancellations $\cancel{X}$. The cancellations $\cancel{X}$ rely on fact that T_2 is obtained by swapping $a \leftrightarrow b$ and $n \leftrightarrow m$ and

thus all terms that are invariant under this swap vanish after taking the difference $T_2 - T_1$. Taking the Tr and resubstituting the value for a and b gives

$$\begin{aligned}\text{Tr } T_1 &= a^2 \langle b, n \rangle^2 - 2a^2 \langle b, n \rangle \langle m, n \rangle - 2\langle a, b \rangle \langle b, n \rangle \\ &= \cancel{\lambda^2 \mu^2 |\mathbf{a}|^2 \langle \mathbf{b}, n \rangle} - 2\lambda^2 \mu |\mathbf{a}|^2 \langle \mathbf{b}, n \rangle \langle m, n \rangle - 2\lambda \mu^2 \langle \mathbf{a}, \mathbf{b} \rangle \langle \mathbf{b}, n \rangle,\end{aligned}$$

where, since $|\mathbf{a}| = |\mathbf{b}|$ and $\langle \mathbf{b}, n \rangle = \langle \mathbf{a}, m \rangle$, the first term cancels with the corresponding term in $\text{Tr } T_2$. Thus we arrive at

$$\begin{aligned}\text{Tr } T_2 - \text{Tr } T_1 &= (\lambda \mu^2 - \lambda^2 \mu) |\mathbf{a}|^2 \langle \mathbf{b}, n \rangle \langle m, n \rangle + 2(\lambda^2 \mu - \lambda \mu^2) \langle \mathbf{a}, \mathbf{b} \rangle \langle \mathbf{b}, n \rangle \\ &\propto \lambda \mu (\lambda - \mu) \stackrel{!}{=} 0,\end{aligned}$$

so that either $\lambda = \mu$, $\lambda = 0$ or $\mu = 0$ as claimed. $\square$

Remark 3.2. The double laminate given by $M = U_1 + \lambda \mathbf{a} \otimes \mathbf{n} + \nu \mathbf{c} \otimes \mathbf{k}$ with $\mathbf{a}$, $\mathbf{n}$ as in Lemma 3.10 and $\mathbf{k} = (0 \ 1 \ \bar{1})$ satisfies $p_3(M) = |M(1 \ 1 \ 1)|^2 = p_3(U)$ for all $(\lambda, \nu) \in [0, 1]^2$. In particular, M lies on the boundary of K^* .

Third Order Laminates

Having our goal in mind, we ought to find third order laminates that remain on the boundary of K^* . We focus on the previous case and require that all constructed third order laminates M still satisfy $p_3(M) = p_3(U)$.

In order to construct a third order laminate we need to find a rank-one connection between two second order laminates that satisfy our boundary condition. Two such double laminates are given by

$$M_1(\lambda_1, \mu_1) = U + \lambda_1 \mathbf{a} \otimes \mathbf{n} + \mu_1 \mathbf{b}_1(\lambda_1) \otimes \mathbf{m}_1, \quad (3.3)$$

$$M_2(\lambda_2, \mu_2) = U + \lambda_2 \mathbf{a} \otimes \mathbf{n} + \mu_2 \mathbf{b}_2(\lambda_2) \otimes \mathbf{m}_2, \quad (3.4)$$

where without loss generality $\mathbf{n} = (1 \ 0 \ \bar{1})$. The vector $\mathbf{a}$ is given by the first solution of Mallard's law (Lemma 2.4) applied to U with $\mathbf{e} = \mathbf{n}$. The vectors $\mathbf{b}_i$ are given as the first solution of Mallard's law (Lemma 2.4) applied to $U + \lambda_i \mathbf{a} \otimes \mathbf{n}$ with $\mathbf{m}_1 = (0 \ 1 \ \bar{1})$ and $\mathbf{m}_2 = (0 \ 1 \ \bar{1})$ or $\mathbf{m}_2 = (1 \ \bar{1} \ 0)$. By Lemma 3.6, $\lambda_1, \lambda_2, \mu_1$ and μ_2 have to be such that

$$\det(M_2^T M_2 - M_1^T M_1) = 0. \quad (3.5)$$

As pointed out before, it is computationally easier to work with the multiplicative form of laminates and thus we write $M = M_i$ as a double shear

$$M = STU,$$

where

$$S = \mathbb{I} + \mu \mathbf{b} \otimes T^{-T} U^{-1} \mathbf{m} \text{ and } T = \mathbb{I} + \lambda \mathbf{a} \otimes U^{-1} \mathbf{n}.$$

Thus we obtain

$$K = M_1^T M_1 - M_2^T M_2 = U(T_1^T S_1^T S_1 T_1 - T_2^T S_2^T S_2 T_2)U.$$

To simplify notation, we set

$$S_i = \mathbb{I} + b_i \otimes m_i, \quad b_i := \mu_i \mathbf{b}_i, \quad m_i := T_i^{-T} U^{-1} \mathbf{m}_i$$

and

$$T_i = \mathbb{I} + a_i \otimes n, \quad a_i = \lambda_i \mathbf{a}, \quad n = U^{-1} \mathbf{n},$$

so that in particular $a_i \perp n$ and $b_i \perp m_i$. By Lemma 3.8, we have $S_i^{-T} = \text{cof } S_i = \mathbb{I} - m_i \otimes b_i$ and $T_i^{-T} = \text{cof } T_i = \mathbb{I} - n \otimes a_i$. Taking out the common factor U we obtain

$$\det U^{-2} \det K = \text{Tr}(T_1^T S_1^T S_1 T_1 \text{cof}(T_2^T S_2^T S_2 T_2)) - \text{Tr}(T_2^T S_2^T S_2 T_2 \text{cof}(T_1^T S_1^T S_1 T_1))$$

and we note that it suffices to calculate the first Tr term. The second Tr term can either be obtained by swapping $1 \leftrightarrow 2$ or by taking cof^T , since for $\det A = \det B = 1$ we have

$$\det(A - B) = \text{Tr}(A \text{cof } B^T) - \text{Tr}(B \text{cof } A^T) = \text{Tr}(A \text{cof } B^T) - \text{Tr}(\text{cof}(A \text{cof } B^T)^T).$$

Using the cyclicity of Tr and the multiplicativity of cof the first term reads

$$\text{Tr}(\text{cof } T_2 T_1^T S_1^T S_1 T_1 \text{cof}(T_2^T) \text{cof}(S_2^T S_2)).$$

We calculate

$$\begin{aligned} T_1 \text{cof}(T_2^T) &= \mathbb{I} + (a_1 - a_2) \otimes n = \mathcal{T}_1, \\ \text{cof } T_2 T_1^T &= \mathbb{I} + n \otimes (a_1 - a_2) =: \mathcal{T}_1^T, \end{aligned}$$

and

$$\begin{aligned} S_1^T S_1 &= (\mathbb{I} + m_1 \otimes b_1)(\mathbb{I} + b_1 \otimes m_1) = \mathbb{I} + b_1 \otimes m_1 + m_1 \otimes b_1 + |b_1|^2 m_1 \otimes m_1, \\ \text{cof } S_2^T \text{cof } S_2 &= (\mathbb{I} - b_2 \otimes m_2)(\mathbb{I} - m_2 \otimes b_2) = \mathbb{I} - b_2 \otimes m_2 - m_2 \otimes b_2 + |m_2|^2 b_2 \otimes b_2. \end{aligned}$$

Thus the requirement (3.5) is equivalent to

$$\begin{aligned} 0 &= \text{Tr} \left(\left(\mathbb{I} - \mu_2 (\mathbf{b}_2 \otimes m_2 + m_2 \otimes \mathbf{b}_2) + \mu_2^2 |m_2|^2 \mathbf{b}_2 \otimes \mathbf{b}_2 \right) \mathcal{T}_1^T S_1^T S_1 \mathcal{T}_1 \right) \\ &\quad - \text{Tr} \left(\left(\mathbb{I} + \mu_2 (\mathbf{b}_2 \otimes m_2 + m_2 \otimes \mathbf{b}_2) + \mu_2^2 |\mathbf{b}_2|^2 m_2 \otimes m_2 \right) \text{cof}(\mathcal{T}_1^T S_1^T S_1 \mathcal{T}_1) \right). \end{aligned}$$

Setting $\mathcal{N}_1 := S_1 \mathcal{T}_1$, which is independent of μ_2 , we thus satisfy (3.5) if μ_2 satisfies the following quadratic equation

$$\begin{aligned}
0 &= \mu_2^2 \left(|m_2|^2 \langle \mathcal{N}_1 \mathbf{b}_2, \mathcal{N}_1 \mathbf{b}_2 \rangle - |\mathbf{b}_2|^2 \langle \text{cof } \mathcal{N}_1 m_2, \text{cof } \mathcal{N}_1 m_2 \rangle \right) \\
&\quad - 2\mu_2 \left(\langle \mathcal{N}_1 \mathbf{b}_2, \mathcal{N}_1 m_2 \rangle + \langle \text{cof } \mathcal{N}_1 \mathbf{b}_2, \text{cof } \mathcal{N}_1 m_2 \rangle \right) + \text{Tr } \mathcal{N}_1^T \mathcal{N}_1 - \text{Tr } \text{cof}(\mathcal{N}_1^T \mathcal{N}_1) \\
&= \mu_2^2 \left(|m_2|^2 |\mathcal{N}_1 \mathbf{b}_2|^2 - |\mathbf{b}_2|^2 |\text{cof } \mathcal{N}_1 m_2|^2 \right) \\
&\quad - 2\mu_2 \left(\langle \mathcal{N}_1 \mathbf{b}_2, \mathcal{N}_1 m_2 \rangle + \langle \text{cof } \mathcal{N}_1 \mathbf{b}_2, \text{cof } \mathcal{N}_1 m_2 \rangle \right) + \text{Tr } \mathcal{N}_1^T \mathcal{N}_1 - \text{Tr } \text{cof}(\mathcal{N}_1^T \mathcal{N}_1).
\end{aligned}$$

In particular, as the solution of a quadratic equation the function $\mu_2 = \mu_2(\lambda_1, \lambda_2, \mu_1)$ can be calculated explicitly and, by construction, all such μ_2 's are such that rank-one connections between two double laminates of the form (3.3) and (3.4) exist.

The next goal is to determine this rank-one connection explicitly. We hope that this rank-one connection has again a normal component orthogonal to $(1 \ 1 \ 1)$ so that the resulting third order laminate stays on the boundary of $p_3 : A \mapsto |A(1 \ 1 \ 1)|^2$. The following theorem provides an important ingredient towards achieving this goal.

Theorem 3.1. ([Šil99])

Let $K = F^T F - G^T G$, $\det F = \det G$ with $\text{eig}_2(K) = 0$ and let $\mathcal{E}_0$ be the eigenspace corresponding to the eigenvalue 0. Let $\mathbf{p} \perp \mathcal{E}_0$ with

$$|\text{cof } F \mathbf{p}|^2 = |\text{cof } G \mathbf{p}|^2.$$

Then $F + \mathbf{c} \otimes \mathbf{p} = RG$ for some $R \in \text{SO}(3)$, where

$$\mathbf{c} = \frac{F \left(\text{cof}(F^T F) - \text{cof}(G^T G) \right) \mathbf{p}}{|\text{cof } F \mathbf{p}|^2} = \frac{\left(\det F \text{cof}(F) - F \text{cof}(G^T G) \right) \mathbf{p}}{|\text{cof } F \mathbf{p}|^2}.$$

Lemma 3.11. Set $F = M_1 = S_1 T_1 U$, $G = M_2 = S_2 T_2 U$ and $K = M_1^T M_1 - M_2^T M_2$, where M_1 and M_2 are the second order laminates defined in (3.3) and (3.4), respectively. Then, in the notation of Theorem 3.1, we have

$$\mathbf{p} \propto \text{cof } K \mathbf{k} \times \mathbf{k},$$

where $\mathbf{k} = (1 \ 1 \ 1)$. In particular, $\mathbf{p} \perp (1 \ 1 \ 1)$.

Proof. Since K is symmetric and $\det K = 0$, the eigenspace $\mathcal{E}_0$ corresponding to the eigenvalue 0 is given by

$$\mathcal{E}_0 = \text{ran cof } K = \text{cof } K \mathbb{R}^3,$$

because $K \text{ cof } K = K^T \text{ cof } K = \det K \mathbb{I} = \mathbb{O}$. Further, since $\mathbf{n}, \mathbf{m}_i \perp \mathbf{k}$ and $M_i = U + \lambda_i \mathbf{a} \otimes \mathbf{n} + \mu_i \mathbf{b} \otimes \mathbf{m}_i$ we have

$$M_1 \mathbf{k} = M_2 \mathbf{k} = U \mathbf{k}$$

To avoid $\mathbf{p} = 0$ we need to make sure that $\mathbf{k} \nparallel \text{cof } K \mathbf{k}$. Let us assume the contrary, i.e. $\text{cof } K \mathbf{k} \propto \mathbf{k}$. Multiplication by K yields $K \mathbf{k} = 0$ and thus since $M_i \mathbf{k} = \mathbf{k}$ we obtain

$$\begin{aligned} M_1^T \mathbf{k} &= M_2^T \mathbf{k} \\ \Leftrightarrow (\mathbb{I} + n \otimes a_1)(\mathbb{I} + m_1 \otimes b_1) \mathbf{k} &= (\mathbb{I} + n \otimes a_2)(\mathbb{I} + m_2 \otimes b_2) \mathbf{k} \\ \Leftrightarrow \mathbf{k} + \langle b_1, \mathbf{k} \rangle m_1 + \langle a_1, \mathbf{k} \rangle n + \langle a_1, m_1 \rangle \langle b_1, \mathbf{k} \rangle n \\ &= \mathbf{k} + \langle b_2, \mathbf{k} \rangle m_2 + \langle a_2, \mathbf{k} \rangle n + \langle a_2, m_2 \rangle \langle b_2, \mathbf{k} \rangle n \\ \Leftrightarrow ((\lambda_1 - \lambda_2) \langle \mathbf{a}, \mathbf{k} \rangle + \lambda_1 \langle \mathbf{a}, m_1 \rangle \langle b_1, \mathbf{k} \rangle - \lambda_2 \langle \mathbf{a}, m_2 \rangle \langle b_2, \mathbf{k} \rangle) n \\ &\quad + \langle b_1, \mathbf{k} \rangle m_1 - \langle b_2, \mathbf{k} \rangle m_2 = 0 \end{aligned}$$

Generically n, m_1, m_2 (excluding the degenerate case $m_1 = m_2$) are linearly independent and thus all coefficients need to be equal to 0. A contradiction.

It remains to check the condition $|\text{cof } F \mathbf{p}|^2 = |\text{cof } G \mathbf{p}|^2$. To this end, we recall the expansion formula for cross products $\langle \mathbf{a} \times \mathbf{b}, \mathbf{c} \times \mathbf{d} \rangle = \langle \mathbf{a}, \mathbf{c} \rangle \langle \mathbf{b}, \mathbf{d} \rangle - \langle \mathbf{b}, \mathbf{c} \rangle \langle \mathbf{a}, \mathbf{d} \rangle$, in

particular $|\mathbf{a} \times \mathbf{b}|^2 = |\mathbf{a}|^2|\mathbf{b}|^2 - \langle \mathbf{a}, \mathbf{b} \rangle^2$, and the transformation rule $\text{cof } A(\mathbf{a} \times \mathbf{b}) = A\mathbf{a} \times A\mathbf{b}$. We thus have

$$\begin{aligned} |\text{cof } M_i \mathbf{p}|^2 &= |M_i \text{cof } K \mathbf{k} \times M_i \mathbf{k}|^2 \\ &= \langle M_i \text{cof } K \mathbf{k}, M_i \text{cof } K \mathbf{k} \rangle |M_i \mathbf{k}|^2 - \langle M_i \text{cof } K \mathbf{k}, M_i \mathbf{k} \rangle^2 \\ &= \langle M_i^T M_i \text{cof } K \mathbf{k}, \text{cof } K \mathbf{k} \rangle |M_i \mathbf{k}|^2 - \langle M_i^T M_i \text{cof } K \mathbf{k}, \mathbf{k} \rangle^2. \end{aligned}$$

To simplify notation let us define $\mathcal{M}_i = M_i^T M_i$ so that $K = \mathcal{M}_1 - \mathcal{M}_2$. Noting that $M_1 \mathbf{k} = M_2 \mathbf{k} = U \mathbf{k}$ we obtain

$$\begin{aligned} |\text{cof } M_1 \mathbf{p}|^2 - |\text{cof } M_2 \mathbf{p}|^2 &= \langle (\mathcal{M}_1 - \mathcal{M}_2) \text{cof } K \mathbf{k}, \text{cof } K \mathbf{k} \rangle |M_i \mathbf{k}|^2 \\ &\quad - \langle \mathcal{M}_1 \text{cof } K \mathbf{k}, \mathbf{k} \rangle^2 + \langle \mathcal{M}_2 \text{cof } K \mathbf{k}, \mathbf{k} \rangle^2 \\ &= -\langle \mathcal{M}_1 \text{cof } K \mathbf{k}, \mathbf{k} \rangle^2 + \langle -\mathcal{M}_1 \text{cof } K \mathbf{k}, \mathbf{k} \rangle^2 = 0, \end{aligned}$$

where we have used that $K \text{cof } K = \mathbb{O}$ and $\mathcal{M}_2 = K - \mathcal{M}_1$. □

Corollary 3.12. *If instead of $M_i = S_i T_i U$ we consider $M_i U^{-1} = S_i T_i$ we have*

$$p = U^{-1} \mathbf{p} \propto \text{cof}((S_1 T_1)^T (S_1 T_1) - (S_2 T_2)^T (S_2 T_2)) U^{-1} \mathbf{k} \times U \mathbf{k}$$

such that $S_1 T_1 + \mathbf{c} \otimes p = R S_2 T_2$ and $\mathbf{c}$ is given by Theorem 3.1 applied with $F \rightarrow S_1 T_1$, $G \rightarrow S_2 T_2$ and $\mathbf{p} \rightarrow p$.

Proof. Writing $M_1 + \mathbf{c} \otimes \mathbf{p} = R M_2 = (S_1 T_1 + \mathbf{c} \otimes U^{-1} \mathbf{p}) U = (R S_2 T_2) U$ we see that

$$S_1 T_1 + \mathbf{c} \otimes U^{-1} \mathbf{p} = R S_2 T_2.$$

□

In particular, we have successfully constructed a third order laminate M that satisfies $p_3(M) = p_3(U)$ and thus stays on the boundary of K^* . Furthermore, this third order

laminate depends on four independent parameters and is thus (most likely)⁴ four dimensional as required.

Duality of Cofactor Bounds

So far, whenever we have used Mallard's law (Lemma 2.4), we have taken the first solution. Let us recall that for a given pair $(A, \mathbf{e})$ the first solution satisfies $\mathbf{n} \parallel \mathbf{e}$ and the second solution $\mathbf{a} \parallel A\mathbf{e}$. Thus, writing the solution of Mallard's law as $A_\lambda = A(\mathbb{I} + \lambda A^{-1}\mathbf{a} \otimes \mathbf{n})$, we see that

$$\text{cof } A_\lambda = \text{cof } A(\mathbb{I} - \lambda \mathbf{n} \otimes A^{-1}\mathbf{a}),$$

where $\mathbf{e} \parallel A^{-1}\mathbf{a}$. So that, as before, taking any vector $\mathbf{f} \perp \mathbf{e}$ we have

$$\text{cof } A_\lambda \mathbf{f} = \text{cof } A \mathbf{f}$$

and thus whenever A satisfies $|\text{cof } A \mathbf{f}|^2 = |\text{cof } A \mathbf{f}|^2$, the sheared matrix A_λ will satisfy the same equality for all λ . If the solution of the twinning equation cannot be obtained through Mallard's law, this method does not apply anymore. However, numerically it is true that always one of the possible solutions from Proposition 2.1 satisfies the cofactor (q_3) bounds and the other the 'normal' (p_3) bounds.

Summary

Since all derived formulas are polynomials and thus continuous, the set of third order laminates is most likely four dimensional. If it is indeed four dimensional, we have determined an open set where the boundary of K^* is attained by elements in K^{lc} . Particularly, in this region the conjectured polyconvex bounds are sharp and we

⁴The pure existence of four parameters does not generally imply four-dimensionality. However, by the continuous dependence of the laminate on four parameters cancellations on an open set seem very unlikely.

have locally determined K^{qc} (and K^{lc} , K^{rc} , K^{pc}). Furthermore, the knowledge of an open set on the boundary of K^{qc} could provide an alternative proof to showing that $\mathbb{I}$ (or even more general matrices) are in the relative interior of K^{qc} (relative to the det constraint). For previous work on this subject see [DK03; Con+07].

3.3 Numerical Considerations

Even though we have (almost surely) succeeded in finding a full-dimensional set on the boundary of K^{qc} , we are still far away from being able to characterise the entire boundary of K^{qc} . Thus, at this point it might be easier to explore numerical methods. Although we have not yet been able to obtain satisfactory results, we briefly outline two possible approaches.

The key idea for these approaches will be the same as in our analytical approach, i.e. matching boundary points of the conjectured polyconvex hull (cf. Conjecture 3.1) with third order laminates. Further details concerning their implementation can be found in Appendix C.

The Mesh Method

Firstly, generate a mesh $\mathcal{M}$ of points in $\mathbb{R}^{3 \times 3}$ that satisfies the polyconvex bound $A \mapsto |A(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2$ with equality and delete all points that violate the conditions of our conjectured polyconvex hull. Secondly, construct a mesh $\mathcal{L}$ of all third order laminates that satisfy $A \mapsto |A(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2 = |U(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2$. Finally, determine the distance $\text{dist}(m, \mathcal{L})$ for all $m \in \mathcal{M}$ and compare it with numerical errors (e.g. resulting from a discrete mesh).

The Minimisation Method

Define a third order laminate function

$$l : [0, 1]^4 \rightarrow \mathbb{R}^{3 \times 3}, (\lambda_1, \lambda_2, \mu_1, \nu) \mapsto l(\lambda_1, \lambda_2, \mu_1, \nu)$$

that satisfies the polyconvex bound $A \mapsto |A(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2$ with equality (cf. the above construction). Pick any point (e.g. at random) $A \in \mathbb{R}^{3 \times 3}$ in the conjectured polyconvex boundary that also satisfies the polyconvex bound $A \mapsto |A(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2 \leq |U(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2$ with equality. Solve the minimisation problem $\min_{\lambda_1, \lambda_2, \mu_1, \nu} \text{dist}(A, l(\lambda_1, \lambda_2, \mu_1, \nu))$ and compare it with numerical errors.

Self-Accommodation

A self-accommodating microstructure is defined as a martensitic microstructure that is macroscopically equivalent to austenite. Materials with this property often show superelastic behaviour and often exhibit the so-called *shape-memory effect*. That is, they can almost deform freely whilst in the martensitic phase and then recover their original shape upon heating. In mathematical terms, this condition can be expressed as the existence of an $F \in K^{\text{qc}}$ with $\text{rank}(F - \mathbb{I}) = 0$. It is clear that this can only happen if the transformation is volume preserving, i.e. $\det U_i = 1$. Further, it can be shown that whenever the austenite is cubic this condition is also sufficient (see [Bha92]). Both conditions shall thus be assumed throughout, so that $K = \text{SO}(3)U_1\mathcal{P}^{24}$ with $\det U_1 = 1$.

4.1 Self-Accommodation in Cubic-to-Tetragonal

At first we consider a cubic-to-tetragonal transformation (cf. Chapter 3) and thus in particular $U_1 = \text{diag}(\alpha^{-2}, \alpha, \alpha)$ for some $\alpha > 0$. The goal is to determine the ‘easiest’ self-accommodating microstructure and characterise it. For related work see also [BC15]. Firstly, we establish the following negative result.

Lemma 4.1. *Let $K = \text{SO}(3)U_1\mathcal{P}^{24}$, where $U_1 = \text{diag}(\alpha^{-2}, \alpha, \alpha)$. Then $\mathbb{I} \notin K^{(2)}$.*

Proof. By Lemma 3.4 we know that $\mathbb{I} \notin K_3^{\text{qc}} := (\text{SO}(3)U_1 \cup \text{SO}(3)U_2)^{\text{qc}}$ and thus we just need to verify the claim for laminates that involve all three wells and are thus of the form described in Lemma 3.10. For convenience of notation let us define the first and second solution operator corresponding to Mallard’s law (Lemma 2.4)

$S(A, \mathbf{e}) := \left(\frac{A^{-T} \mathbf{e}}{|A^{-T} \mathbf{e}|^2} - A \mathbf{e} \right) \otimes \mathbf{e}$ and $T(A, \mathbf{e}) := \frac{2}{|A \mathbf{e}|^2} A \mathbf{e} \otimes (|A \mathbf{e}|^2 \mathbf{e} - A^T A \mathbf{e})$. Without loss of generality we start from the well U_1 . Then any simple laminate between U_1 and U_2 is given by

$$L(\mu) = U_1 + \mu S(U_1, \mathbf{e}),$$

where we can without loss generality only consider the first solution with $\mathbf{e} = [1 \ 1 \ 0]$. This is because the second solution will just give L^T and choosing the normal $\mathbf{e} = [1 \ \bar{1} \ 0]$ just swaps the first and second solution. Now consider the two distinct second order laminates

$$M_1(\mu, \lambda) := L(\mu) + \lambda S(L(\mu), \mathbf{f}),$$

$$M_2(\mu, \lambda) := L(\mu) + \lambda T(L(\mu), \mathbf{f}),$$

where $\mathbf{f} = [1 \ 0 \ 1]$. And again the solutions for $\mathbf{f} = [1 \ 0 \ \bar{1}]$ is symmetry related by conjugation with $R[180^\circ, \mathbf{e}_2]$. In order to achieve the identity we need to satisfy

$$M_i^T M_i = \mathbb{I}.$$

But we have

$$\begin{aligned} (M_1^T M_1)_{12} &= -\frac{(\lambda - 1)(\mu - 1)\mu(\eta_2 - \eta_1)^2(\eta_2 + \eta_1)^2}{\eta_1^2 + \eta_2^2} \\ &\propto (\lambda - 1)(\mu - 1)\mu \\ (M_2^T M_2)_{13} &= -\frac{\lambda(\lambda - 1)(\mu - 1)^2(-\eta_1^2\mu + \eta_2^2\mu - \eta_1^2 - \eta_2^2)^2(\eta_2 + \eta_1)^2(\eta_2 - \eta_1)^2}{(\eta_1^2 + \eta_2^2)(\eta_1^4\mu^2 - 2\eta_1^2\eta_2^2\mu^2 + \eta_2^4\mu^2 + 2\eta_1^2\eta_2^2\mu - 2\eta_2^4\mu + \eta_1^4 + 2\eta_1^2\eta_2^2 + \eta_2^4)} \\ &\propto \lambda(\lambda - 1)(\mu - 1)^2, \end{aligned}$$

where $\eta_1 = \alpha$ and $\eta_2 = \alpha^{-2}$. So that in either case we are reduced to a two well situation and thus $\mathbb{I} \notin K^{(2)}$. $\square$

However, we have the following positive result.

Lemma 4.2. *Let $K = \text{SO}(3)U_1\mathcal{P}^{24}$, where $U_1 = \text{diag}(\alpha^{-2}, \alpha, \alpha)$. Then $\mathbb{I} \in K^{(4)}$.*

To show this assertion we will make use of the following.

Theorem 4.1. ($K^{\text{qc}} \cap \text{diag}$)

Let $K = \text{SO}(3)U_1\mathcal{P}^{24}$, $U_1 = \text{diag}(\eta_2, \eta_1, \eta_1)$. Then if $\eta_1 < \eta_2$ we have

$$K^{\text{qc}} \cap \text{diag} = \left\{ F = \text{diag}(\alpha, \beta, \gamma) : \alpha \in [\eta_1, \eta_2], \beta \in [\eta_1, \frac{\eta_1\eta_2}{\alpha}], \gamma = \frac{\eta_1^2\eta_2}{\alpha\beta} \right\},$$

and if $\eta_1 > \eta_2$ we have

$$K^{\text{qc}} \cap \text{diag} = \left\{ F = \text{diag}(\alpha, \beta, \gamma) : \alpha \in [\eta_2, \eta_1], \beta \in [\eta_2, \frac{\eta_1\eta_2}{\alpha}], \gamma = \frac{\eta_1^2\eta_2}{\alpha\beta} \right\}.$$

Proof. Let us first assume $\eta_1 < \eta_2$ and calculate an outer bound of $K^{\text{qc}} \cap \text{diag}$ by considering the polyconvex function

$$p(A) = \sum_{i=1}^3 \rho(|A\mathbf{e}_i|^2 - \eta_2^2) + \sum_{i=1}^3 \rho(|\text{cof } A\mathbf{e}_i|^2 - \eta_1^2\eta_2^2) + |\det A - \eta_1^2\eta_2|,$$

where $\rho : \mathbb{R} \rightarrow \mathbb{R}_+$ is a convex C^∞ function with $\rho(x) = 0$ iff $x \leq 0$. Thus we have

$$\begin{aligned} K^{\text{qc}} \cap \text{diag} &\subset K^{\text{pc}} \cap \text{diag} \subset p^{-1}(0) \cap \text{diag} \\ &= \{F = \text{diag}(\alpha, \beta, \gamma) : \alpha, \beta, \gamma \in [\eta_1, \eta_2], \alpha\beta\gamma = \eta_1^2\eta_2\} \\ &= \left\{ F = \text{diag}(\alpha, \beta, \gamma) : \alpha \in [\eta_1, \eta_2], \beta \in [\eta_1, \frac{\eta_1\eta_2}{\alpha}], \gamma = \frac{\eta_1^2\eta_2}{\alpha\beta} \right\} =: K^*. \end{aligned}$$

Next, we use the result on the two-well problem to show the attainment of these bounds by higher order laminates. We recall that by Lemma 3.4 the quasiconvex hull of $K_i = \text{SO}(3)U_j \cup \text{SO}(3)U_k$, $(i, j, k) \in \mathcal{S}_3$ is given by

$$K_i^{\text{qc}} = \{F : \det F = \eta_1^2\eta_2, F^T F \mathbf{e}_i = \eta_1^2 \mathbf{e}_i, |F(\mathbf{e}_j \pm \mathbf{e}_k)|^2 \leq \eta_1^2 + \eta_2^2\}, \quad (4.1)$$

and coincides with the lamination convex hull $K_i^{(2)}$ of second order. In particular, each element in K_i^{qc} can be achieved by at most a second order laminate. We claim

that each element in K^* can be achieved by at most a 4th order laminate and is thus contained in $K^{\text{lc}} \cap \text{diag}$. To this end consider any element

$$K^* \ni F = \text{diag}(\alpha, \beta, \gamma),$$

where $\alpha \in [\eta_1, \eta_2]$, $\beta \in [\eta_1, \frac{\eta_1 \eta_2}{\alpha}]$ and $\gamma = \frac{\eta_1^2 \eta_2}{\alpha \beta}$. In a first step we use second order laminates to construct the matrices

$$V = \text{diag}(\alpha, \frac{\eta_1 \eta_2}{\alpha}, \eta_1) \in K_3^{\text{qc}}$$

and

$$W = \text{diag}(\alpha, \eta_1, \frac{\eta_1 \eta_2}{\alpha}) \in K_2^{\text{qc}}.$$

We note that these matrices satisfy the conditions in (4.1) since the function $a \mapsto a^2 + \frac{\eta_1^2 \eta_2^2}{a^2}$ is convex in a and achieves its maximum at the boundary, i.e. for $a \in \{\eta_1, \eta_2\}$. By the $\text{SO}(3)$ invariance of the wells also $\text{SO}(3)V, \text{SO}(3)W \subset K^{\text{lc}}$. Thus, using the two well result once more with the wells given by $\text{SO}(3)V \cup \text{SO}(3)W$, we obtain the result and conclude that $K^{\text{lc}} \cap \text{diag} = K^{\text{qc}} \cap \text{diag} = K^{\text{pc}} \cap \text{diag} = K^*$. The case $\eta_1 > \eta_2$ can be proved analogously. $\square$

Proof. (of Lemma 4.2) The proof is an easy consequence of Theorem 4.1. In the notation of the theorem we can achieve $V = \text{diag}(1, \alpha, \alpha^{-1}) \in K_3^{\text{qc}}$ and $W = \text{diag}(1, \alpha^{-1}, \alpha) \in K_2^{\text{qc}}$ by a second order laminate and then $\mathbb{I} \in (\text{SO}(3)V \cup \text{SO}(3)W)^{\text{qc}}$ by another second order laminate (of second order laminates). $\square$

The previous constructions allows us to give an estimate on the ‘easiest’ possible microstructure that can be self-accommodating. That is, a self-accommodating microstructure that involves as few different martensitic variants as possible. In other words we are looking for a GYM ν supported on K with $\bar{\nu} = \mathbb{I}$ and $|\text{supp } \nu| \rightarrow \min$.

Lemma 4.3. *There exists a GYM ν supported on K with $\bar{\nu} = \mathbb{I}$ and $|\text{supp } \nu| \leq 9$.*

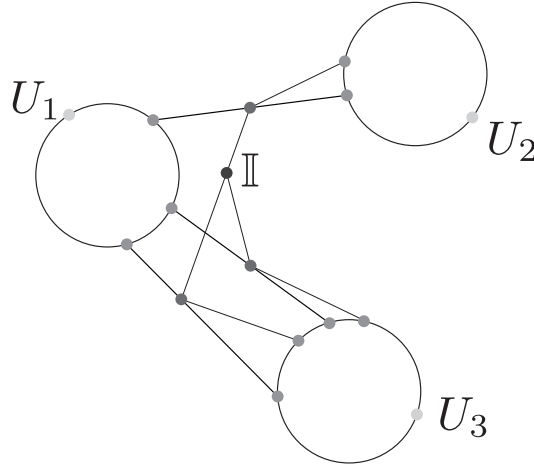


Fig. 4.1. Schematic representation of a 4th order laminate that is supported on nine matrices and has macroscopic deformation gradient $\mathbb{I}$. Circles represent the wells $\text{SO}(3)U_i$ corresponding to the variants U_i .

Proof. By the two well result (cf. Lemma 3.4) and by the construction of Lemma 4.2, we need exactly three martensitic variants to construct $V \in K_3^{\text{qc}}$ and $W \in K_2^{\text{qc}}$. To construct the self-accommodating laminate we need another three variants from our new wells given by $\text{SO}(3)V$ and $\text{SO}(3)W$ and thus we need a total of $3 \times 3 = 9$ martensitic variants. Figure 4.1 illustrates the construction. $\square$

The above inclusions naturally raise the question whether $\mathbb{I} \in K^{(3)}$?

Conjecture 4.1. *Let $K = \text{SO}(3)U_1\mathcal{P}^{24}$, where $U_1 = \text{diag}(\alpha^{-2}, \alpha, \alpha)$. Then $\mathbb{I} \notin K^{(3)}$.*

This conjecture is based on the explicit knowledge of all second order laminates (cf. Lemma 3.10) and that $\mathbb{I}$ cannot be on the boundary of the K^{qc} (cf. [DK03]). With the help of a computer algebra program, rank-one connections between these (possibly trivial) second order laminates were computed and after squaring ($F \mapsto F^{\text{T}}F$) compared to $\mathbb{I}$. The computations of the rank-one connections were performed as described in Chapter 3 (see also Appendix C).

4.2 Volume Fractions

In this section, we would like to gain further insight into the properties of any self-accommodating microstructure by establishing bounds on the possible volume fractions. That is, we give estimates what percentage of each well $\text{SO}(3)U_i$ needs to be present in *any* self-accommodating microstructure. In the case of a cubic-to-tetragonal phase transformation we also comment on whether these theoretical bounds can be attained by a construction.

Lemma 4.4. (*Volume fractions in cubic-to-tetragonal*)

Let $K = \bigcup_{i=1}^3 \text{SO}(3)U_i$, where $U_1 = \text{diag}(\alpha^{-2}, \alpha, \alpha) = \alpha \mathbb{I} + (\alpha^{-2} - \alpha)\mathbf{e}_1 \otimes \mathbf{e}_1$, $U_2 = \text{diag}(\alpha, \alpha^{-2}, \alpha)$ and $U_3 = \text{diag}(\alpha, \alpha, \alpha^{-2})$ are the three martensitic variants in a volume preserving cubic-to-tetragonal phase transformation. Let further ν be a GYM supported on K with $\bar{\nu} = \mathbb{I}$ and decompose ν into three probability measures μ_i that are supported on the three wells, i.e.

$$\nu = \sum_{i=1}^3 \lambda_i \mu_i,$$

where $\text{supp } \mu_i \subset \text{SO}(3)U_i$ and $\mu_i(\mathbb{R}^{3 \times 3}) = 1$. Then, for $\alpha < 1$ and $j = 1, 2, 3$, we have

$$\frac{\alpha^2}{\alpha^2 + \alpha + 1} \leq \lambda_j(\alpha) \leq \frac{1}{\alpha^2 + \alpha + 1}. \quad (4.2)$$

For $\alpha > 1$ the inequalities reverse (cf. Figure 4.2).

Proof. Let us first suppose that $\alpha < 1$ and consider the duality pairing between ν and cof given by

$$\langle \nu, \text{cof} \rangle = \sum_{i=1}^3 \lambda_i \langle \mu_i, \text{cof} \rangle.$$

Then

$$\langle \mu_i, \text{cof} \rangle = \int_{\text{SO}(3)U_i} \text{cof}(A) \, d\mu_i(A) = \int_{\text{SO}(3)} \text{cof}(RU_i) \, d\mu_i^*(R) = \int_{\text{SO}(3)} R \, d\mu_i^*(R) \, \text{cof } U_i,$$

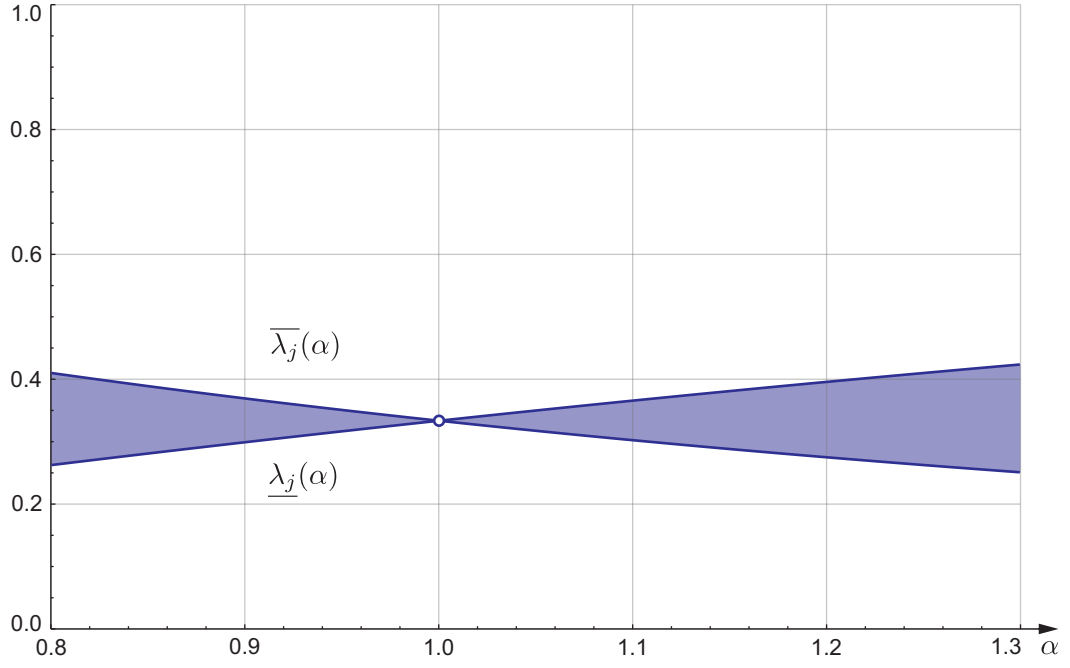


Fig. 4.2. Upper and lower bounds on the volume fractions of each cubic-to-tetragonal well in a self-accommodating microstructure.

where $\mu_i^*(R) := \mu_i(RU_i)$ is also a probability measure. Let us now define

$$T_i := \int_{\text{SO}(3)} R \, d\mu_i^*(R) \in \text{SO}(3)^c$$

to obtain

$$\mathbb{I} = \lambda_1 T_1 \text{cof } U_1 + \lambda_2 T_2 \text{cof } U_2 + \lambda_3 T_3 \text{cof } U_3, \quad (4.3)$$

where $\text{cof } U_1 = \text{diag}(\alpha^2, \frac{1}{\alpha}, \frac{1}{\alpha})$, $\text{cof } U_2 = \text{diag}(\frac{1}{\alpha}, \alpha^2, \frac{1}{\alpha})$ and $\text{cof } U_3 = \text{diag}(\frac{1}{\alpha}, \frac{1}{\alpha}, \alpha^2)$.

Analogously we obtain

$$\mathbb{I} = \lambda_1 T_1 U_1 + \lambda_2 T_2 U_2 + \lambda_3 T_3 U_3. \quad (4.4)$$

Multiplying (4.4) by $\mathbf{e}_j$ from the right gives

$$\mathbf{e}_j = \sum_{k=1}^3 \lambda_k (\alpha + \delta_{kj}(\alpha^{-2} - \alpha)) T_k \mathbf{e}_j$$

and taking the norm for each j yields

$$\begin{aligned} 1 &\leq \lambda_1 \alpha^{-2} + \alpha(\lambda_2 + \lambda_3) = \lambda_1 \alpha^{-2} + \alpha(1 - \lambda_1) = \alpha + \lambda_1(\alpha^{-2} - \alpha), \\ 1 &\leq \lambda_2 \alpha^{-2} + \alpha(\lambda_1 + \lambda_3) = \lambda_2 \alpha^{-2} + \alpha(1 - \lambda_2) = \alpha + \lambda_2(\alpha^{-2} - \alpha), \\ 1 &\leq \lambda_3 \alpha^{-2} + \alpha(\lambda_1 + \lambda_2) = \lambda_3 \alpha^{-2} + \alpha(1 - \lambda_3) = \alpha + \lambda_3(\alpha^{-2} - \alpha), \end{aligned}$$

where we used that $\|T_j\| \leq 1$. Thus, since $\alpha^{-2} - \alpha > 0$, we obtain

$$\lambda_j \geq \frac{1 - \alpha}{\alpha^{-2} - \alpha} = \frac{\alpha^2}{\alpha^2 + \alpha + 1}$$

for $j = 1, 2, 3$. The inequalities from the cofactor relations are obtained analogously. We arrive at $1 \leq \alpha^{-1} + \lambda_j(\alpha^2 - \alpha^{-1})$ for $j = 1, 2, 3$. Finally, since $\alpha^2 - \alpha^{-1} < 0$, we obtain

$$\lambda_j \leq \frac{1 - \alpha^{-1}}{\alpha^2 - \alpha^{-1}} = \frac{1}{\alpha^2 + \alpha + 1}$$

for $j = 1, 2, 3$. For $\alpha > 1$ the computations are exactly the same with the inequalities reversed. $\square$

In particular, from (4.2) we see that $\lim_{\alpha \rightarrow 1, \alpha \neq 1} \lambda_j(\alpha) = \frac{1}{3}$ and thus, whenever the lattice parameters are very close to unity, all martensite wells have to be contained in almost equal volume fractions. Of course, the limit case, $\alpha = 1$, is not admissible as all variants would collapse to the austenite.

Attainment of the Bounds on Volume Fractions

Having established upper and lower bounds on the volume fractions that can build a self-accommodating microstructure it is natural to ask whether these bounds can be attained by an explicit construction of a self-accommodating microstructure. To simplify notation we will henceforth write $\lambda_{\min}^Y(X) := \lambda_{\min}(\text{SO}(3)X)$ to denote the minimum volume fraction of the matrix Y on the well $\text{SO}(3)X$. The following theorem will provide a crucial tool for our estimates.

Theorem 4.2. ([Iqb99, Theorem 4.5 and Section 4.2])

Let $U_1 = \text{diag}(\eta_1, \eta_2)$, $U_2 = \text{diag}(\eta_2, \eta_1)$ and denote by $\mathcal{A}$ the set of probability measures supported on $\text{SO}(3)U_1 \cup \text{SO}(3)U_2$ with centres of mass F . Then the minimum and maximum possible volume fractions on $\text{SO}(3)U_1$ are given by

$$\lambda_{\min}^F(U_1) = \frac{\sqrt{(\eta_2 F_{21} + \eta_1 F_{12})^2 + (\eta_2 F_{11} - \eta_1 F_{22})^2}}{|\eta_2^2 - \eta_1^2|}, \quad (4.5)$$

$$\lambda_{\max}^F(U_1) = 1 - \frac{\sqrt{(\eta_2 F_{12} + \eta_1 F_{21})^2 + (\eta_1 F_{11} - \eta_2 F_{22})^2}}{|\eta_2^2 - \eta_1^2|}. \quad (4.6)$$

The value $\lambda_{\min}$ is attained for measures in $\mathcal{A}$ whose restriction to $\text{SO}(3)U_1$ is a Dirac mass and the value $\lambda_{\max}$ for measures in $\mathcal{A}$ whose restriction to $\text{SO}(3)U_2$ is a Dirac mass. Further, each of the volume fractions in the range $[\lambda_{\min}, \lambda_{\max}]$ can be attained by a homogeneous gradient Young measure.

We would like to answer the following two questions:

- Can we construct a self-accommodating microstructure with equal volume fractions (i.e. $\lambda_i = \frac{1}{3}$) for any α ?
- Can we construct a self-accommodating microstructure that attains the theoretical minimal/maximal volume fractions on e.g. U_1 from Lemma 4.4?

We will try to answer these questions by using the same construction as in Lemma 4.2.

We note that the two-well problem is essentially two dimensional and thus Theorem 4.2 is applicable with $U_1 = \text{diag}(\alpha^{-2}, \alpha, \alpha)$. We recall that in the construction of Lemma 4.2 we have $V = \text{diag}(1, \alpha^{-1}, \alpha) \in (\text{SO}(3)U_1 \cup \text{SO}(3)U_2)^{\text{qc}}$, $W = \text{diag}(1, \alpha, \alpha^{-1}) \in (\text{SO}(3)U_1 \cup \text{SO}(3)U_3)^{\text{qc}}$ and thus

$$\mathbb{I} \in (\text{SO}(3)V \cup \text{SO}(3)W)^{\text{qc}}.$$

Now let us determine the minimum volume fraction on e.g. $\text{SO}(3)U_1$. By (4.5) we have

$$\lambda_{\min}^W(U_1) = \lambda_{\min}^V(U_1) = \frac{|\alpha^{-2} \cdot 1 - \alpha \cdot \alpha^{-1}|}{|\alpha^{-4} - \alpha^2|} = \frac{\alpha^2}{\alpha^4 + \alpha^2 + 1}.$$

We note that since $\lambda_{\min}^W(U_1) = \lambda_{\min}^V(U_1)$ we cannot minimise with respect to the volume fraction on $SO(3)U_1$ in the third (and final) step. We conclude that

$$\lambda_{\min}^{\mathbb{I}}(U_1) = \frac{\alpha^2}{\alpha^4 + \alpha^2 + 1},$$

and analogously by using (4.6) instead of (4.5) we conclude that

$$\lambda_{\max}^{\mathbb{I}}(U_1) = 1 - \frac{|\alpha \cdot 1 - \alpha^{-2} \cdot \alpha^{-1}|}{|\alpha^{-4} - \alpha^2|} = \frac{\alpha^4 - \alpha^3 + \alpha^2 - \alpha + 1}{\alpha^4 + \alpha^2 + 1}.$$

It is obvious that we can achieve any volume fraction between the extremal values. In particular, we can have the same volume fractions on each well. Figure 4.3 shows a comparison between our construction and the theoretical bounds from Lemma 4.4.

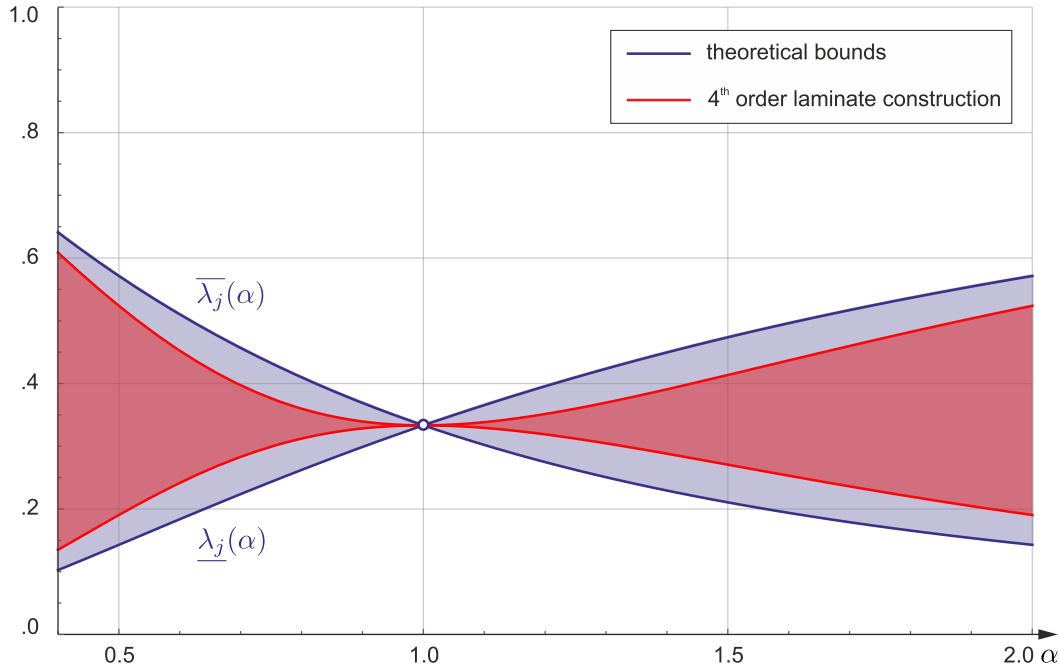


Fig. 4.3. Comparison between the theoretical bounds on the volume fractions for each tetragonal well and the achieved volume fractions by a self-accommodating 4th order laminate construction.

Cubic-to-Orthorhombic

We derive bounds on the volume fractions of a self-accommodating microstructure in a cubic-to-orthorhombic transformation.¹ By the algorithm from Chapter 1 (or see e.g. [Dol03, Ch. 5.3]) the transformation strains are given by

$$U_1 = \begin{pmatrix} \xi & \eta & 0 \\ \eta & \xi & 0 \\ 0 & 0 & \zeta \end{pmatrix}, U_2 = \begin{pmatrix} \xi & -\eta & 0 \\ -\eta & \xi & 0 \\ 0 & 0 & \zeta \end{pmatrix}, U_3 = \begin{pmatrix} \xi & 0 & \eta \\ 0 & \zeta & 0 \\ \eta & 0 & \xi \end{pmatrix},$$

$$U_4 = \begin{pmatrix} \xi & 0 & -\eta \\ 0 & \zeta & 0 \\ -\eta & 0 & \xi \end{pmatrix}, U_5 = \begin{pmatrix} \zeta & 0 & 0 \\ 0 & \xi & \eta \\ 0 & \eta & \xi \end{pmatrix}, U_6 = \begin{pmatrix} \zeta & 0 & 0 \\ 0 & \xi & -\eta \\ 0 & -\eta & \xi \end{pmatrix},$$

with $\xi = \frac{\alpha+\gamma}{2} > \eta = \frac{\alpha-\gamma}{2} > 0$, $\zeta = \beta > 0$, $\alpha\beta\gamma = 1$ and thus $\zeta = \beta = (\xi^2 - \eta^2)^{-1}$.

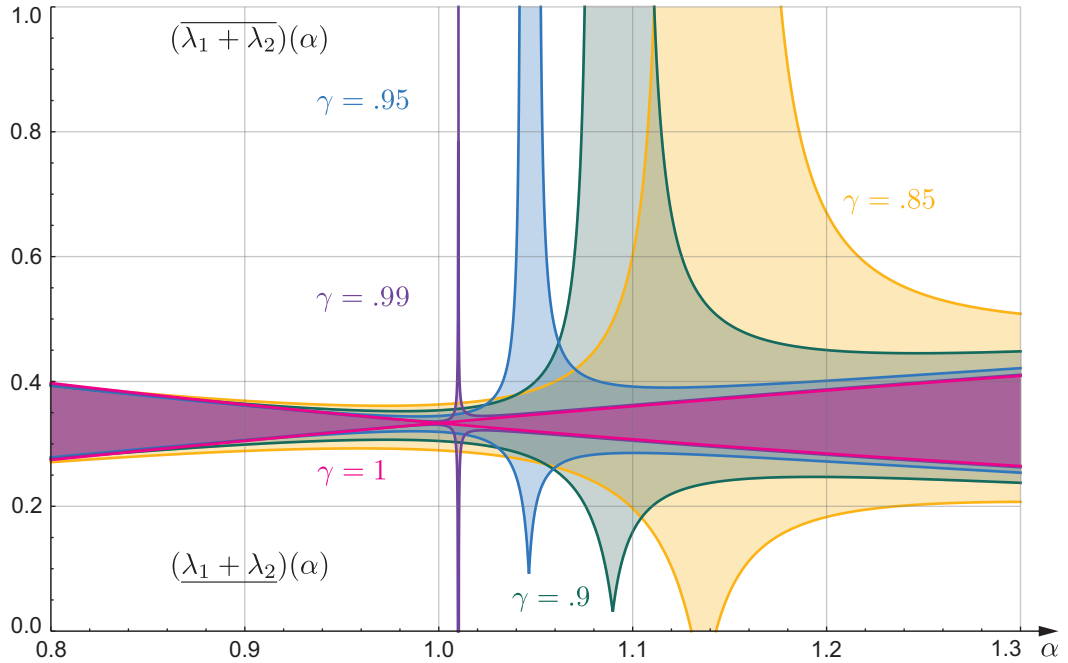


Fig. 4.4. Upper and lower bounds on the volume fractions of the first two orthorhombic wells in a self-accommodating microstructure for different values of $\gamma \in \{.85, .9, .95, .99, 1\}$.

Lemma 4.5. (*Volume fractions in cubic-to-orthorhombic*)

Let $K = \bigcup_{i=1}^6 \text{SO}(3)U_i$, where U_i denotes the set of martensitic variants in a volume preserving cubic-to-orthorhombic phase transformation (see above). Let further ν be

¹We note that the proposed method would not work for the unphysical (non-observed) cubic-to-orthorhombic transformation, where $U_i = \text{diag}(\pi_i(\alpha, \beta, (\alpha\beta)^{-1}))$, $\pi_i \in \mathcal{S}_3$.

a GYM supported on K with $\bar{\nu} = \mathbb{I}$ and decompose ν into six probability measures μ_i that are supported on the six wells, i.e. $\nu = \sum_{i=1}^6 \lambda_i \mu_i$, where $\text{supp } \mu_i \subset \text{SO}(3)U_i$ and $\mu_i(\mathbb{R}^{3 \times 3}) = 1$. Then if $2\beta^2 = 2\alpha^{-2}\gamma^{-2} > \alpha^2 + \gamma^2$ we have

$$\lambda_1 + \lambda_2 \geq \frac{\alpha\gamma - \alpha\gamma\sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}{1 - \alpha\gamma\sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}$$

and the opposite inequality for $2\alpha^{-2}\gamma^{-2} < \alpha^2 + \gamma^2$. And if $2\beta^{-4} = 2\alpha^4\gamma^4 < \alpha^2 + \gamma^2$ we have

$$\lambda_1 + \lambda_2 \leq \frac{\alpha\gamma - \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}{\alpha^2\gamma^2 - \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}$$

and the opposite inequality for $2\alpha^4\gamma^4 > \alpha^2 + \gamma^2$. The same inequalities hold for $\lambda_3 + \lambda_4$ and $\lambda_5 + \lambda_6$. In general, we always have (possibly trivial, i.e. ≥ 1) upper bounds and we do not have lower bounds whenever $2\alpha^{-2}\gamma^{-2} < \alpha^2 + \gamma^2$ and $2\alpha^4\gamma^4 < \alpha^2 + \gamma^2$. Figure 4.4 shows the bounds on the volume fractions of $\lambda_1 + \lambda_2$ for $\alpha \in [0.8, 1.3]$ and $\gamma \in \{.85, .9, .95, .99, 1\}$.

Proof. The cofactor matrices are given by

$$\begin{aligned} \text{cof } U_1 &= \zeta \begin{pmatrix} \xi & -\eta & 0 \\ -\eta & \xi & 0 \\ 0 & 0 & \zeta^{-2} \end{pmatrix}, \text{cof } U_2 = \zeta \begin{pmatrix} \xi & \eta & 0 \\ \eta & \xi & 0 \\ 0 & 0 & \zeta^{-2} \end{pmatrix}, \text{cof } U_3 = \zeta \begin{pmatrix} \xi & 0 & -\eta \\ 0 & \zeta^{-2} & 0 \\ -\eta & 0 & \xi \end{pmatrix}, \\ \text{cof } U_4 &= \zeta \begin{pmatrix} \xi & 0 & \eta \\ 0 & \zeta^{-2} & 0 \\ \eta & 0 & \xi \end{pmatrix}, \text{cof } U_5 = \zeta \begin{pmatrix} \zeta^{-2} & 0 & 0 \\ 0 & \xi & -\eta \\ 0 & -\eta & \xi \end{pmatrix}, \text{cof } U_6 = \zeta \begin{pmatrix} \zeta^{-2} & 0 & 0 \\ 0 & \xi & \eta \\ 0 & \eta & \xi \end{pmatrix}. \end{aligned}$$

Since by assumption $\det U_1 = 1$, we can find $T_i \in \text{SO}(3)^c, i = 1, \dots, 6$ such that

$$\mathbb{I} = \sum_{i=1}^6 \lambda_i T_i U_i \quad (4.7)$$

and

$$\mathbb{I} = \sum_{i=1}^6 \lambda_i T_i \text{cof } U_i. \quad (4.8)$$

Multiplying (4.8) from the right with $\mathbf{e}_3$ and taking the Euclidean norm gives

$$\begin{aligned} 1 &\leq \left(\sum_{i=3}^6 \lambda_i\right) \zeta \sqrt{\xi^2 + \eta^2} + (\lambda_1 + \lambda_2) \zeta^{-1} \\ &= \zeta \sqrt{\xi^2 + \eta^2} + (\lambda_1 + \lambda_2) (\zeta^{-1} - \zeta \sqrt{\xi^2 + \eta^2}) \\ &= \beta \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)} + (\lambda_1 + \lambda_2) \left(\beta^{-1} - \beta \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)} \right), \end{aligned}$$

where we have used that $\sum_{i=1}^6 \lambda_i = 1$ and $2(\xi^2 + \eta^2) = \alpha^2 + \gamma^2$. Thus if $2\beta^{-4} = 2\alpha^4\gamma^4 < \alpha^2 + \gamma^2$ we have

$$\lambda_1 + \lambda_2 \leq \frac{\alpha\gamma - \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}{\alpha^2\gamma^2 - \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}$$

and the opposite inequality for $2\alpha^4\gamma^4 > \alpha^2 + \gamma^2$. Multiplying (4.7) from the right with $\mathbf{e}_3$ and taking the Euclidean norm gives

$$\begin{aligned} 1 &\leq \left(\sum_{i=3}^6 \lambda_i\right) \sqrt{\xi^2 + \eta^2} + (\lambda_1 + \lambda_2) \zeta \\ &= \sqrt{\xi^2 + \eta^2} + (\lambda_1 + \lambda_2) (\zeta - \sqrt{\xi^2 + \eta^2}) \\ &= \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)} + (\lambda_1 + \lambda_2) \left(\beta - \sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)} \right). \end{aligned}$$

Thus if $2\beta^2 = 2\alpha^{-2}\gamma^{-2} < \alpha^2 + \gamma^2$ we have

$$\lambda_1 + \lambda_2 \leq \frac{\alpha\gamma - \alpha\gamma\sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}{1 - \alpha\gamma\sqrt{\frac{1}{2}(\alpha^2 + \gamma^2)}}$$

and the opposite inequality for $2\alpha^{-2}\gamma^{-2} > \alpha^2 + \gamma^2$. The inequalities for $\lambda_3 + \lambda_4$ and $\lambda_5 + \lambda_6$ can be derived analogously. Finally, we investigate the case when we only have one-sided bounds on $\lambda_1 + \lambda_2$. To this end, we note that if $2\alpha^{-2}\gamma^{-2} > \alpha^2 + \gamma^2$ and $2\alpha^4\gamma^4 > \alpha^2 + \gamma^2$ then, since $\alpha^2 + \gamma^2 > 2ac$, we have $1 > a^3c^3$ and $1 > a^{-3}c^{-3}$, a contraction and thus we always have upper bounds. $\square$

Cubic-to-Trigonal

In a cubic-to-trigonal transformation the four transformation strains are given by

$$U_1 = \begin{pmatrix} \alpha & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{pmatrix}, U_2 = \begin{pmatrix} \alpha & -\beta & \beta \\ -\beta & \alpha & -\beta \\ \beta & -\beta & \alpha \end{pmatrix},$$

$$U_3 = \begin{pmatrix} \alpha & \beta & -\beta \\ \beta & \alpha & -\beta \\ -\beta & -\beta & \alpha \end{pmatrix}, U_4 = \begin{pmatrix} \alpha & -\beta & -\beta \\ -\beta & \alpha & \beta \\ -\beta & \beta & \alpha \end{pmatrix},$$

with $\det U_1 = (\alpha + 2\beta)(\alpha - \beta)^2 = 1$, $\alpha > \beta$ and thus we may write $\alpha = \alpha(\beta)$.

Lemma 4.6. (*Volume fractions in cubic-to-trigonal*)

Let $K = \bigcup_{i=1}^4 \text{SO}(3)U_i$, where U_i denotes the set of martensitic variants in a volume preserving cubic-to-orthorhombic phase transformation (see above). Let further ν be a GYM supported on K with $\bar{\nu} = \mathbb{I}$ and decompose ν into four probability measures μ_i that are supported on the four wells, i.e. $\nu = \sum_{i=1}^4 \lambda_i \mu_i$, where $\text{supp } \mu_i \subset \text{SO}(3)U_i$ and $\mu_i(\mathbb{R}^{3 \times 3}) = 1$. Then if $\beta > 0$ we have

$$\lambda_1 \geq \frac{1}{4} - \frac{\beta}{2} + \frac{\beta^2}{12} + \frac{\beta^3}{18} + \mathcal{O}(\beta^4)$$

and

$$\lambda_1 \leq \frac{1}{4} + \frac{\beta}{2} - \frac{5\beta^2}{12} + \frac{5\beta^3}{18} + \mathcal{O}(\beta^4).$$

For $\beta < 0$ the inequalities reverse (cf. Figure 4.5).

Proof. Let us first assume that $\beta > 0$. Multiplication of the equivalent of (4.7) by $\mathbf{n} = \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3$ and taking the norm yields

$$\begin{aligned} \sqrt{3} &\leq \lambda_1 \sqrt{3}(\alpha + 2\beta) + (1 - \lambda_1) \sqrt{(\alpha - 2\beta)^2 + 2\alpha^2} \\ &= \sqrt{(\alpha - 2\beta)^2 + 2\alpha^2} + \lambda_1 \left(\sqrt{3}(\alpha + 2\beta) - \sqrt{(\alpha - 2\beta)^2 + 2\alpha^2} \right). \end{aligned}$$

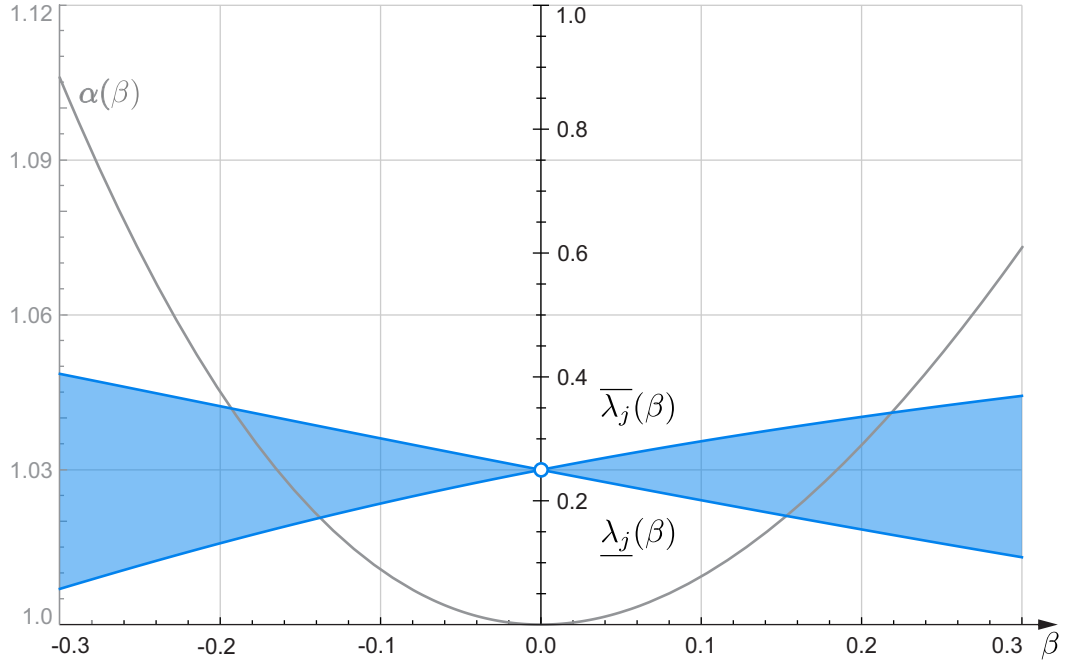


Fig. 4.5. Upper and lower bounds on the volume fractions of each cubic-to-trigonal well in a self-accommodating microstructure. The dependence $\alpha = \alpha(\beta)$ that allows self-accommodation is plotted in grey.

Thus

$$\lambda_1 \geq \frac{\sqrt{3} - \sqrt{(\alpha - 2\beta)^2 + 2\alpha^2}}{\sqrt{3}(\alpha + 2\beta) - \sqrt{(\alpha - 2\beta)^2 + 2\alpha^2}},$$

where we used that for $\beta > 0$ the denominator is always positive. The bounds for $\lambda_i, i = 2, 3, 4$ can be derived analogously. Similarly, multiplying the equivalent of (4.8) by $\mathbf{n} = \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3$ and using the norm gives

$$\sqrt{3} \leq (\alpha - \beta)\sqrt{3\alpha^2 + 10\alpha\beta + 11\beta^2} + \lambda_1 \left(\sqrt{3}(\alpha - \beta)^2 - (\alpha - \beta)\sqrt{3\alpha^2 + 10\alpha\beta + 11\beta^2} \right)$$

and thus

$$\lambda_1 \leq \frac{\sqrt{3} - (\alpha - \beta)\sqrt{3\alpha^2 + 10\alpha\beta + 11\beta^2}}{\sqrt{3}(\alpha - \beta)^2 - (\alpha - \beta)\sqrt{3\alpha^2 + 10\alpha\beta + 11\beta^2}},$$

where we have used that for $\beta > 0$ the denominator is always negative. The case $\beta < 0$ can be treated analogously and the inequalities reverse. By using the explicit dependence $\alpha(\beta)$ and performing a Taylor expansion about $\beta = 0$ we obtain the desired bounds. $\square$

We conclude this chapter by recalling that, within the Ball-James model, a self-accommodating martensitic microstructure is able to fit stress free within austenite. In the next chapter, we investigate what happens if the martensite fails to be self-accommodating and determine whether in this situation it is still energetically favourable to nucleate martensite within austenite.

Interior Nucleation of Martensite

In this chapter, contrary to the previous chapter, we will always assume that the microstructure cannot be self-accommodating (i.e. $\det U_1 \neq 1$) and we investigate whether in such a case a microstructure, that is not fully supported on the martensite wells, can still be energetically preferable over pure austenite and thus lead to interior nucleation. The results presented in this chapter have been published in [Mue15].

5.1 Background and Motivation

The high growth velocity of heterogeneous temperature induced nucleation of martensite, which is of the order of magnitude of the speed of sound ([BM53], [Chr02, p.977 ff.]), is one of the reasons why the process of nucleation is not yet satisfactorily understood. As pointed out in [Chr02, Ch. 23] “*the kinetics of martensitic transformations are dependent mainly on the nucleation process as each plate grows rapidly to its limiting size*” and as a consequence “*it is often found that the plates of martensite formed [...] have a constant length:thickness ratio*” until “*growth ceases because of plastic deformation*”. Different models (e.g. [Bal+11; Coo73; OC79; OR92]) have been proposed to explain the formation and predict properties of such plates. It has been shown theoretically and experimentally that the availability of a free surface can have a significant influence on the nucleation process. In [Kra+89] a single crystal of Fe-Ni was coated with a Ni-rich surface layer to inhibit nucleation from the free surface with the effect that the formation of martensite was completely suppressed during slow cooling. Applying a similar procedure to an In-Cd alloy

however did not show a difference between the coated and uncoated crystal. In a related experiment on Cu-Al-Ni single- and polycrystals with varying grain-sizes it has been shown in [SC79] that the energy needed for bulk nucleation is significantly higher than that required for corner nucleation or to move a planar interface. A single crystal of the same alloy was considered in [Bal+11] where it was shown experimentally and theoretically that corner nucleation is energetically preferable over interior nucleation. However, if a free surface is not available, for instance because of a relatively large grain-size or by a coating as described above, it is of interest to establish criteria for interior nucleation.

We will use the Ball-James Model (cf. Chapter 2) to obtain estimates on the energy of interior nuclei. In contrast to [OR92], where a nucleus forms within an array of interfacial dislocation, we assume that the material deforms purely elastically and we do not consider plasticity. Furthermore, interfacial energy is not taken into account.

In Chapter 4, we have seen that whenever the austenite has cubic symmetry and the transformation is volume-preserving the material can be self-accommodating and thus the martensite is able to match the austenite along any interface. In particular, in this situation interior nucleation is energetically equivalent to nucleation from the boundary. However, in general we expect to have a volume change during transformation, so that any inclusion of martensite within austenite necessarily has a region where it is neither on the austenite nor on the martensite wells. We will refer to this region as the *interpolation layer* and it can loosely be understood as the elastic equivalent to having interfacial energy and plasticity. By the classical theory of heterogeneous nucleation, in order to transform a given region of austenite to martensite, *“the negative free energy change resulting from the formation of a given volume of a more stable phase [the martensite] is opposed by a positive free energy change due to the creation of an interface [the interpolation layer] between the initial phase and the new phase”* ([Chr02, p. 4]). Thus, our criterion for interior nucleation is that the energy of the inclusion is lower than the energy of the parent phase, i.e.

the austenite. It seems to have first been shown qualitatively in [Bal13] that, for a sufficiently flat cylindrical inclusion, nucleation is always energetically preferable over pure austenite. In the present work, we develop quantitative estimates on the energy difference between a nucleus and the austenite. The estimates will depend on the temperature and the assumed growth of the free energy density away from the wells.

5.2 A Mathematical Model for Interior Nucleation

We adopt the setting of non-linear elasticity described in Chapter 2 and thus look for minimising sequences of

$$E(y) := \int_{\Omega} W_{\theta}(Dy(x)) \, dx, \quad (\text{E})$$

where $\Omega \subset \mathbb{R}^3$ represents the undistorted austenite. The free energy density W_{θ} is minimised at $K_m = \text{SO}(3)U_1(\theta)\mathcal{P}^{24}$, $U_1(\theta) = \text{diag}(\eta_2, \eta_1, \eta_1)$ below the transformation temperature θ_c and minimised at $\alpha(\theta)\text{SO}(3)$ above the transformation temperature. For notational convenience and without loss of generality we henceforth fix a temperature $\theta^* < \theta_c$ and assume that $\alpha(\theta^*) = 1$. We set

$$W = \begin{cases} 0 & \text{on } \text{SO}(3), \\ -\tau & \text{on } K_m, \end{cases} \quad (5.1)$$

so that in particular $W > -\tau$ on $\mathbb{R}^{3 \times 3} \setminus K_m$. Further, since we are interested in interior nucleation, the boundary condition is always the austenite and thus by frame indifference we may assume that $y(x)|_{\Omega} = x$, $Dy(x)|_{\Omega} = \mathbb{I}$.

To determine whether nucleation of martensite within austenite is energetically favourable we need to find configurations containing martensite that have lower energy than pure austenite. Clearly, the energy functional (E) is bounded from below by $E(y) \geq -\tau|\Omega|$. Hence, any sequence $\{y_j\}_j \subset W^{1,\infty}(\Omega)$ such that $E(y_j) \rightarrow -\tau|\Omega|$

corresponds to a microstructure that can only contain variants of martensite and thus can only exist if the volume does not change during transformation. If the transformation does involve a change in volume, i.e. $\det U_1 \neq 1$, it is of interest to find the minimum value of the free energy (E). Since the energy is proportional to the volume of the inclusion the relevant quantity is the macroscopic free energy density W^{qc} . In particular, $W^{\text{qc}}(\mathbb{I})$ equals the free energy density of a region that has been macroscopically deformed by the identity map. By Definition 2.5, W^{qc} can be characterised by

$$W^{\text{qc}}(\mathbb{I}) = \frac{1}{|\Omega|} \inf_{\phi \in W_0^{1,\infty}(\Omega)} \int_{\Omega} W(\mathbb{I} + D\phi(x)) \, dx,$$

so that $\inf E(y) = |\Omega|W^{\text{qc}}(\mathbb{I})$. In particular whenever $W^{\text{qc}}(\mathbb{I}) < 0$ there exists a deformation $y(x) = x + \phi(x)$ that is energetically preferable over the pure austenite.

5.3 Construction of Martensitic Nuclei

Our goal is to construct a test function ϕ such that the corresponding deformation $y(x) = x + \phi(x)$ has negative total free energy and is thus energetically preferable over the pure austenite corresponding to $y(x) = x$. We will explore two different approaches. In the first approach we only allow deviations from the austenite and we show that the geometry of the inclusion plays a crucial rôle. In the second approach we only allow deviations from the martensite wells and use the principle of self-accommodation to derive our estimates.

Deviations from the Austenite

We have seen that a laminate between two martensitic variants can be compatible with austenite. That is, there exists a rank-one matrix $\mathbf{b} \otimes \mathbf{m}$, $\mathbf{b} \in \mathbb{R}^3$, $\mathbf{m} \in S^2$ such that

$$\lambda \hat{R}U_1 + (1 - \lambda) \hat{R}RU_2 = \mathbb{I} + \mathbf{b} \otimes \mathbf{m}, \quad (5.2)$$

where $\hat{R}U_1, \hat{R}RU_2 \in K_m$ such that $U_1 - RU_2 = \mathbf{a} \otimes \mathbf{n}$, $\mathbf{a} \in \mathbb{R}^3$, $\mathbf{n} \in S^2$ and $\lambda \in (0, 1)$.

We consider an inclusion with a core of pure martensite. Since the volumes do not agree we have a transition layer where the deformation gradients cannot be supported on the wells. We show that the energy penalty from the transition layer can be overcome by the decrease in energy due to the presence of the martensite as long as the inclusion is flat and thin.

Definition 5.1. (Cylindrically symmetric inclusion with a simple laminate core)

Let $\Omega = \Omega_1 \cup \Omega_2$ be such that the core Ω_1 consists of a simple laminate of martensite that is compatible with the austenite in the sense of (5.2). By rotating the entire system we may assume without loss of generality that $\mathbf{m} = \mathbf{e}_3$. We define the two regions as follows

$$\Omega_1 := \{x \in \mathbb{R}^3 | x_3 \in [0, \varphi(r)]\}, \quad \Omega_2 := \{x \in \mathbb{R}^3 | x_3 \in (\varphi(r), \sigma\varphi(r)]\},$$

where $r^2 = x_1^2 + x_2^2$, $\sigma > 1$ and $0 \leq \varphi(r) \in W^{1,\infty}([0, \infty))$, $\lim_{r \rightarrow \infty} \varphi(r) = 0$. Note that we assume symmetry with respect to the $x_1 - x_2$ plane and only define the upper half of the inclusion. Further, we assume that $\text{Vol}(\Omega_1) = 2\pi \int_0^\infty r\varphi(r) dr = 1$ and thus $\text{Vol}(\Omega_2) = \sigma - 1$. We define our test function $\phi \in W_0^{1,\infty}(\Omega)$ in the regions Ω_1 and Ω_2 separately. In Ω_1 we set $\phi_1(x) \equiv \phi|_{\Omega_1} := \mathbf{b} \cdot x_3$ and in Ω_2 we interpolate linearly in x_3 direction from $\mathbf{b} \cdot \varphi(r)$ to 0 by defining

$$\phi_2(x) \equiv \phi|_{\Omega_2} := \frac{\mathbf{b}}{1 - \sigma} \cdot (x_3 - \sigma\varphi(r)),$$

so that $\phi = \phi_1 + \phi_2 \in W_0^{1,\infty}(\Omega)$.

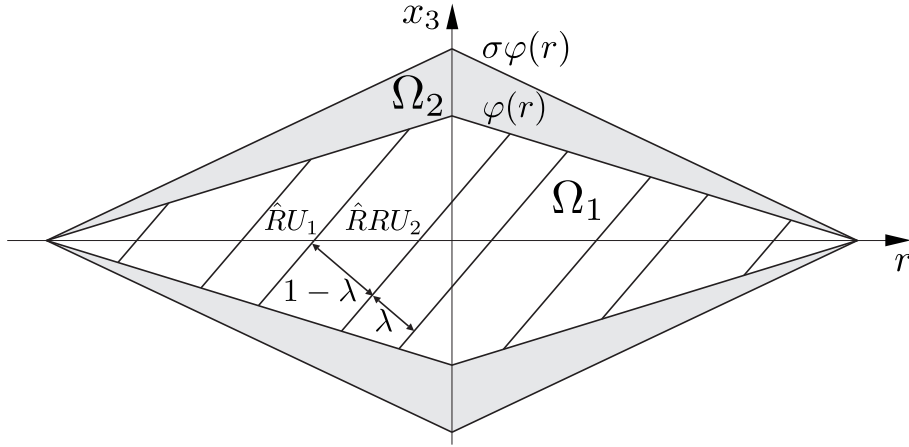


Fig. 5.1. Schematic representation of the cross section at $x_2 = 0$ in the $x_1 - x_3$ plane of an interior nuclei with a simple laminate core.

Theorem 5.1. *Let W be as in (5.1) and assume the following upper bound on W away from the austenite*

$$W(\mathbb{I} + H) \leq C |H|^2. \quad (5.3)$$

Then the inclusion given by Definition 5.1 provides the following upper bound

$$W^{\text{qc}}(\mathbb{I}) \leq -\tau \left(1 + 2\beta + 2\sqrt{\beta + \beta^2} \right)^{-1}, \quad (5.4)$$

where $\beta := \frac{C}{\tau} |\mathbf{b}|^2$.

Proof. In Ω_1 the gradients of ϕ are supported on the martensite wells and therefore $E(\phi_1) = -\tau \text{Vol}(\Omega_1) = -\tau$. In Ω_2 we estimate the energy using the upper bound on $W(\mathbb{I} + H)$. We have $D\phi_2(x) = \frac{\mathbf{b}}{1-\sigma} \otimes \nabla u(x)$ with $\nabla u(x) = (-\sigma\phi'(r)\frac{x_1}{r}, -\sigma\phi'(r)\frac{x_2}{r}, 1)^T$. Noting that $D\phi_2(x)$ is independent of x_3 and using the coarea formula (see [Fed96, Ch. 3]) we arrive at

$$E(\phi_2) \leq \frac{C}{(\sigma - 1)} |\mathbf{b}|^2 + \frac{\sigma^2}{(\sigma - 1)} \gamma,$$

where $\gamma := C\pi |\mathbf{b}|^2 \int_0^\infty r\phi(r)\phi'(r)^2 dr$. Combining the two estimates we obtain

$$E(\phi) \leq -\tau + \frac{C}{(\sigma - 1)} |\mathbf{b}|^2 + \frac{\sigma^2}{(\sigma - 1)} \gamma$$

and thus for $\gamma \rightarrow 0$ and since $|\Omega| = \sigma$ we have

$$W^{\text{qc}}(\mathbb{I}) \leq \tau \left(-\frac{1}{\sigma} + \frac{C}{\tau} \frac{1}{\sigma(\sigma-1)} |\mathbf{b}|^2 \right) = \tau \left(-\frac{1}{\sigma} + \frac{\beta}{\sigma(\sigma-1)} \right),$$

where $\beta := \frac{C}{\tau} |\mathbf{b}|^2$. Minimisation with respect to σ gives the desired bound. $\square$

Remark 5.1. We note that we derived this upper bound by taking the limit $\gamma \rightarrow 0$ and thus $\int_0^\infty r \varphi(r) \varphi'(r)^2 dr \rightarrow 0$ which corresponds to $\varphi'(r) \rightarrow 0$ as the volume is fixed. Thus, within the class of inclusions under consideration, the lowest energy is achieved by a very flat and thin inclusion.

We can derive the same upper bound on $W^{\text{qc}}(\mathbb{I})$ by using the general result that $W^{\text{qc}} \leq W^{\text{rc}}$ (cf. Remark 2.5). Even though this argument is simpler, it does not give information on the structure of the inclusion.

Lemma 5.1. *Under the same assumptions as in Theorem 5.1 an upper bound on $W^{\text{rc}}(\mathbb{I})$ and thus on $W^{\text{qc}}(\mathbb{I})$ is given by*

$$W^{\text{rc}}(\mathbb{I}) \leq -\tau \left(1 + 2\beta + 2\sqrt{\beta + \beta^2} \right)^{-1},$$

where $\beta := \frac{C}{\tau} |\mathbf{b}|^2$.

Proof. An upper bound on W^{rc} (see [Dac07, Thm. 6.10]) is in its simplest form given by

$$W^{\text{rc}}(A) \leq \inf \{ \lambda W(A_1) + (1-\lambda)W(A_2) : \lambda A_1 + (1-\lambda)A_2 = A, \text{rank}(A_1 - A_2) \leq 1 \}. \quad (5.5)$$

The estimate can be refined by applying the same estimate to each of the terms $W(A_i), i = 1, 2$ on the right-hand side. We now decompose

$$\mathbb{I} = \lambda(\mathbb{I} + \mathbf{b} \otimes \mathbf{m}) + (1-\lambda)(\mathbb{I} + \varepsilon \mathbf{b} \otimes \mathbf{m}),$$

where $\varepsilon = \frac{\lambda}{\lambda-1}$ and $\mathbb{I} + \mathbf{b} \otimes \mathbf{m} = \lambda R_1 U_1 + (1 - \lambda) R_2 U_2$, $R_1, R_2 \in \text{SO}(3)$ such that $\text{rank}(R_1 U_1 - R_2 U_2) = 1$. Then by using (5.3) and (5.5) we arrive at

$$W^{\text{rc}}(\mathbb{I}) \leq \lambda W^{\text{rc}}(\mathbb{I} + \mathbf{b} \otimes \mathbf{m}) + (1 - \lambda) W(\mathbb{I} + \frac{\lambda}{\lambda-1} \mathbf{b} \otimes \mathbf{m}) \leq \tau \left(-\lambda + \beta \frac{\lambda^2}{1 - \lambda} \right)$$

with $\beta := \frac{C}{\tau} |\mathbf{b}|^2$. Minimisation with respect to λ gives the desired estimate. $\square$

Deviations from the Martensite

In many materials $\det U_1 \approx 1$, so that matrices in a relatively small neighbourhood of the martensite wells have unit determinant. Allowing deviations from the martensite wells we now consider an inclusion with a core of variants that are close to the martensite wells and allow self-accommodation and thus do not require a transition layer.

Theorem 5.2. *Let $|\det U^{-1/3} - 1| \ll |\eta_1 - 1|, |\eta_2 - 1|$, $U \in K_m = \bigcup_{i=1}^3 \text{SO}(3) U_i$ and let W be as (5.1) with*

$$W(V) \leq W(U) + C \text{dist}^2(V, K_m) \quad (5.6)$$

for all $V \in \mathbb{R}^{3 \times 3}$ such that $\text{dist}(V, K_m) \leq |1 - \det U^{-1/3}|$. Then

$$W^{\text{qc}}(\mathbb{I}) \leq W^{\text{rc}}(\mathbb{I}) \leq -\tau + C(\det U^{-1/3} - 1)^2 |U|^2. \quad (5.7)$$

Proof. By Lemma 4.2 we know that in a cubic-to-tetragonal phase transformation there exist laminates with macroscopic deformation gradient $\mathbb{I}$. Therefore let us set $\tilde{U}_i := (\det U)^{-1/3} U_i$ so that $\det \tilde{U}_i = 1$. By (5.6) we have

$$W(\tilde{U}_i) \leq -\tau + C \left(1 - \det U^{-1/3} \right)^2 |U|^2$$

and thus, using the refined version of (5.5), we can estimate

$$W^{\text{qc}}(\mathbb{I}) \leq W^{\text{rc}}(\mathbb{I}) \leq W(U) + C \left(1 - \det U^{-1/3}\right)^2 |U|^2.$$

□

Remark 5.2. We note that unlike Theorem 5.1 this construction is only preferable over the pure austenite for τ sufficiently large, corresponding to a temperature θ^* sufficiently far below the transition temperature θ_c , or for $\det U$ sufficiently close to 1. A comparison with the estimates in Theorem 5.1 reveals that (5.7) provides a better bound than (5.4) for small volume changes and a worse bound on $W^{\text{qc}}(\mathbb{I})$ for large volume changes. For $\det U \rightarrow 1$ we recover the case of self-accommodation, i.e.

$$-\tau \leq W^{\text{qc}}(\mathbb{I}) \leq -\tau + \lim_{\det U \rightarrow 1} C(\det U^{-1/3} - 1)^2 |U|^2 = -\tau.$$

Remark 5.3. For simplicity we have only considered a cubic-to-tetragonal phase transformation. However, in the first part the only assumption on the material was the existence of an interface between a microstructure of martensite and austenite. In the second part, the only assumption on the material was that it almost satisfies a criterion of self-accommodation (e.g. in a cubic-to-* transformation this holds iff $\det U_i \approx 1$, cf. Chapter 4). Thus, as long as either or both assumptions are satisfied, all respective conclusions remain the same.

Part II

A NEW APPROACH TO STEELS

Steel has always been and still is one of the most important materials. It is ubiquitous and indispensable in construction and present in almost every building and machine we use. The term ‘steel’ can be traced back to the Proto-Germanic term ‘stakhla’ which means standing firm [Har16]. And indeed, even though new and improved high-tech materials are developed every year, steel remains one of the most durable and more importantly, cost-effective materials available on a large scale. It is thus no surprise that it is considered the ‘gold-standard’¹ against which emerging structural materials are compared.

Historically, and most commonly, the term steel is associated with an alloy of iron with 0.05% – 3% carbon. However, today, a wide range of other alloying elements, such as chromium, manganese, nitrogen, and various combinations of them are common-place. The natural allotropes of iron are the body-centred cubic α -phase (ferrite), the face-centred cubic γ -phase (austenite) and the hexagonal close-packed ϵ -phase. However, the ϵ -phase only occurs at low temperatures and under very high pressure and the vast majority of steels rely on the transition from γ to α (cf. Chapter 1). Furthermore, following the classification of [BH11, Fig. 1.6] one can

¹Following the words of [BH11].

distinguish between two types of steel according to their transformation mechanism: reconstructive (i.e. diffusion of atoms) and displacive (diffusionless). Martensite falls into the second category and will be the focus of the theoretical treatment of steels in the present work. In spite of its iconic name, it seems that martensitic steel has not been addressed thoroughly within the framework of non-linear elasticity before. A possible reason may be the large transformation strains (cf. Chapter 1) that prevent elastic behaviour. Another reason might be the differences in terminology between the metallurgical and the mathematical community.

Our goal is to change this situation by the introduction of tools, familiar to the mathematical community, to the modelling of steels. This introduction will be conducted on two different levels. In Chapter 6, we develop a dictionary that translates between the experimentally observable orientation relationships, which are central quantities in the metallurgy community, and the actual transformation strains U_i , which are central to most mathematical models (cf. Chapter 2). In Chapter 7, we show how fundamental statements and procedures used in phenomenological approaches can be recast in mathematical language.

Aside from the simplification and generalisation of existing theories, the main advantage of the mathematical treatment is that often fewer or no input parameters are required. For instance, in Chapter 6 most of the commonly known orientation relationships are derived under very fundamental assumptions on invariant planes and directions and the results on optimal lattice transformations from Chapter 1. In Section 7.3, which concerns a new approach to the modelling of low carbon steels, we show how a mathematical theory that requires essentially no input parameters can recast and improve the most commonly used phenomenological theories which require no less than 7 fitted parameters. The absence of curve fitting provides new insight into the underlying mechanism and leads to a prediction of a new microscopic structure of low carbon steels. While these predictions seem to contravene common belief, recent independent experiments suggest that they may in fact be true.

A Theoretical Investigation of Orientation Relationships and Transformation Strains in Steels

The identification of orientation relationships (ORs) plays a crucial rôle in the understanding of solid phase transformations. In steels, the most common models of ORs are the ones by Nishiyama-Wassermann (NW) and Kurdjumov-Sachs (KS). The defining feature of these and other OR models is the matching of directions and planes in the face-centred cubic γ -phase to ones in the body-centred cubic/tetragonal α/α' -phase.

We introduce a novel method that identifies transformation strains with ORs and use it to develop a new strain-based approach to phase transformation models in steels. Whenever the product phase is cubic, we show that the transformation strains that leave a close packed plane in the γ -phase and a close packed direction within that plane unrotated are precisely those giving rise to the NW and KS ORs. Further, it is outlined how, by choosing different pairs of unrotated planes and directions, other common ORs such as the ones by Pitsch (P) and Greninger-Troiano (GT) can be derived.

One of the advantages of our approach is that it leads to a natural generalisation of the NW, KS and other ORs for different ratios of tetragonality r of the product bcc α' -phase. These generalised ORs predict a sharpening of the transformation textures with increasing tetragonality and are thus in qualitative agreement with experiments on steels with varying alloy concentration.

The results presented in this chapter have been published in [KM16a].

Background

The transformation mechanism from the face-centred cubic (fcc) to the body-centred cubic/tetragonal (bcc/bct) phase of steel has received widespread attention and the most influential early studies include [Bai24; KS30; Nis34; Was35]. In his seminal paper, Bain [Bai24] proposed a mechanism that transforms the fcc γ -phase of iron to its bcc α -phase (cf. Chapter 1). His conceived mechanism, although now widely accepted, was not without criticism from his contemporaries. Among the critics were Kurdjumov & Sachs [KS30] who conducted X-ray diffraction measurements on 1.4% carbon steel and measured the orientation relationships between austenite and pure bcc α -iron as well as between austenite and 1.4% C α' -steel.¹ The most important feature of their mechanism was the parallelism between the $(111)_\gamma$ and the $(011)_{\alpha'}$ plane as well as the $[10\bar{1}]_\gamma$ and the $[1\bar{1}1]_{\alpha'}$ direction and they explained how these conditions can be satisfied by a combination of three shears. They concluded that the resulting orientation relationship for pure iron differs from the one for 1.4% C steel (see Tables 2 in [KS30] and [Ott60]). In 1934, using the same methods, Nishiyama [Nis34] investigated a Fe-30% Ni single crystal which, like pure iron, undergoes an fcc-to-bcc transformation. Based on his observations, Nishiyama proposed a different orientation relationship that has the same parallel planes but the direction $[10\bar{1}]_\gamma$ parallel to $[100]_{\alpha'}$. One year later, Wassermann [Was35] independently postulated the same relationships and also confirmed the earlier results by Kurdjumov & Sachs. Apart from the Nishiyama-Wassermann (NW) and Kurdjumov-Sachs (KS) orientation relationships (ORs) several other ORs, e.g. by Pitsch [Pit59] (P) and Greninger-Troiano [GT49] (GT), have been proposed and they all share the common feature of matching directions and planes in the parent phase to ones in the product phase.

¹Henceforth, we adopt the convention from [Nis78] of using the symbol α' for the low temperature phase of steels irrespectively of whether it is cubic or tetragonal.

Our goal is to shift this paradigm towards a derivation of orientation relationships based on the transformation strains. Compared to previous approaches (see e.g. [Guo+04; He+05; Cay+10]), our approach brings the following novelties:

1. The only necessary inputs are the lattice parameters of the two phases and the knowledge of a plane and a direction that is left unrotated.
2. Each derived strain can be uniquely identified with an OR and the parallelisms between planes and directions in the two phases follow.
3. The additional knowledge of the actual underlying deformation of the material can e.g. be used to unambiguously determine twin relationships (cf. Section 6.2) and generally lay the groundwork for mathematical theories of steels based on energy minimisation (see e.g. [Bha03] and Chapter 7.3).
4. Our method takes into account the ratio of tetragonality $r = c/a$ of the bct α' -phase. Thus, the derived strains and orientation relationships also depend on r and can be expressed explicitly as functions of r .

For $r = 1$, corresponding to bcc, we recover the original NW, KS and P ORs. However, for $r > 1$, our approach predicts a deviation from the original ORs. We show how this leads to a sharpening of the transformation textures and how it can be used to explain the deviation from the exact parallelism condition in the GT ORs.

Notation and Useful Identities

We recall the identities

$$(\mathbf{m} \times \mathbf{u}) \cdot (\mathbf{n} \times \mathbf{v}) = (\mathbf{m} \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{v}) - (\mathbf{u} \cdot \mathbf{n})(\mathbf{v} \cdot \mathbf{m}) \quad (6.1)$$

and

$$A\mathbf{u} \times A\mathbf{v} = \text{cof } A(\mathbf{u} \times \mathbf{v}), \quad (6.2)$$

where $\mathbf{u}, \mathbf{v}, \mathbf{m}, \mathbf{n} \in \mathbb{R}^3$ and $A \in \mathbb{R}^{3 \times 3}$. In particular, the matrix of cofactors, $\text{cof } A$, measures how a vector normal to $\mathbf{u}$ and $\mathbf{v}$ deforms whenever $\mathbf{u}$ and $\mathbf{v}$ are deformed by A . Further, we uniquely identify any rotation $R \in \text{SO}(3)$ as a counterclockwise rotation by an angle ϕ about a vector $\mathbf{u}$ and we write $R = R[\phi, \mathbf{u}]$, where $\mathbf{u}$ is always expressed in the standard basis $\mathbf{e}_1 = (1, 0, 0)^T$, $\mathbf{e}_2 = (0, 1, 0)^T$, $\mathbf{e}_3 = (0, 0, 1)^T$. The magnitude of the angle of rotation is given by $|\phi| = \arccos((\text{Tr } R - 1)/2)$ and the sign of ϕ is given by $\text{sgn}(\phi) = \text{sgn}((\mathbf{n} \times R\mathbf{n}) \cdot \mathbf{u})$, where $\mathbf{n}$ is any vector that is not parallel to the axis of rotation $\mathbf{u}$. In particular, reversing the sign of the axis $\mathbf{u} \rightarrow -\mathbf{u}$ is equivalent to reversing the sign of the angle of rotation $\phi \rightarrow -\phi$. Finally, we recall that $\mathcal{P}^{24}$ (see Definition 0.5 and Appendix F) denotes the point group of a cube and that (see Definition 0.6) two vectors $\mathbf{n}, \mathbf{n}'$ are *crystallographically equivalent* iff $\mathbf{n}' = P\mathbf{n}$ for some $P \in \mathcal{P}^{24}$.

6.1 A Unified Approach to Phase Transformation

Models in Steels

Since Bain's seminal paper [Bai24] (see also Chapter 1) it is well known that the pure stretches required to transform an fcc lattice to a bcc/bct lattice are given by the three Bain strains

$$U_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}, U_2 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}, U_3 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad (6.3)$$

where $\alpha = \frac{\sqrt{2}a}{a_0}$ and $\beta = \frac{c}{a_0}$. Here a_0 is the lattice parameter of the fcc phase and $c \geq a$ are the lattice parameters of the bct phase ($a = c$ for bcc). An additional rigid body rotation R does not change the bcc/bct lattice structure and hence any lattice transformation T from fcc to bcc/bct is of the form

$$T = RU_i \text{ for some } i = 1, 2, 3.$$

Now suppose that the transformation T leaves a plane with normal $\mathbf{n}$ and a direction $\mathbf{v}$ within that plane unrotated, i.e.

$$\frac{\text{cof } T\mathbf{n}}{|\text{cof } T\mathbf{n}|} = R \frac{\text{cof } U_i\mathbf{n}}{|\text{cof } U_i\mathbf{n}|} = \mathbf{n} \text{ and } \frac{T\mathbf{v}}{|T\mathbf{v}|} = R \frac{U_i\mathbf{v}}{|U_i\mathbf{v}|} = \mathbf{v}. \quad (6.4)$$

Defining $\mathbf{m}_i = \text{cof } U_i\mathbf{n}/|\text{cof } U_i\mathbf{n}|$, $\mathbf{u}_i = U_i\mathbf{v}/|U_i\mathbf{v}|$, we observe that

$$\mathbf{m}_i \cdot \mathbf{u}_i \propto \text{cof } U_i\mathbf{n} \cdot U_i\mathbf{v} = U_i^T \text{cof } U_i\mathbf{n} \cdot \mathbf{v} \propto \mathbf{n} \cdot \mathbf{v} = 0,$$

where we have used that $\text{cof } U_i \propto U_i^{-T}$ and that $\mathbf{v} \perp \mathbf{n}$.² In particular, the pairs $\mathbf{m}_i, \mathbf{u}_i$ and $\mathbf{n}, \mathbf{v}$ are both orthonormal and thus there is a unique rotation $R = R_i$ such that $R_i\mathbf{m}_i = \mathbf{n}$ and $R_i\mathbf{u}_i = \mathbf{v}$ given by

$$R_i = \begin{pmatrix} | & | & | \\ \mathbf{n} & \mathbf{v} & \mathbf{n} \times \mathbf{v} \\ | & | & | \end{pmatrix} \begin{pmatrix} - & \mathbf{m}_i & - \\ - & \mathbf{u}_i & - \\ -\mathbf{m}_i \times \mathbf{u}_i- \end{pmatrix}. \quad (6.5)$$

Consequently, for each $i = 1, 2, 3$ there is exactly one transformation strain, $T_i = R_i U_i$, from fcc to bcc/bct that leaves the plane with normal $\mathbf{n}$ and the direction $\mathbf{v}$ within that plane unrotated.

Identifying Strains with Orientation Relationships

Given the transformation strain T_i , we show how to compute the corresponding orientation relationship (OR). For simplicity, we focus on the case $i = 2$; the remaining two cases can be treated analogously. From the pure Bain mechanism it is clear that the transformation U_2 results in a bcc/bct unit cell with edges along the directions $\mathbf{e}_1 - \mathbf{e}_3$, $\mathbf{e}_2$ and $\mathbf{e}_1 + \mathbf{e}_3$ (see Figure 6.1). The additional rotation R_2 in the transformation T_2 then results in a bcc/bct unit cell with edges along the directions

$$R_2(\mathbf{e}_1 - \mathbf{e}_3), R_2\mathbf{e}_2 \text{ and } R_2(\mathbf{e}_1 + \mathbf{e}_3),$$

²Recall that $x \propto y$ if there is a constant $c \in \mathbb{R}$ such that $x = cy$.

which form the natural basis for the bcc/bct lattice. Noting that $\mathbf{e}_1 - \mathbf{e}_3 = R[45^\circ, \mathbf{e}_2]\mathbf{e}_1$

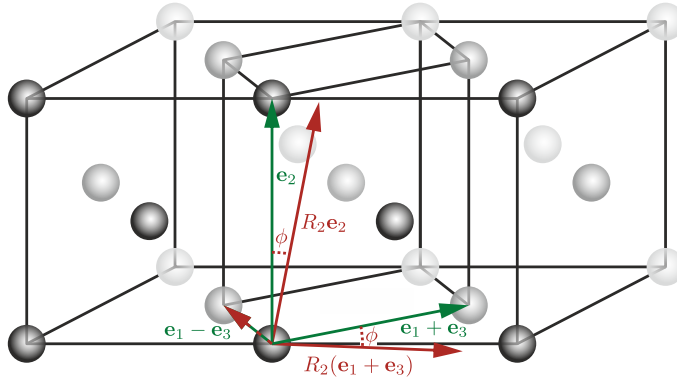


Fig. 6.1. The green vectors $\mathbf{e}_1 - \mathbf{e}_3, \mathbf{e}_2, \mathbf{e}_1 + \mathbf{e}_3$ are along the edges of the body-centred tetragonal cell that is contained in the face-centred cubic lattice and the red vectors are obtained through the rotation R_2 .

and $\mathbf{e}_1 + \mathbf{e}_3 = R[45^\circ, \mathbf{e}_2]\mathbf{e}_3$ we see that the change of basis matrix between fcc and bcc/bct is given by $R_2R[45^\circ, \mathbf{e}_2]$, i.e. $\mathbf{x} = [x_1 \ x_2 \ x_3]_\gamma = [\hat{x}_1 \ \hat{x}_2 \ \hat{x}_3]_{\alpha'}$, where

$$\begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \end{pmatrix} = R[-45^\circ, \mathbf{e}_2]R_2^T \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} =: O_2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \quad (6.6)$$

In particular, through the matrix $O_2 = R[-45^\circ, \mathbf{e}_2]R_2^T$ one can express the coordinates of the unrotated plane $\mathbf{n}$ and direction $\mathbf{v}$ in the new bcc/bct (α' -) basis and hence determine the *orientation relationship*. In general, the orientation relationship corresponding to $T_i = R_iU_i$ is given through the matrix

$$O_i = R[-45^\circ, \mathbf{e}_i]R_i^T, \quad (6.7)$$

which we henceforth call the *orientation relationship matrix*. We note that $R[45^\circ, \mathbf{e}_i] = R[90^\circ, \mathbf{e}_i]R[-45^\circ, \mathbf{e}_i]$ with $R[90^\circ, \mathbf{e}_i] \in \mathcal{P}^{24}$, i.e. choosing the opposite sign for the 45° rotation about $\mathbf{e}_i$ simply leads to a crystallographically equivalent normal and direction. In summary, starting from the transformation T_i , we obtain the *orientation relationship*

$$(n_1 \ n_2 \ n_3)_\gamma \parallel (\hat{n}_1 \ \hat{n}_2 \ \hat{n}_3)_{\alpha'} \text{ and } [v_1 \ v_2 \ v_3]_\gamma \parallel [\hat{v}_1 \ \hat{v}_2 \ \hat{v}_3]_{\alpha'}, \quad (6.8)$$

where the coordinates $\hat{n}_i$ and $\hat{v}_i$ are obtained by using the *orientation relationship matrix* O_i from (6.7) in (6.6).

Conversely, suppose that an OR of the form (6.8) is given with the property that the normal $(n_1 \ n_2 \ n_3)_\gamma$ and the direction $[v_1 \ v_2 \ v_3]_\gamma$ are left unrotated by the transformation. By the above process, we can compute three possible transformation strains T_i and corresponding OR matrices O_i . For each OR matrix O_i we can calculate the bcc/bct coordinates of $(n_1 \ n_2 \ n_3)_\gamma$ and $[v_1 \ v_2 \ v_3]_\gamma$. For one of the matrices O_i , the calculated coordinates must agree, up to crystallographic equivalence, with the given OR and, hence, we may uniquely identify the Bain variant U_i , and the corresponding transformation strain T_i , that gives rise to the OR. If the coordinates do not agree for any O_i , then the OR cannot be compatible with the Bain mechanism.

Generating Variants Through Crystallographic Equivalence in the γ -Phase

Given a transformation strain T (or equivalently the corresponding OR matrix O) we are able to generate further variants of T through the application of $\mathcal{P}^{24}$ in the reference configuration. To this end, we recall that, given the fcc basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, all crystallographically equivalent fcc bases are given by $\{P\mathbf{e}_1, P\mathbf{e}_2, P\mathbf{e}_3\}$ for $P \in \mathcal{P}^{24}$. Thus, letting T as in (6.4) and using the identity $P_i^T P_i = \mathbb{I}$, we infer that

$$\frac{\text{cof}(P_i T P_i^T) P_i \mathbf{n}}{|\text{cof } T \mathbf{n}|} = P_i \mathbf{n} \text{ and } \frac{(P_i T P_i^T) P_i \mathbf{v}}{|T \mathbf{v}|} = P_i \mathbf{v}.$$

That is, for each $i = 1, 2, \dots, 24$, the deformation $P_i T P_i^T$ leaves the plane with normal $P_i \mathbf{n}$ and the direction $P_i \mathbf{v}$ within that plane unrotated and thus describes a *strain variant* of the original transformation strain T . Similarly, $P_i O P_i^T$ describes the corresponding *orientation relationship variant*. We note that in general, it may happen (see e.g. the NW model) that $P_i T P_i^T = P_j T P_j^T$ for some $i \neq j$ and thus there

can be less than 24 distinct variants for a given transformation strain (or equivalently for a given OR).

6.2 The NW and KS Models

In this section, we derive the NW and KS models. Both models have the attractive feature of leaving a close-packed $\{111\}_\gamma$ plane and a close-packed $\langle\bar{1}10\rangle$ direction within that plane unrotated (see also Appendix A for a detailed illustration of the mechanism). Owing to this feature they seem to be the most natural candidates for OR models. To carry out the derivation we apply our unified approach from Section 6.1 with

$$\mathbf{n} = (111)_\gamma \text{ and } \mathbf{v} = [10\bar{1}]_\gamma.$$

The Transformation with Stretch Component U_2

Let us consider the second Bain variant U_2 . Noting that $\mathbf{v}$ is an eigenvector of U_2 , we immediately deduce that, by (6.4), $R_2\mathbf{v} = \mathbf{v}$ and thus $\mathbf{v}$ is the axis of rotation. Regarding the angle of rotation we calculate

$$\text{Tr } R_2 = \mathbf{m}_2 \cdot \mathbf{n} + \mathbf{u}_2 \cdot \mathbf{v} + (\mathbf{m}_2 \times \mathbf{u}_2) \cdot (\mathbf{n} \times \mathbf{v}) = 2\mathbf{m}_2 \cdot \mathbf{n} + 1,$$

where we used that $\mathbf{u}_2 = \mathbf{v}$ and (6.1). Hence, the angle of rotation is given by

$$\arccos\left(\frac{\text{cof } U_2 \mathbf{n} \cdot \mathbf{n}}{|\text{cof } U_2 \mathbf{n}|}\right) \text{sgn}((\mathbf{m}_2 \times \mathbf{n}) \cdot \mathbf{v}) = \arccos\left(\frac{1 + \sqrt{2}r}{\sqrt{3}\sqrt{1+r^2}}\right) =: \phi(r), \quad (6.9)$$

where $r = c/a = \sqrt{2}\beta/\alpha$ is the ratio of tetragonality of the bct cell. In particular, for $r = 1$ corresponding to a bcc product lattice we obtain $\phi(1) = \arccos\left(\frac{1+\sqrt{2}}{\sqrt{6}}\right) \approx 9.7356^\circ$.

Hence, the only transformation from fcc to bcc/bct with stretch component U_2 which leaves the plane $(1\ 1\ 1)_\gamma$ and the direction $[1\ 0\ \bar{1}]_\gamma$ unrotated is

$$T_2 = R_2 U_2 = R[\phi(r), [1\ 0\ \bar{1}]] U_2. \quad (6.10)$$

Regarding the orientation relationships corresponding to T_2 , through (6.10) and (6.7), we infer that $O_2 = R[-45^\circ, \mathbf{e}_2] R[-\phi(r), [1\ 0\ \bar{1}]]$ (cf. Figure 6.1). Consequently,

$$(1\ 1\ 1)_\gamma \parallel (0\ 1\ r)_{\alpha'} \text{ and } [1\ 0\ \bar{1}]_\gamma \parallel [1\ 0\ 0]_{\alpha'}. \quad (6.11)$$

Note that, as expected, the latter is a closest packed plane in the resulting bct lattice containing the bct direction $[1\ 0\ 0]_{\alpha'}$. Thus for $r = 1$ (bcc) the transformation T_2 gives rise to the OR NW1 (see Table 6.1) and henceforth we denote $T_2 = T_{\text{NW1}}$. The OR matrix O_{NW1} between fcc and bcc is given by

$$O_{\text{NW1}} = R[-45^\circ, \mathbf{e}_2] R[-9.7356^\circ, [1\ 0\ \bar{1}]] \approx \begin{pmatrix} 0.7071 & 0 & -0.7071 \\ 0.1196 & 0.9856 & 0.1196 \\ 0.6969 & -0.1691 & 0.6969 \end{pmatrix},$$

and the corresponding transformation T_{NW1} is given by

$$T_{\text{NW1}} = R[9.7356^\circ, [1\ 0\ \bar{1}]] U_2 \approx \begin{pmatrix} 1.1144 & 0.0949 & -0.0081 \\ -0.1342 & 0.7823 & -0.1342 \\ -0.0081 & 0.0949 & 1.1144 \end{pmatrix}.$$

Next, we characterise the remaining NW variants. Following our unified approach, they are given by $P_i T_{\text{NW1}} P_i^T$. Since $T_{\text{NW1}} = R[\phi(r), [1\ 0\ \bar{1}]] U_2$, $P_2 [1\ 0\ \bar{1}]_\gamma = [1\ 0\ \bar{1}]_\gamma$ and $P_2 U_2 P_2^T = U_2$ we deduce that $P_2 T_{\text{NW1}} P_2^T = T_{\text{NW1}}$ and similarly that $P_{2j} T_{\text{NW1}} P_{2j}^T = P_{2j-1} T_{\text{NW1}} P_{2j-1}^T$ for any $j = 2, \dots, 12$. Thus there are only 12 NW strain variants given by

$$T_{\text{NW}j} := P_{2j-1} T_{\text{NW1}} P_{2j-1}^T = R[\phi(r), P_{2j-1} [1\ 0\ \bar{1}]] P_{2j-1} U_2 P_{2j-1}^T,$$

for $j = 1, 2, \dots, 12$. In particular, $T_{\text{NW}j}$ has a stretch component $P_{2j-1}U_2P_{2j-1}^T$ followed by a rotation of $\phi(r)$ about $P_{2j-1}[1\ 0\ \bar{1}]_\gamma$. The corresponding OR matrices are obtained by the same conjugation. That is

$$O_{\text{NW}j} = P_{2j-1}O_{\text{NW}1}P_{2j-1}^T = R[-45^\circ, P_{2j-1}\mathbf{e}_2] R[-\phi(r), P_{2j-1}[1\ 0\ \bar{1}]],$$

for $j = 1, 2, \dots, 12$. Thus, by (6.11), $O_{\text{NW}j}$ maps the fcc normal $P_{2j-1}\mathbf{n}$ and fcc vector $P_{2j-1}\mathbf{v}$ to the bcc/bct normal $P_{2j-1}(0\ 1\ r)_{\alpha'}$ and the bcc/bct direction $P_{2j-1}[1\ 0\ 0]_{\alpha'}$ (see Table D1 in the Appendix). It is easy to verify that, for $r = 1$, the resulting bcc vectors are crystallographically equivalent (through P_{2j-1}^T) to the bcc vector $[1\ 0\ 0]_{\alpha'}$ and the bcc normal $(0\ 1\ 1)_{\alpha'}$, giving the NW variants as in Table 6.1. We note that the choice of sign for the 45° rotation about $\mathbf{e}_2$, as well as the enumeration of $\mathcal{P}^{24}$, has been carefully made so that the OR NW j is obtained through P_{2j-1}^T . A choice of the opposite sign and/or a different enumeration of $\mathcal{P}^{24}$, will not alter the result but will lead to bcc/bct coordinates that are crystallographically equivalent to the ones in Table 6.1 through different elements of $\mathcal{P}^{24}$.

Tab. 6.1. The NW orientation relationships. The corresponding variants in each row are given by $T_{\text{NW}j} = R[\phi(r), \mathbf{v}_j] U_j$.

O.R. ^a	fcc plane ^b	bcc plane	fcc direction ^c	bcc direction	Bain Variant ^d
NW1	$(1\ 1\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[1\ 0\ \bar{1}]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_2
NW2	$(1\ 1\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[\bar{1}\ 1\ 0]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_3
NW3	$(1\ 1\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[0\ \bar{1}\ 1]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_1
NW4	$(\bar{1}\ 1\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[1\ 0\ 1]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_2
NW5	$(\bar{1}\ 1\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[\bar{1}\ \bar{1}\ 0]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_3
NW6	$(\bar{1}\ 1\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[0\ 1\ \bar{1}]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_1
NW7	$(1\ \bar{1}\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[\bar{1}\ 0\ 1]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_2
NW8	$(1\ \bar{1}\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[1\ 1\ 0]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_3
NW9	$(1\ \bar{1}\ 1)_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[0\ \bar{1}\ \bar{1}]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_1
NW10	$(1\ 1\ \bar{1})_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[\bar{1}\ 0\ \bar{1}]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_2
NW11	$(1\ 1\ \bar{1})_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[1\ \bar{1}\ 0]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_3
NW12	$(1\ 1\ \bar{1})_\gamma$	$(0\ 1\ 1)_{\alpha'}$	$[0\ 1\ 1]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_1

^a NW j ^b $P_{2j-1}(1\ 1\ 1)_\gamma$ ^c $\mathbf{v}_j = P_{2j-1}[1\ 0\ \bar{1}]_\gamma$ ^d $U_j = P_{2j-1}U_2P_{2j-1}^T$

The Transformation with Stretch Component U_3

Similarly, using U_3 instead of U_2 in (6.4) gives rise to a rotation R_3 satisfying

$$R_3 \mathbf{m}_3 = \mathbf{n} \text{ and } R_3 \mathbf{u}_3 = \mathbf{v}. \quad (6.12)$$

Noting that $R_{NW2} \mathbf{m}_3 = \mathbf{n}$ we immediately see that $R_3 R_{NW2}^T \mathbf{n} = \mathbf{n}$ and

$$R_3 = R[\theta, \mathbf{n}] R_{NW2} = R[\theta, [1\ 1\ 1]] R[\phi(r), [\bar{1}\ 1\ 0]]$$

for some angle $\theta = \theta(r)$. Let us first determine the sign of $\theta(r)$. By (6.12), we have that $R[\theta, \mathbf{n}] R_{NW2} \mathbf{u}_3 = \mathbf{v}$ and thus $\text{sgn } \theta(r) = \text{sgn}(R_{NW2} \mathbf{u}_3 \times \mathbf{v}) \cdot \mathbf{n} = 1$. For the angle itself we deduce from (6.5) that

$$\theta(r) = \arccos \left(\frac{\text{Tr } R[\theta, \mathbf{n}] - 1}{2} \right) = \arccos \left(\frac{\sqrt{3}\sqrt{r^2 + 1} + 1}{2\sqrt{r^2 + 2}} \right). \quad (6.13)$$

For $r = 1$ (bcc) this angle is given by $\theta(1) = \arccos \left(\frac{1+\sqrt{6}}{2\sqrt{3}} \right) \approx 5.2644^\circ$. Hence, the only transformation from fcc to bcc/bct with stretch component U_3 which leaves the plane $(1\ 1\ 1)_\gamma$ and the direction $[1\ 0\ \bar{1}]_\gamma$ unrotated is

$$T_3 = R_3 U_3 = R[\theta(r), [1\ 1\ 1]] R[\phi(r), [\bar{1}\ 1\ 0]] U_3. \quad (6.14)$$

Regarding the corresponding orientation relationships, by (6.7), we deduce that

$$O_3 = R[45^\circ, \mathbf{e}_3] R[-\phi(r), [\bar{1}\ 1\ 0]] R[-\theta(r), [1\ 1\ 1]] \quad (6.15)$$

and, consequently,

$$(1\ 1\ 1)_\gamma \parallel (0\ r\ 1)_{\alpha'} \text{ and } [1\ 0\ \bar{1}]_\gamma \parallel [1\ 1\ \bar{r}]_{\alpha'}. \quad (6.16)$$

In particular, the resulting α' -normal is a closest packed plane in the bcc/bct lattice and the resulting α' -direction is a closed packed direction within that plane. Clearly,

for $r = 1$ (bcc), the transformation T_3 gives rise to the OR KS1 (see Table 6.2) and henceforth we denote $T_3 = T_{\text{KS1}}$. The OR matrix O_{KS1} between fcc and bcc is then given by

$$O_{\text{KS1}} = R[45^\circ, \mathbf{e}_3] R[-9.7356^\circ, [\bar{1} 1 0]] R[-5.2644^\circ, [1 1 1]] \\ \approx \begin{pmatrix} 0.7416 & -0.6667 & -0.0749 \\ 0.6498 & 0.7416 & -0.1667 \\ 0.1667 & 0.07492 & 0.9832 \end{pmatrix}$$

and the transformation strain by

$$T_{\text{KS1}} = R[5.2644^\circ, [1 1 1]] R[9.7356^\circ, [\bar{1} 1 0]] U_3 \approx \begin{pmatrix} 1.1044 & -0.0728 & 0.1323 \\ 0.0595 & 1.1177 & 0.0595 \\ -0.1917 & -0.0728 & 0.7803 \end{pmatrix}.$$

The remaining KS strain variants are $T_{\text{KS}j} := P_j T_{\text{KS1}} P_j^T$ and by (6.14) they are given by

$$T_{\text{KS}j} = R[\theta(r), P_j[1 1 1]] R[\phi(r), P_j[\bar{1} 1 0]] P_j U_3 P_j^T.$$

In particular, $T_{\text{KS}j}$ leaves the close packed plane $P_j \mathbf{n}$ and the close packed direction $P_j \mathbf{v}$ within that plane unrotated. The corresponding OR variants are given by $O_{\text{KS}j} = P_j O_{\text{KS1}} P_j^T$ and $O_{\text{KS}j}$ maps the fcc normal $P_j \mathbf{n}$ and fcc direction $P_j \mathbf{v}$ to the bcc/bct normal $P_j(0 \ r \ 1)_{\alpha'}$ and the bcc/bct direction $P_j[1 \ 1 \ \bar{r}]_{\alpha'}$ (see Table D2 in the Appendix).

The Transformation with Stretch Component U_1

Let us, for example, consider $P = P_2$. Then

$$P_2 \mathbf{n} = -\mathbf{n}, P_2 \mathbf{v} = \mathbf{v} \text{ and } P_2 U_3 P_2^T = U_1$$

and thus $T_{KS2} = R[-\theta(r), [1\ 1\ 1]] R[\phi(r), [\bar{1}\ 1\ 0]] U_1$ is the only transformation with stretch component U_1 that leaves the close packed plane $(1\ 1\ 1)_\gamma$ and the close packed direction $[1\ 0\ \bar{1}]_\gamma$ unrotated. It is therefore the third and last solution of (6.4).

Just like in the derivation of the NW variants, care has been taken so that all odd $KS(2j - 1)$ variants correspond immediately to the entries in Table 6.2 and the crystallographic equivalence in the bcc/bct lattice is given by P_{2j-1}^T . However, unlike the NW variants, $T_{KS2} = P_2 T_{KS1} P_2^T \neq T_{KS1}$ are distinct and thus the ORs are different. To illustrate this, let us take $O_{KS2} = P_2 O_{KS1} P_2^T$ and investigate its action on the fcc plane with normal $\mathbf{n} = (1\ 1\ 1)_\gamma$ and the fcc direction $\mathbf{v} = [1\ 0\ \bar{1}]_\gamma$. We have

$$O_{KS2}\mathbf{n} = P_2 O_{KS1}(-\mathbf{n}) = -P_2 0 r 1_{\alpha'} = 1 r 0_{\alpha'}$$

$$\text{and } O_{KS2}\mathbf{v} = P_2 O_{KS1}\mathbf{v} = P_2 [1\ 1\ \bar{r}]_{\alpha'} = [r\ \bar{1}\ \bar{1}]_{\alpha'},$$

which are the closest packed plane and close packed direction in that plane in the resulting bct lattice. If $r = 1$ (bcc), noting that $P_3(1\ r\ 0)_{\alpha'} = (0\ 1\ r)_{\alpha'}$ and $P_3[r\ \bar{1}\ \bar{1}]_{\alpha'} = [\bar{1}\ r\ \bar{1}]_{\alpha'}$ we obtain, up to crystallographic equivalence in the bcc lattice (by P_3)³, the OR associated to KS2 (cf. Table 6.2). The ORs for the remaining even $KS(2j)$ are obtained analogously and the required crystallographic equivalence transformation in the bcc lattice is given by $P_3 P_{2j}^T$. Figure 6.2 shows the relations between all Bain, NW and KS variants.

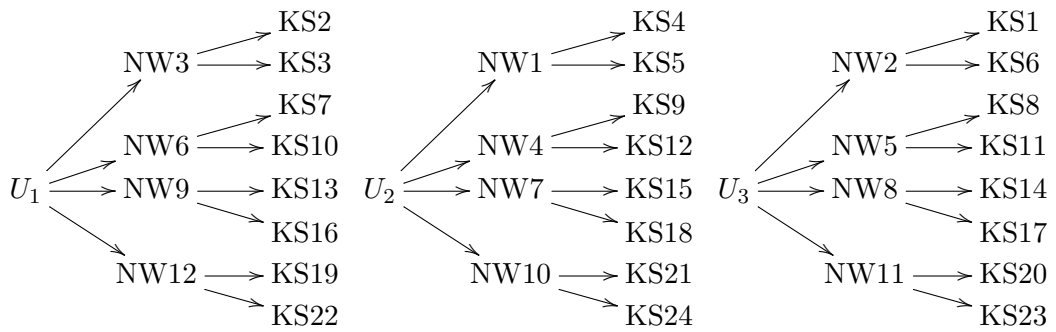


Fig. 6.2. An arrow from a Bain variant U_k to an NW variant NW_j signifies that $T_{NWj} = R[\phi(r), \mathbf{v}_j] U_k$ (cf. Table 6.1). Respectively, an arrow from an NW variant NW_j to a KS variant KS_i signifies that $T_{KS_i} = R[(-1)^{i+1}\theta(r), \mathbf{n}_i] T_{NW_j}$ (cf. Table 6.2).

³Nevertheless, P_3 is not a lattice invariant rotation for the resulting bct lattice.

Tab. 6.2. The KS orientation relationships. The corresponding variants in each row are given by $T_{KSj} = R[(-1)^{j+1}\theta(r), \mathbf{n}_j] R[\phi(r), P_j[\bar{1}10]] U_j$.

O.R. ^a	fcc plane ^b	bcc plane	fcc direction ^c	bcc direction	Bain Variant ^d
KS1	$(111)_\gamma$	$(011)_{\alpha'}$	$[10\bar{1}]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_3
KS2	$(111)_\gamma$	$(011)_{\alpha'}$	$[10\bar{1}]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_1
KS3	$(111)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}10]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_1
KS4	$(111)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}10]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_2
KS5	$(111)_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}1]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_2
KS6	$(111)_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}1]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_3
KS7	$(\bar{1}11)_\gamma$	$(011)_{\alpha'}$	$[101]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_1
KS8	$(\bar{1}11)_\gamma$	$(011)_{\alpha'}$	$[101]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_3
KS9	$(\bar{1}11)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}\bar{1}0]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_2
KS10	$(\bar{1}11)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}\bar{1}0]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_1
KS11	$(\bar{1}11)_\gamma$	$(011)_{\alpha'}$	$[01\bar{1}]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_3
KS12	$(\bar{1}11)_\gamma$	$(011)_{\alpha'}$	$[01\bar{1}]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_2
KS13	$(1\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}01]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_1
KS14	$(1\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}01]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_3
KS15	$(1\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[110]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_2
KS16	$(1\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[110]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_1
KS17	$(1\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}\bar{1}]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_3
KS18	$(1\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}\bar{1}]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_2
KS19	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[\bar{1}0\bar{1}]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_1
KS20	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[\bar{1}0\bar{1}]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_3
KS21	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[1\bar{1}0]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_2
KS22	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[1\bar{1}0]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_1
KS23	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[011]_\gamma$	$[11\bar{1}]_{\alpha'}$	U_3
KS24	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[011]_\gamma$	$[\bar{1}1\bar{1}]_{\alpha'}$	U_2

^a KSj ^b $\mathbf{n}_j = (-1)^{j+1} P_j(111)_\gamma$ ^c $P_j[10\bar{1}]_\gamma$ ^d $U_j = P_j U_3 P_j^T$

Relation to Other Descriptions

In the literature (see e.g. [Kal+76; RJ90; Bun13]) the NW ORs are sometimes described as $\zeta = \arccos\left(\frac{1}{\sqrt{6}} - \frac{1}{2}\right) \approx 95.264^\circ$ rotations about $\langle hkl \rangle$ where $(h, k, l) = (1 + \sqrt{2} + \sqrt{3}, \sqrt{2}, -1 + \sqrt{2} + \sqrt{3})$ and the KS ORs as 90° rotations about $\langle 112 \rangle$. We show that these descriptions follow, up to crystallographic equivalence, from

the above derivation. Let us start with the OR for NW1. With the choice $P_3 = R[120^\circ, [1\ 1\ 1]]$ we obtain

$$P_3 O_{\text{NW1}} = R[\zeta, [h\ k\ l]] \approx R[95.264^\circ, (0.85, 0.29, 0.44)]$$

and thus $P_{2j-1} P_3 O_{\text{NW1}} P_{2j-1}^T = P O_{\text{NW}j} = R[\zeta, P_{2j-1}[h\ k\ l]]$ for some⁴ $P \in \mathcal{P}^{24}$. That is, up to crystallographic equivalence in the bcc lattice, $O_{\text{NW}j}$ is a $\zeta \approx 95.264^\circ$ rotation about $P_{2j-1}[h\ k\ l]$ (see Table 6.3).

Tab. 6.3. The OR matrices corresponding to the NW orientation relationships. The components of $[h\ k\ l]$ are given by $(h, k, l) = (1 + \sqrt{2} + \sqrt{3}, \sqrt{2}, -1 + \sqrt{2} + \sqrt{3}) \approx (0.85, 0.29, 0.44)$.

OR	OR matrix	OR	OR matrix
NW1	$R[95.264^\circ, [h\ k\ l]]$	NW7	$R[95.264^\circ, [l\ \bar{k}\ h]]$
NW2	$R[95.264^\circ, [l\ h\ k]]$	NW8	$R[95.264^\circ, [h\ \bar{l}\ k]]$
NW3	$R[95.264^\circ, [k\ l\ h]]$	NW9	$R[95.264^\circ, [k\ \bar{h}\ l]]$
NW4	$R[95.264^\circ, [\bar{l}\ k\ h]]$	NW10	$R[95.264^\circ, [l\ k\ \bar{h}]]$
NW5	$R[95.264^\circ, [\bar{h}\ l\ k]]$	NW11	$R[95.264^\circ, [h\ l\ \bar{k}]]$
NW6	$R[95.264^\circ, [\bar{k}\ h\ l]]$	NW12	$R[95.264^\circ, [k\ h\ \bar{l}]]$

Next, let us consider the OR for KS1. With the choice $P_{10} = R[-120^\circ, [1\ \bar{1}\ 1]]$ we obtain

$$P_{10} O_{\text{KS1}} = R[90^\circ, [\bar{1}\ 2\ \bar{1}]]$$

and thus $P_j P_{10} O_{\text{KS1}} P_j^T = P O_{\text{KS}j} = R[90^\circ, P_j[\bar{1}\ 2\ \bar{1}]]$ for some⁵ $P \in \mathcal{P}^{24}$, i.e. up to crystallographic equivalence in the bcc lattice, $O_{\text{KS}j}$ is a 90° rotation about $P_j[\bar{1}\ 2\ \bar{1}]$ (see Table 6.4).

⁴ $P = P_3$ for $j \in \{1, 2, 3\}$, $P = P_{18}$ for $j \in \{4, 5, 6\}$, $P = P_{24}$ for $j \in \{7, 8, 9\}$ and $P = P_{12}$ for $j \in \{10, 11, 12\}$.

⁵ $P = P_j P_{10} P_j^T$.

Tab. 6.4. The OR matrices corresponding to the KS orientation relationships.

OR	OR matrix	OR	OR matrix
KS1	$R[+90^\circ, [\bar{1} \ 2 \ \bar{1}]]$	KS13	$R[+90^\circ, [\bar{1} \ \bar{2} \ \bar{1}]]$
KS2	$R[-90^\circ, [\bar{1} \ 2 \ \bar{1}]]$	KS14	$R[-90^\circ, [\bar{1} \ \bar{2} \ \bar{1}]]$
KS3	$R[+90^\circ, [\bar{1} \ \bar{1} \ 2]]$	KS15	$R[+90^\circ, [\bar{1} \ 1 \ 2]]$
KS4	$R[-90^\circ, [\bar{1} \ \bar{1} \ 2]]$	KS16	$R[-90^\circ, [\bar{1} \ 1 \ 2]]$
KS5	$R[+90^\circ, [2 \ \bar{1} \ \bar{1}]]$	KS17	$R[+90^\circ, [2 \ 1 \ \bar{1}]]$
KS6	$R[-90^\circ, [2 \ \bar{1} \ \bar{1}]]$	KS18	$R[-90^\circ, [2 \ 1 \ \bar{1}]]$
KS7	$R[+90^\circ, [1 \ 2 \ \bar{1}]]$	KS19	$R[+90^\circ, [\bar{1} \ 2 \ 1]]$
KS8	$R[-90^\circ, [1 \ 2 \ \bar{1}]]$	KS20	$R[-90^\circ, [\bar{1} \ 2 \ 1]]$
KS9	$R[+90^\circ, [1 \ \bar{1} \ 2]]$	KS21	$R[+90^\circ, [\bar{1} \ \bar{1} \ \bar{2}]]$
KS10	$R[-90^\circ, [1 \ \bar{1} \ 2]]$	KS22	$R[-90^\circ, [\bar{1} \ \bar{1} \ \bar{2}]]$
KS11	$R[+90^\circ, [2 \ \bar{1} \ \bar{1}]]$	KS23	$R[+90^\circ, [2 \ \bar{1} \ 1]]$
KS12	$R[-90^\circ, [2 \ \bar{1} \ \bar{1}]]$	KS24	$R[-90^\circ, [2 \ \bar{1} \ 1]]$

Twin Relationships Between KS Variants

With the knowledge of the transformation strains we are able to unambiguously identify pairs of KS variants KS_k and KS_l that are twin related, i.e. variant pairs whose relative deformation is an invariant plane strain. That is

$$T_{KS_k} = T_{KS_l}(\mathbb{I} + \mathbf{b} \otimes \mathbf{m}),$$

where $\mathbf{b} \otimes \mathbf{m}$ is the 3×3 matrix with components $(\mathbf{b} \otimes \mathbf{m})_{ij} = b_i m_j$. In particular, this implies that a fully coherent interface of normal $\mathbf{m}$ can be formed between the two variants. We show that this can only happen between the pairs $KS(2j-1)$ and $KS(2j)$ and whenever this is the case the lattices on either side of the interface are related by a 180° rotation about the common invariant fcc direction $P_{2j-1}[1 \ 0 \ \bar{1}] = \mathbf{v}_j$ (cf. Table 6.1). We start with KS1 and assume that

$$M_i := T_{KS_i} - T_{KS1} = P_i T_{KS1} P_i^T - T_{KS1} = \mathbf{b} \otimes \mathbf{m}. \quad (6.17)$$

Whenever P_i does not leave $\mathbf{v}_1$ invariant we have $(T_{KS_i} - T_{KS1})\mathbf{v}_1 \neq 0$ and $(T_{KS_i} - T_{KS1})P_i\mathbf{v}_1 \neq 0$ and thus $\mathbf{m} \parallel \mathbf{v}_1 \times P_i\mathbf{v}_1$. Similarly, whenever P_i does not leave

$\mathbf{n}_1 = (111)_\gamma$ invariant, i.e. $i \geq 7$, we have⁶ $M_i^T \mathbf{n}_1 \neq 0$ and $M_i^T \mathbf{n}_i \neq 0$ and thus $\mathbf{b} \parallel \mathbf{n}_1 \times \mathbf{n}_i$, where $\mathbf{n}_i := P_i \mathbf{n}_1$. Hence for $i \geq 7$ it holds that

$$M_i^T \mathbf{n}_i \propto \mathbf{m} \otimes (\mathbf{n}_1 \times \mathbf{n}_i) \mathbf{n}_i = \langle \mathbf{n}_1 \times \mathbf{n}_i, \mathbf{n}_i \rangle \mathbf{m} = 0$$

and thus, since $\mathbf{n}_i$ is an eigenvector of $T_{KS_i}^T$, it must also be an eigenvector of T_{KS1}^T . However, we know that this can only be the case for $i \leq 6$ (cf. Table 6.2), a contradiction. For the remaining cases, i.e. $2 \leq i \leq 6$, we have

$$M_i P_i \mathbf{v}_1 \propto \langle \mathbf{v}_1 \times P_i \mathbf{v}_1, P_i \mathbf{v}_1 \rangle \mathbf{b} = 0$$

and thus since $P_i \mathbf{v}_1$ is an eigenvector of T_{KS_i} it must also be an eigenvector of T_{KS1} which is again, unless $i = 2$, a contradiction. Finally,

$$T_{KS2} - T_{KS1} = P_2 T_{KS1} P_2^T - T_{KS1} = \frac{2^{1/6}}{\sqrt{3}} \mathbf{v}_1 \otimes [101],$$

where P_2 is a 180° rotation about the common fcc direction $\mathbf{v}_1$. Through conjugation with P_{2j-1} we obtain that the relative deformations between T_{KS2j-1} and $T_{KS2j} = P_{2j-1} T_{KS2} P_{2j-1}^T$ are also invariant plane strains.

The Influence of Tetragonality on the Orientation Relationships

For many compositions of steel the α' -phase is not cubic ($r = 1$) but slightly tetragonal ($r > 1$). For instance, the addition of carbon leads to a ratio of tetragonality approximately given by

$$r = \frac{c}{a} = 1 + 0.045 \text{ wt-\%C}, \quad (6.18)$$

⁶For an invertible matrix A , v is an eigenvector of $\text{cof } A$ iff it is an eigenvector of A^T .

for C in the range 0.4–2 wt-%C (see [Rob53; WC62]).⁷ Similarly, the addition of nitrogen instead of carbon leads to a tetragonality ratio of

$$r = \frac{c}{a} = 0.995 + 0.0383 \text{ wt-\%N}$$

for N in the range 0.6–2.9 wt-%N (after [Nis78, Fig. 2.2]). For small carbon content and certain Fe-Ni alloys, such as the Fe-30% Ni alloy investigated in [Nis34] and [Was35], the α' -phase is likely to be cubic, however, alloying additional elements such as Cr, Mn or Ti leads again to a tetragonal α' -phase.

Our derivation in Section 6.2 takes the tetragonality of the α' -phase into account and the transformation strains, as well as the ORs, are derived for any ratio of tetragonality $1 \leq r < \sqrt{2}$.⁸ In particular, the angles of rotations $\phi(r)$ and $\theta(r)$ in (6.9) and (6.13) respectively decrease with increasing tetragonality and thus our theory predicts a narrower distribution of peaks in the pole figures. This prediction agrees very well with [RJ90] which summarises that “*investigators have shown that the chemical composition of steel has a significant effect on the nature and sharpness of the final transformation texture*” and that increasing alloy content (i.e. higher tetragonality) leads to sharper textures (see e.g. [RJ90, Fig. 11-16]). Figure 6.3 depicts the changes in the NW and KS ORs for different ratios of tetragonality obtained through (6.18) for a carbon content increasing from 0% to 2%.

6.3 Other Orientation Relationship Models

In this section, we briefly comment on how our approach can be used to derive the Pitsch (see [Pit59]), Greninger-Troiano (GT) (see [GT49]) and inverse Greninger-Troiano GT'(see [He+06]) OR models.

⁷Related experiments on Fe-7% Al-C in [WW71b] showed that the tetragonality does not increase for carbon above 2%.

⁸Note that $r = \sqrt{2}$ corresponds to an fcc lattice and thus there is no phase transformation.

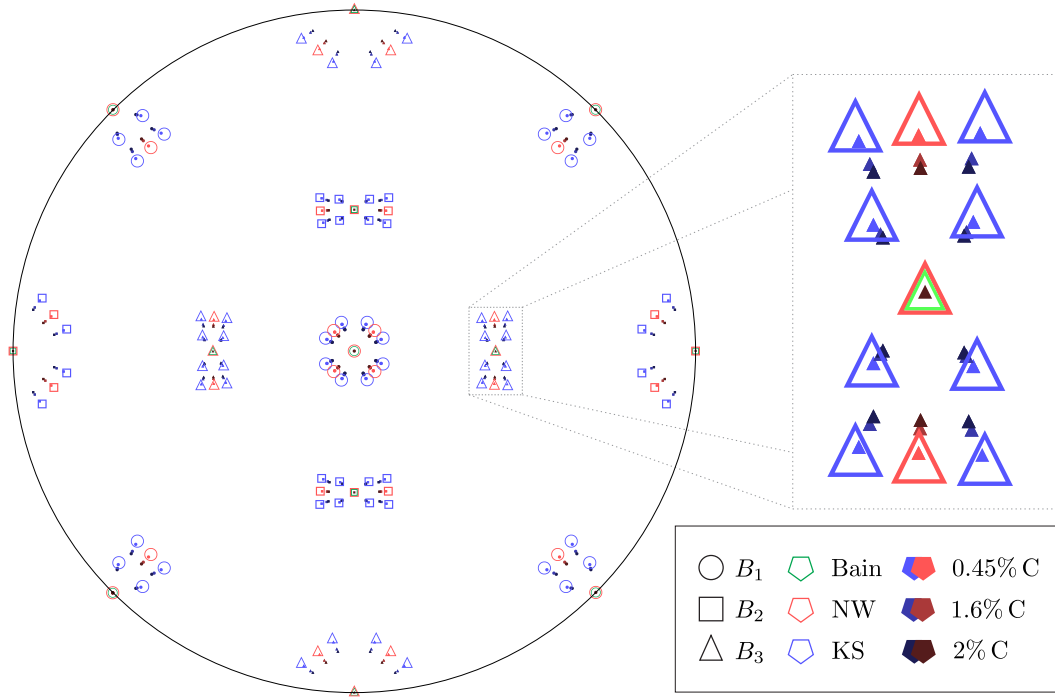


Fig. 6.3. $\{100\}$ pole figures showing the change in the ORs with increasing carbon content. Hollow circles, squares and triangles correspond respectively to the fcc-to-bcc transformations with stretch components U_1 , U_2 and U_3 . The colours blue, red and green correspond respectively to KS, NW and Bain. The solid shapes correspond to increasing carbon content from lighter to darker shading and with values 0.45, 1.6 and 2 wt-%C respectively.

The Pitsch Model

Following [Pit59] the Pitsch ORs (P) are given as

$$(110)_\gamma \parallel (\bar{1}\bar{1}\bar{2})_{\alpha'} \text{ and } [001]_\gamma \parallel [1\bar{1}0]_{\alpha'}.^9 \quad (6.19)$$

Using our unified approach from Section 6.1 with $\mathbf{n} = (110)$ and $\mathbf{v} = [1\bar{1}0]$ we obtain $T_{P1} = R[-\psi(r), [001]]U_2$ and $O_{P1} = R[-45^\circ, \mathbf{e}_2]R[\psi(r), [001]]$, where $\psi(r) = \arccos\left(\frac{\sqrt{2}+r}{\sqrt{2}\sqrt{2+r^2}}\right)$. The remaining eleven Pitsch OR and strain variants are given through conjugation with $\mathcal{P}^{24}$. We note that for $r = 1$, $\psi(1) = \phi(1)$, where $\phi(r)$ is given by (6.9) in the derivation of the NW variants, and that $O_{P1} = O_{NW7}^T$ (similarly $O_{Pj} = O_{NW_i}^T$ for some i). If instead of (6.19) one uses the parallelisms $(010)_\gamma \parallel (101)_{\alpha'}$ and $[101]_\gamma \parallel [\bar{1}\bar{1}1]_{\alpha'}$ (as e.g. in [He+06; Nol04]) the resulting

⁹In [Pit59] a third parallelism $[1\bar{1}0]_\gamma \parallel [\bar{1}\bar{1}1]_{\alpha'}$ is provided, which is not required for our derivation but, nevertheless, follows from it.

strains and ORs are the same. Finally, we remark that occasionally [Pit62] is also cited for the Pitsch ORs. However, the measurements in [Pit62] are for cementite which has an orthorhombic crystal structure and thus our unified approach from Section 6.1 does not apply directly. Nevertheless, the underlying mechanism remains applicable if in (6.4) one replaces the Bain strain by the respective strain required to transform austenite to cementite.

The Greninger-Troiano and Inverse

Greninger-Troiano Models

In [GT49], Greninger-Troiano (GT) studied a Fe-20%Ni-0.8%C crystal with $r = c/a = 1.045$ and observed the following approximate parallelisms

$$(111)_\gamma : (101)_{\alpha'} \approx 1^\circ, (112)_\gamma : [10\bar{1}]_{\alpha'} \approx 2^\circ \text{ and } (110)_\gamma : [11\bar{1}]_{\alpha'} \approx 2.5^\circ.$$

Apart from these original ORs (up to crystallographic equivalence), several authors use slightly different approximate parallelisms as defining features of the Greninger-Troiano (GT) orientation relationships. For instance, [BH11; Tsa+02] report $\{111\}_\gamma : \{011\}_{\alpha'} \approx 0.2^\circ$ and $(10\bar{1})_\gamma : (11\bar{1})_{\alpha'} \approx 2.7^\circ$ and [He+06] uses the parallelisms

$$\{111\}_\gamma \parallel \{011\}_{\alpha'} \text{ and } \langle 51217 \rangle_\gamma \parallel \langle 71717 \rangle_{\alpha'} \quad (6.20)$$

to approximate the GT ORs. Using the parallelism condition (6.20) our unified approach can capture the slight misorientations as an effect of the increased tetragonality of the bct lattice. With $\mathbf{n} = (111)_\gamma$ and $\mathbf{v} = [\bar{5}17\bar{1}2]_\gamma$ we obtain $T_{GT1} = R[\xi(r), [111]]R[\phi(r), [\bar{1}10]]U_3$ and

$$O_{GT1} = R[45^\circ, \mathbf{e}_3]R[-\phi(r), [\bar{1}10]]R[-\xi(r), [111]]$$

with $\xi(r) = \arccos\left(\frac{7^2+17^2\sqrt{3}\sqrt{1+r^2}}{\sqrt{2}\sqrt{5^2+12^2+17^2}\sqrt{7^2+17^2+17^2r^2}}\right)$. In particular, we have $(111)_\gamma \parallel (0r1)_{\alpha'}$ and $[\bar{1}2\bar{5}17]_\gamma \parallel [\bar{7}\bar{1}717r]_{\alpha'}$ and thus for the value $r = 1.045$ studied in

[GT49] we obtain $(111)_\gamma \parallel (01.0451)_{\alpha'} : (011)_{\alpha'} \approx 1.26^\circ$, $[11\bar{2}]_\gamma : [01\bar{1}]_{\alpha'} \approx 2.8^\circ$ and $[10\bar{1}]_\gamma : [11\bar{1}]_{\alpha'} \approx 2.9^\circ$.

The inverse GT, introduced in [He+06], satisfy the conditions $(\bar{1}\bar{7}\bar{7}17)_\gamma \parallel (\bar{5}\bar{1}\bar{2}17)_{\alpha'}$ and $[101]_\gamma \parallel [111]_{\alpha'}$ and as before our unified approach can be used to derive the corresponding strains and ORs. For further details on the P, GT GT' and also on the NW and KS ORs we refer to Appendix D.

Energy Based Models for Steels and Their Relationship to Phenomenological Theories

Henceforth, due to the results from Chapter 6, we do not need to distinguish strictly between orientation relationships and transformation strains. In particular, the established one-to-one correspondence will simplify our comparison between mathematical models based on energy minimisation and existing phenomenological theories. Before starting this comparison we will give a brief overview of steels or rather of ferrous martensites. We follow [MW92] and classify ferrous martensites according to the observed habit plane normals. Table 7.1 (p. 148 overleaf) gives an overview over the features of steels that undergo a pure γ -to- α transformations. The transformation from the γ -phase to a mixture of the body-centred α' and the hexagonal ϵ -phase lies outside the scope of both theories and will thus be omitted.

Tab. 7.1. Overview over three common types of ferrous martensites.

Habit plane	$(3\ 10\ 15)_\gamma / (2\ 5\ 9)_\gamma$	$(2\ 2\ 5)_\gamma / (4\ 4\ 9)_\gamma$	$(5\ 5\ 7)_\gamma / (1\ 1\ 1)_\gamma$
found in e.g.	highly tetragonal steels [EW67, Fe-24.5Pt(at %)] [DB69, Fe-22Ni-.8C] ^a [WW71b, Fe-7Al-2C] ^{a,b}	[DB69, Fe-6Mn-.95C] ^a [BM64, Fe-(1.13-1.19)C] ^a	low carbon steels [Mor+03, Fe-(.0026-.61)C] ^a [SW83, Fe-(.2-.4)C] ^a
substructure	plate-like with twins along $(1\ 1\ 0)_\gamma$	plate-like complex substructure w/o satisfactory characterisation	lath often no retained austenite high-dislocation density (but cf. Ch. 7.3)
ORS	close to GT	$(1\ \bar{1}\ 0)_\gamma : (1\ 0\ 1)_\alpha \approx .3 - .5^\circ$ $[\bar{1}\ 1\ 0]_\gamma : [\bar{1}\ \bar{1}\ 1]_\alpha \approx .3 - .7^\circ$ for [DB72, Fe-6Mn-.95C]	various reported; complete transformation often inhibits observation
common theories	Single shear theories with very good agreement	various proposed theories w/o satisfactory agreement	double or even triple shear theories good agreement but heavy parameter fitting

^a all values in wt-% unless specified otherwise; $(x-y)$ symbolises that the study including several alloys with wt-% ranging from x to y

^b [MW92] also lists Fe-(29-35%)Ni and [Was35; Nis34; GT49; PW66] as references. However, even though the former three investigate Fe-Ni alloys, no habit plane normals were determined. The latter paper mainly concerns twinning of martensite and it is found that twinning is heavier for higher Nickel content. The habit plane normals are not measured but rather mentioned as being “the only habit plane variants theoretically consistent with the results”. We also note that [Bha03, Table 7.1] claims to have taken experimental data for habit plane normals from [GT49] even though they are not provided in the (available) original paper.

Review of Phenomenological Theories

The crystallographic theory of martensite was first proposed by Wechsler, Lieberman & Read (WLR) [Wec+53] and has proven very successful in explaining features of various martensitic transformations. However, when applied to steels it was only successful in a few well-behaved cases, such as the $(3\ 10\ 15)_\gamma$ (cf. Section 7.1) transformation, and failed to give adequate predictions for e.g. the $(2\ 2\ 5)_\gamma$ (cf. Section 7.2) or the $(5\ 5\ 7)_\gamma$ (cf. Section 7.3) transformations. This inadequateness gave rise to various extensions of the original theory. However, none of these extensions achieved equally convincing results. A good overview over the original theory and its various extensions can e.g. be found in [DW71].

The fundamental idea of the crystallographic theory is, just like in the Ball-James model, that a pure (martensitic) Bain variant U_i cannot be compatible with the austenite (cf. Chapter 2). Or equivalently, in the language of metallurgy, any rotation $R \in \text{SO}(3)$ of a Bain variant U_i cannot give rise to an invariant plane strain, i.e. $RU_i \neq \mathbb{I} + \mathbf{a} \otimes \mathbf{n}$ for any $\mathbf{a}, \mathbf{n} \in \mathbb{R}^3$ (cf. Proposition 2.1). However, an additional lattice invariant shear S of the martensitic variant can achieve

$$\mathbb{I} + \mathbf{a} \otimes \mathbf{n} = RUS. \quad (7.1)$$

In [Wec+53] the lattice invariant shear S arises (macroscopically) from fine twinning of two martensitic variants. The theory developed by Bowles and MacKenzie [BM54] is, even though written differently, equivalent to (7.1). Instead of looking for an invariant plane strain, they multiply (7.1) with the inverse of the shear to get an invariant line strain (i.e. a matrix that differs from $\mathbb{I}$ by a rank-2 matrix) which can be represented by $RU = (\mathbb{I} + \mathbf{a}_1 \otimes \mathbf{n}_1)(\mathbb{I} + \mathbf{a}_2 \otimes \mathbf{n}_2)$. Another equivalent treatment was developed in [BC56], where dislocation theory was used to justify the choice of the simple shear.

In an attempt to account for a wider range of habit plane normals, [RC70; AB69] developed so-called double shear theories. In their theories, the single shear matrix S in (7.1) is replaced by the product of two shear matrices $S_1 S_2$. The most important application of their theories is the explanation of the $(\bar{5} \ 5 \ 7)$ habit planes observed in lath martensite (see e.g. [Kel92; Qi+14]). A shortcoming of these theories is that, due to the large number of degrees of freedom to choose two shears, large trial and error computations are necessary to obtain the desired results. The need for such extensive calculations indicates that the underlying principles are not understood well enough. We address and propose a solution to this issue in Section 7.3.

Translating Between Shear Theories and Models Based on Energy Minimisation

Even though in the WLR model the overall deformation is represented as a shear followed by the Bain strain and an overall rotation (cf. (7.1)), the shear was not chosen arbitrarily but rather as the one arising from simple twinning. More generally, on a macroscopic level, a twin is always equivalent to a simple shear, whereas the reverse does not hold. Similarly, one may ask in the set-up of double shear theories, whether the shears can arise from a double twin, i.e. an element in $K^{(2)}$ (cf. Definition 2.7).

Before we start a detailed comparison between the shear theories and (extensions of) the Ball-James model, it is convenient to clear up some differences in notation. Table 7.2 lists terms in material science/metallurgy and their counterparts in the language of mathematics.

Tab. 7.2. Comparison between terminology in metallurgy/materials science and mathematics.

Metallurgy	Mathematics (in formulas)
invariant plane strain	rank-one connected to $\mathbb{I}$ ($\text{rank } F - \mathbb{I} = 1$)
principal stretches/elongations	singular values ($\nu_i(F) = \sqrt{\lambda_i(F^T F)}$)
twins in martensite	1 st order laminate (macroscopically $K^{(1)}$)
twins within twins in martensite	2 nd order laminate (macroscopically $K^{(2)}$)

Macroscopic Equivalence of Twins and Shears

Given a fine twin of two martensitic variants according to Mallard's law (Lemma 2.4)

$F = (1 - \lambda)U_1 + \lambda RU_2 = U_1 + \lambda \mathbf{a} \otimes \mathbf{n}$ we can factor out U_1 to obtain

$$F = U_1(\mathbb{I} + U_1^{-1} \mathbf{a} \otimes \mathbf{n}) =: U_1 S,$$

where, since $U_1^{-1} \mathbf{a} \perp \mathbf{n}$ the deformation S is indeed a simple shear. The following lemma establishes the corresponding result for double twins.

Lemma 7.1. *(Macroscopic equivalence of twins within twins and double shears)*

Let F arise from a double twin (cf. Lemma 3.10), i.e.

$$F = R(U_1 + \lambda_1 \mathbf{a}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{a}_2 \otimes \mathbf{n}_2).$$

Then, in the notation of [RC70], this relation can be expressed as a double shear of the form

$$F = RPS_2S_1$$

where $P = U_1$, $S_1 = \mathbb{I} + \lambda_1 U_1^{-1} \mathbf{a}_1 \otimes \mathbf{n}_1$ and $S_2 = \mathbb{I} + \lambda_2 U_1^{-1} \mathbf{a}_2 \otimes S_1^{-T} \mathbf{n}_2$. Further, using the representation $S_i = \mathbb{I} + g_i \mathbf{l}_i \otimes \mathbf{m}_i$, $i = 1, 2$ of a shear as in [RC70] we can relate the individual components by $g_1 = \lambda_1 |U_1^{-1} \mathbf{a}_1|$, $\mathbf{l}_1 = N(U_1^{-1} \mathbf{a}_1)$, $\mathbf{m}_1 = \mathbf{n}_1$ and $g_2 = \lambda_2 |U_1^{-1} \mathbf{a}_2| |S_1^{-T} \mathbf{n}_2|$, $\mathbf{l}_2 = N(U_1^{-1} \mathbf{a}_2)$, $\mathbf{m}_2 = N(S_1^{-T} \mathbf{n}_2)$, where $N(\mathbf{v}) := \mathbf{v} / |\mathbf{v}|$ is the projection on the unit sphere.

Proof. By straightforward verification. □

Austenite-Martensite Habit Planes

Another central question in both the phenomenological and the mathematical theories is the determination of the habit plane between austenite and the sheared/twinned martensite. In formulas this amounts to finding a rotation R such that

$$RF = \mathbb{I} + \mu \mathbf{d} \otimes \boldsymbol{\nu}, \quad (7.2)$$

where, in the notation of [RC70], μ is the shearing magnitude, $\mathbf{d} \in \mathbb{R}^3$ is the shearing direction and $\boldsymbol{\nu} \in \mathbb{S}^2$ is the shearing/habit plane normal. In both theories it is understood that a necessary condition for F to form a stress free interface with the austenite, i.e. F can be represented in the form (7.2), is that one of its singular values is equal to 1¹. In the Ball-James model, the information of the precise form of the rank-one connection and the rotation needed is elegantly given through Proposition 2.1. In the metallurgy literature, even in recent papers (e.g. [Mor+03; Qi+14]), an elaborate procedure (which requires additional, unnecessary assumptions) going back to [RC70] is employed to reach the same results. Below, we first review this procedure and then show its equivalence to Proposition 2.1 (after dropping the unnecessary additional assumptions).

Starting from the overall deformation F determine $\boldsymbol{\nu}$ first. To this end consider a unit vector $\mathbf{u}$ and its image $\mathbf{v} = S_2 S_1 \mathbf{u}$ under the shears. Then require that $|\mathbf{u}| = |\mathbf{v}|$, $|P\mathbf{v}| = |\mathbf{v}|$ and that $|\mathbf{v}| = 1$.² Next, solve numerically the resulting quartic equation for $|\mathbf{v}|$ and obtain four solutions. Then calculate the four corresponding solutions $\mathbf{u}$ through $\mathbf{u} = S_1^{-1} S_2^{-1} \mathbf{v}$. Taking all possible six choices of pairs $\mathbf{v}_1, \mathbf{v}_2$ arising from the four solutions, single

¹Additionally, in the mathematical model it is known that this condition is sufficient if it is the middle eigenvalue.

²Recall that, in the notation of [RC70], P denotes the Bain strain U_1 .

out the correct two pairs by requiring that $\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = \langle P\mathbf{v}_1, P\mathbf{v}_2 \rangle$. Finally, arrive at $\boldsymbol{\nu} = \frac{\mathbf{u}_1 \times \mathbf{u}_2}{|\mathbf{u}_1 \times \mathbf{u}_2|}$. With the knowledge of $\boldsymbol{\nu}$ solve

$$F^T F = \mathbb{I} + \mu(\mathbf{d} \otimes \boldsymbol{\nu} + \boldsymbol{\nu} \otimes \mathbf{d}) + \mu^2 \boldsymbol{\nu} \otimes \boldsymbol{\nu} \quad (7.3)$$

for $\mathbf{d}$, where $\mu = \sqrt{\text{Tr } F^T F - 2 \det F - 1}$. Ross, 1970

To simplify our forthcoming comparison of the results, we use a shortened version of this derivation that includes all necessary steps: find two linear independent vectors $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^3$ such that

$$\langle F\mathbf{u}_i, F\mathbf{u}_j \rangle = \langle \mathbf{u}_i, \mathbf{u}_j \rangle \quad (7.4)$$

for all $i, j = 1, 2$. Then $\boldsymbol{\nu} = \frac{\mathbf{u}_1 \times \mathbf{u}_2}{|\mathbf{u}_1 \times \mathbf{u}_2|}$ and thus one is able to solve (7.3) as above.

Lemma 7.2. *(Equivalence of the results for habit planes)*

Let $\nu_2(F) = 1$ and let $\mu_i, \boldsymbol{\nu}_i, \mathbf{d}_i, \mathbf{u}_i, i = 1, 2$ be given by the above algorithm. Then the result of the algorithm coincides with the result obtained from Proposition 2.1 applied to F with, in the notation of Proposition 2.1, $\mathbf{b}_i = \mu_i \mathbf{d}_i$ and $\mathbf{m}_i = \boldsymbol{\nu}_i, i = 1, 2$. In particular, the algorithm gives the correct solution.

Proof. Consider the singular value decomposition of F given by $F = QDP$, where $P, Q \in \text{SO}(3)$ and $D = \text{diag}(\nu_1, \nu_2 = 1, \nu_3)$. Now consider the symmetric matrix $P^T D P$ which has an orthonormal eigenbasis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. Let $\mathbf{u}_i = (u_i^1, u_i^2, u_i^3)$ be the representation of $\mathbf{u}_i$ in this basis. Then using $i = j$ in (7.4) we obtain

$$|F\mathbf{u}_i|^2 = |\mathbf{u}_i|^2 \Leftrightarrow (\nu_1^2 - 1)(u_i^1)^2 - (\nu_3^2 - 1)(u_i^3)^2 = 0$$

and thus $u_i^3 = \kappa_i \sqrt{\frac{1-\nu_1^2}{\nu_3^2-1}} u_i^1, \kappa_i \in \{\pm 1\}$. The condition on the angles ($i \neq j$) becomes

$$\begin{aligned} \langle F\mathbf{u}_1, F\mathbf{u}_2 \rangle &= \langle \mathbf{u}_1, \mathbf{u}_2 \rangle \Leftrightarrow (\nu_1^2 - 1)u_1^1 u_2^1 + (\nu_3^2 - 1)u_1^3 u_2^3 = 0 \\ &\Leftrightarrow (\nu_1^2 - 1)u_1^1 u_2^1 + \kappa_1 \kappa_2 \frac{1 - \nu_1^2}{\nu_3^2 - 1} (\nu_3^2 - 1)u_1^1 u_2^1 = 0 \\ &\Leftrightarrow \kappa_1 \kappa_2 = 1. \end{aligned}$$

and thus $\kappa_1 = \kappa_2$ and we may drop the index on κ . We also note that the two choices of κ lead to two different pairs of vectors $\mathbf{u}_1, \mathbf{u}_2$, just as in the long derivation of [RC70]. Now calculate

$$\mathbf{u}_1 \times \mathbf{u}_2 = (u_1^2 u_2^3 - u_1^3 u_2^2, u_1^3 u_2^1 - u_1^1 u_2^3, u_1^1 u_2^2 - u_1^2 u_2^1)$$

and note that $u_1^3 u_2^1 = \kappa \sqrt{\frac{1-\nu_1^2}{\nu_3^2-1}} u_1^1 u_2^1 = u_1^1 \kappa \sqrt{\frac{1-\nu_1^2}{\nu_3^2-1}} u_2^1 = u_1^1 u_2^3$. Thus $(\mathbf{u}_1 \times \mathbf{u}_2)^2 \equiv (\mathbf{u}_1 \times \mathbf{u}_2) \cdot \mathbf{e}_2 = 0$. For the first component we compute

$$u_1^2 u_2^3 - u_1^3 u_2^2 = \kappa \sqrt{\frac{1-\nu_1^2}{\nu_3^2-1}} (u_1^2 u_2^1 - u_1^1 u_2^2) = -\kappa \sqrt{\frac{1-\nu_1^2}{\nu_3^2-1}} (\mathbf{u}_1 \times \mathbf{u}_2)^3$$

and thus, up to normalisation,

$$\boldsymbol{\nu} \propto \mathbf{u}_1 \times \mathbf{u}_2 \propto -\kappa \sqrt{1-\nu_1^2} \mathbf{e}_1 + \sqrt{\nu_3^2-1} \mathbf{e}_3, \quad \kappa \in \{\pm 1\}$$

as claimed in Proposition 2.1. The calculation for $\mathbf{b}_i = \mu_i \mathbf{d}_i$ is similar. $\square$

Twinning in Terms of Rotations vs. Rank-One Connections

Another difference in terminology concerns the notion of twinning. As outlined in ‘Twin Relationships Between KS Variants’ in Chapter 6, from the point of view of orientation relationships, which is more common in materials science, twins are described as two phases being related by a 180° degree rotation. On the contrary, in the mathematical literature a twin is characterised by a rank-one connection between two phases. We show that, whenever the twin relationship can be obtained by Mallard’s law (Lemma 2.4), these interpretations coincide.

Lemma 7.3. *Let U' and U be two (not necessarily symmetric) matrices related by a 180° degree rotation $P = -\mathbb{I} + 2\mathbf{e} \otimes \mathbf{e}$ about $\mathbf{e}$, i.e. $U' = PUP$. Let $R_i, i = 1, 2$ be*

the rotation that allows the rank-one connection between the two wells according to Mallard's law, i.e.

$$R_i U' = U + \mathbf{a}_i \otimes \mathbf{n}_i, \quad i = 1, 2$$

where $(\mathbf{a}_i, \mathbf{n}_i), i = 1, 2$ is the i -th solution of Mallard's law. Let further $\{\mathbf{e}_j^A\}_{j=1}^3$ be the lattice vectors in the reference configuration (austenite), and $\{\mathbf{f}_j\}_j = \{R_i U' \mathbf{e}_j^A\}_j$ and $\{\mathbf{g}_j\}_j = \{U \mathbf{e}_j^A\}_j$ be the lattice vectors of the deformed configuration on either side of the interface. Then, up to $\mu \in \text{SL}(3, \mathbb{Z})$, for $j = 1, 2, 3$ we have

$$\mathbf{f}_j = \mu S_i \mathbf{g}_j,$$

where $S_i = R_i P$ is a 180° degree rotation about the twin plane $\mathbf{K}_1 = \frac{U^{-T} \mathbf{n}_1}{|U^{-T} \mathbf{n}_1|}$ for $i = 1$ and a 180° degree rotation about the shearing direction $\boldsymbol{\eta}_1 = \frac{\mathbf{a}_2}{|\mathbf{a}_2|}$ for $i = 2$.

Proof. For ease of notation we will drop the index i indicating whether we have used the first or second solution of Mallard's law (Lemma 2.4). By definition of the lattice vectors we have for $j = 1, 2, 3$

$$\mathbf{f}_j = R U' \mathbf{e}_j^A = R P U P \mathbf{e}_j^A = \sum_{k=1}^3 R P U \mu_j^k \mathbf{e}_k^A = \sum_k \mu_j^k R P U \mathbf{e}_k^A = \sum_k \mu_j^k S \mathbf{g}_k,$$

where $S = R P$ and we have used that $P \in \mathcal{P}^{24} \subset \text{SL}(3, \mathbb{Z})$ generates an equivalent lattice. Recall that $R U' = R P U P = U + \mathbf{a} \otimes \mathbf{n}$ and thus $R P = U P U^{-1} + \mathbf{a} \otimes U^{-T} P \mathbf{n}$. Therefore, using the definition of P , we obtain

$$S = R P = -\mathbb{I} + 2U \mathbf{e} \otimes U^{-T} \mathbf{e} - \mathbf{a} \otimes U^{-T} \mathbf{n} + 2\langle \mathbf{e}, \mathbf{n} \rangle \mathbf{a} \otimes U^{-T} \mathbf{n}.$$

Using the first solution we thus arrive at

$$\begin{aligned} S_1 = R_1 P &= -\mathbb{I} + 2U \mathbf{e} \otimes U^{-T} \mathbf{e} + \mathbf{a}_1 \otimes U^{-T} \mathbf{e} \\ &= -\mathbb{I} + 2U \mathbf{e} \otimes U^{-T} \mathbf{e} + 2 \frac{U^{-T} \mathbf{e}}{|U^{-T} \mathbf{e}|^2} \otimes U^{-T} \mathbf{e} - 2U \mathbf{e} \otimes U^{-T} \mathbf{e} \\ &= -\mathbb{I} + 2\mathbf{K}_1 \otimes \mathbf{K}_1 \end{aligned}$$

and using the second solution we obtain

$$\begin{aligned}
S_2 = R_2 P &= -\mathbb{I} + 2U\mathbf{e} \otimes U^{-T}\mathbf{e} + \mathbf{a}_2 \otimes U^{-T}P\mathbf{n}_2 \\
&= -\mathbb{I} + 2U\mathbf{e} \otimes U^{-T}\mathbf{e} + 2U\mathbf{e} \otimes U^{-T}P\mathbf{e} - 2U\mathbf{e} \otimes U^{-T}P \frac{U^2\mathbf{e}}{|U\mathbf{e}|^2} \\
&\stackrel{P\mathbf{e}=\mathbf{e}}{=} -\mathbb{I} + 4U\mathbf{e} \otimes U^{-T}\mathbf{e} + 2U\mathbf{e} \otimes \frac{U\mathbf{e}}{|U\mathbf{e}|^2} - 4U\mathbf{e} \otimes U^{-T}\mathbf{e} \frac{|U\mathbf{e}|^2}{|U\mathbf{e}|^2} \\
&= -\mathbb{I} + 2\boldsymbol{\eta}_1 \otimes \boldsymbol{\eta}_1.
\end{aligned}$$

□

Thus indeed, whenever a twin is given by Mallard's law, the lattices on either side of the interface are related by a 180° rotation. However, generically this will not be the case and thus the notation of rank-one connections is more general in this sense. Furthermore, as already pointed out in Chapter 6, since the conditions on having a 180° rotation does not take into account the stretch components of the deformations, it can result in 'twins' between the same Bain variants and in particular they will not be rank-one connected (cf. Lemma 2.2) and thus not twins in the mathematical sense.

7.1 The $(3\ 10\ 15)_\gamma$ or $(2\ 5\ 9)_\gamma$ Transformation

In this section, we compare the results of the Ball-James model with the ones from the original crystallographic theory for the $(3\ 10\ 15)_\gamma$ or $(2\ 5\ 9)_\gamma$ transformation. Before doing so, we stress that the term $(3\ 10\ 15)_\gamma$ transformation only means that a habit plane with coordinates near $(3\ 10\ 15)_\gamma$ is observed. In particular $(2\ 5\ 9)_\gamma$ is near $(3\ 10\ 15)_\gamma$ and thus both transformations fall into the same category (cf. Figure 7.1).

Habit planes of normal approximately $(3\ 10\ 15)_\gamma$ are observed in e.g. Fe-7AL-2C [WW71a] and Fe-24.5 at-% Pt [EW67] and habit planes of normal $(2\ 5\ 9)_\gamma$ e.g. in

Fe-22Ni-.8C [DB69]. In all cases the substructure is plate-like with complete internal $(112)_\alpha (= (110)_\gamma)$ twins and agreement between the (original) crystallographic theory and experiment has been shown to be excellent in all three cases. Due to the macroscopic equivalence of the Ball-James theory and the original crystallographic theory, the results agree macroscopically. Moreover, the Ball-James model predicts the microstructure of fine $(110)_\gamma$ twins. A comparison between experimental values from [WW71a] has been established in [Bha03, Table 4.1]. To illustrate the theory we conduct a detailed comparison between the results from the Ball-James model and the experimental results (see Table 7.3) for three different alloys.

Tab. 7.3. Experimental results for the habit plane normals $\mathbf{n}$ and shearing vectors $\mathbf{a}$ for three alloys undergoing a $(31015)_\gamma$ or $(259)_\gamma$ transformation.

Alloy	Fe-22Ni-.8C	Fe-7Al-2C	Fe-24.5 at-% Pt
$\mathbf{a}$	$[-.034, -.132, .135]$	$[-.017, -.077, .093]$	$[-.028, -.157, .145]$
$\mathbf{n}$	$(.175, .548, .818)$	$(.127, .576, .808)$	$(.191, .621, .760)$
$r = c/a$	1.040	1.14	1.0
Reference	[DB69]	[WW71a]	[EW67]

We recall that, by Theorem 2.1, given two tetragonal martensitic variants with lattice parameters η_1, η_2 the volume fractions that allow an interface with austenite are given by

$$\lambda_{\pm} = \frac{1}{2} \pm \frac{1}{2} \frac{1}{\eta_2^2 - \eta_1^2} \sqrt{(2 - \eta_2^2 - \eta_1^2)(\eta_1^2 - 2\eta_1^2\eta_2^2 + \eta_2^2)}. \quad (7.5)$$

We emphasise that it is important to check that it is indeed the middle eigenvalue of the macroscopic deformation that is equal to one. For each of the values λ_i , we can

calculate two pairs of habit plane normals and shears according to Proposition 2.1³.

For λ_- , one of these pairs is given by the (normalised) normal (h, k, l) , where

$$\begin{aligned} h &= \frac{1}{2\eta_1} \frac{1}{\sqrt{1-\eta_2^2}} \left(\sqrt{\eta_1^2 + \eta_2^2 - 2\eta_1^2\eta_2^2} - \sqrt{2 - \eta_1^2 - \eta_2^2} \right), \\ k &= -\frac{1}{2\eta_1} \frac{1}{\sqrt{1-\eta_2^2}} \left(\sqrt{\eta_1^2 + \eta_2^2 - 2\eta_1^2\eta_2^2} + \sqrt{2 - \eta_1^2 - \eta_2^2} \right), \\ l &= \frac{1}{\eta_1} \frac{\sqrt{\eta_1^2 - 1}}{\sqrt{1 - \eta_2^2}}, \end{aligned}$$

and the shear (r, s, t) , where

$$\begin{aligned} r &= -\frac{\eta_1}{2} \sqrt{\frac{1-\eta_2}{1+\eta_2}} \left(\sqrt{\eta_1^2 + \eta_2^2 - 2\eta_1^2\eta_2^2} - \sqrt{2 - \eta_1^2 - \eta_2^2} \right), \\ s &= \frac{\eta_1}{2} \sqrt{\frac{1-\eta_2}{1+\eta_2}} \left(\sqrt{\eta_1^2 + \eta_2^2 - 2\eta_1^2\eta_2^2} + \sqrt{2 - \eta_1^2 - \eta_2^2} \right), \\ t &= \frac{\eta_1\eta_2\sqrt{(\eta_1^2 - 1)(1 - \eta_2^2)}}{1 + \eta_2}. \end{aligned}$$

All remaining possible pairs are given as $\mathcal{P}^{24}$ conjugates. In particular, up to permutations and sign changes, all normals and shears are the same, irrespectively of the choice of λ_i or the first or second solution. Figure 7.1 depicts the dependence of the habit plane normals for a range of parameters η_1, η_2 .

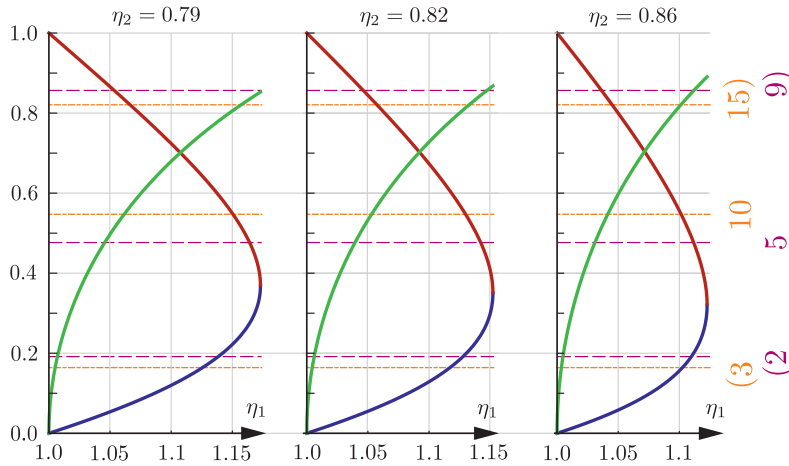


Fig. 7.1. Coordinates of habit plane normal (blue, red, green) arising from simple twinning for different values of η_1, η_2 .

³The formulas can also be found in [BJ87, (5.68)]. However, be aware that in the formula for δ it should be $(1 + \eta_2)^{-1}$ instead of $(1 - \eta_2)^{-1}$

Let us compare these results with the experimental values from Table 7.3. To apply our results we ought to recover the lattice parameters from the ratio of tetragonality r and the volume change ΔV via

$$(\eta_1, \eta_2) = \left(\frac{2^{1/6}(\Delta V)^{1/3}}{r^{1/3}}, \frac{r^{2/3}(\Delta V)^{1/3}}{2^{1/3}} \right).$$

The results (and the experimental values for comparison) are listed in Table 7.4. The overall agreement is good, particularly for the habit plane in Fe-24.5 at-% Pt. To put the comparison into perspective one should remember that the measured values are averaged over 6 samples with a scattering of up to 20% of the values.

Tab. 7.4. Computed values for alloys undergoing a $(3\ 10\ 15)_\gamma$ or $(2\ 5\ 9)_\gamma$ Transformation compared to the experimental values from Table 7.3.

Alloy	Fe-22Ni-.8C		Fe-7Al-2C		Fe-24.5 at-% Pt	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
a	$\begin{pmatrix} -.033 \\ .146 \\ .139 \end{pmatrix}$	$\begin{pmatrix} -.034 \\ -.132 \\ .135 \end{pmatrix}$	$\begin{pmatrix} -.018 \\ .090 \\ .102 \end{pmatrix}$	$\begin{pmatrix} -.017 \\ -.077 \\ .093 \end{pmatrix}$	$\begin{pmatrix} -.044 \\ .162 \\ .157 \end{pmatrix}$	$\begin{pmatrix} -.028 \\ -.157 \\ .145 \end{pmatrix}$
n	$\begin{pmatrix} .147 \\ -.643 \\ .752 \end{pmatrix}$	$\begin{pmatrix} .175 \\ .548 \\ .818 \end{pmatrix}$	$\begin{pmatrix} .122 \\ -.604 \\ .787 \end{pmatrix}$	$\begin{pmatrix} .127 \\ .576 \\ .808 \end{pmatrix}$	$\begin{pmatrix} .169 \\ -.626 \\ .761 \end{pmatrix}$	$\begin{pmatrix} .191 \\ .621 \\ .760 \end{pmatrix}$
(η_1, η_2)	(1.110, 0.816)		(1.083, 0.873)		(1.126, 0.796)	

7.2 The $(2\ 2\ 5)_\gamma$ Transformation

The $(2\ 2\ 5)_\gamma$ transformation is observed in e.g. Fe-(0.5 – 1.4%)C alloys [BM64], Fe-Cr-C [Way+61] and Fe-Mn-C alloys [DB69]. Unlike $(3\ 10\ 15)_\gamma$ steels, the substructure is less regular and significantly more complex. Even though $(1\ 1\ 2)_\alpha$ twins are still observed consistently, they do not extend completely through the plate and the edges are irregular. Further, the twins are accompanied by various defects and the midribs are much less well defined (cf. [MW92; DW71]). Owing to the irregular structure it is perhaps no surprise that attempts to apply the original (single

shear) crystallographic theory have proven unsuccessful (cf. Figure 7.1 and note that $(2\ 2\ 5) \approx (.35, .35, .87)$).

In an attempt to fit the experimental observations with the theory, [BM64] made use of an extension of the Bowles & MacKenzie theory (cf. [MB57]), which introduced an adjustable uniform dilatation parameter δ . This parameter corresponds to changing the requirement of having a rank-one connection to $\mathbb{I}$ (invariant plane strain) to having it to $\delta\mathbb{I}$. This approach has been criticised heavily in [DW71] as experiments did not show any evidence for such a dilatation. Other approaches by [Lie66] (triple shear model), [AB69] and [RC70] (double shear model) tend to give better predictions but again rely heavily on experimental input to guess the additional parameters. Moreover, in spite of these additional degrees of freedom, the agreement between experiment and theory is still unsatisfactory. We conclude that there seems to be a fundamental lack of understanding in the underlying mechanism and that in order to obtain better predictions one should first try to find a more suitable model.

7.3 The $(5\ 5\ 7)_\gamma$ Transformation and a New Approach

The $(5\ 5\ 7)_\gamma$ transformation is commonly observed in low carbon ($< 0.4\%$) steels [MW92]. Because of its morphology consisting of so-called laths which are part of blocks and packets (see Figure 7.2) it is known as *lath martensite*. Conventionally, lath martensite is also associated with high dislocation density, slip and plasticity and the absence of transformation twins (see e.g. [WW81]⁴). However, the forthcoming theory predicts the existence of very fine twins instead. A possible explanation for these differences may be the lack of high enough resolution images leading to a

⁴Comment from the anonymous reviewer: “Indeed, it is well known in the literature that lath martensite forming in low carbon steels contains a high density of dislocations but no transformation twins.”

misinterpretation of very fine microstructures as dislocations. The results presented in this section have been published in [KM15].

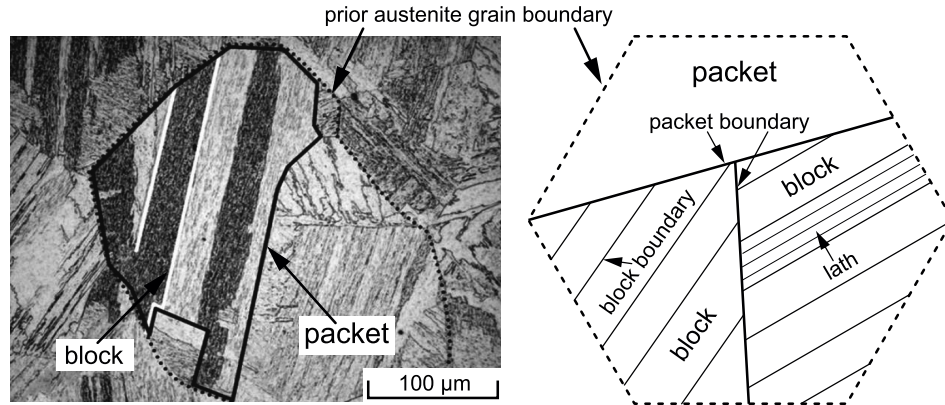


Fig. 7.2. A micrograph and schematic representation of lath martensite (after [Mor+03]). Each packet is divided into layers of blocks, each consisting of layers of laths.

As can be seen from Figure 7.1 (note that $(5\ 5\ 7) \approx (.5, .5, .7)$) any reasonable choice of lattice parameters in the classical crystallographic theory cannot result in $\{5\ 5\ 7\}$ habit plane normals. However, (phenomenological) double shear theories have widely been used to explain the observed habit plane normals and some of the most accurate calculations go back to an algorithm developed by Kelly [Kel92]. A short-coming of double shear theories is the lack of a selection mechanism that picks the right lattice invariant shearing systems (see e.g. [Kel92, Table 1] or [Qi+14]), in turn leading to a large number of input parameters.

To overcome this insufficiency, we propose a new approach that, similarly to the original crystallographic theory, only allows shearing *systems* that arise from mechanical twinning. From Lemma 7.1 it is clear that this is, on a macroscopic level, equivalent to considering a double laminate (or twins within twins). Apart from being able to explain the $\{5\ 5\ 7\}$ habit plane normals with fewer parameters, we are also able to show that it is in fact the only possible family of habit planes that satisfies a condition of maximal compatibility and a condition of small overall atomic movement.

The Setup of Our New Approach

To derive our theory we employ the Ball-James model (cf. Chapter 2) and we expand on previous work by Ball & Carstensen [BC97] on the possibility of *non-classical* austenite-martensite interfaces. Here, non-classical stands for any interface between elements in K^{qc} that are not contained in $K^{(1)}$ (cf. Definition 2.7). An important difference between our approach and the one in [BC97] is that we consider interfaces between austenite and martensitic structures supported on *all* three martensite wells. By doing so, we are able to obtain microstructures whose macroscopic deformation can be closer to self-accommodation (cf. Chapter 4) and thus fit within austenite with smaller strains. Since we are in the setting of low carbon steels (cf. Chapter 1), we assume the Bain strains

$$U_1 = \text{diag}(\eta_2, \eta_1, \eta_1), \quad U_2 = \text{diag}(\eta_1, \eta_2, \eta_1), \quad U_3 = \text{diag}(\eta_1, \eta_1, \eta_2),$$

where $\eta_1 = \frac{\sqrt{2}a}{a_0}$ and $\eta_2 = \frac{c}{a_0}$. Here a_0 is the lattice parameter of the fcc austenite and a, c are the lattice parameters of the bct martensite ($a = c$ for bcc).

A Double Shear Theory Derived from Internal Twinning

By Lemma 3.10 we know that any a double laminate, which is supported on all three wells, is a laminate between two simple laminates related by a 180° degree rotation. Let us consider the two simple laminates with average strain $U_1 + \lambda \mathbf{a} \otimes \mathbf{n}$ and $U_1 + \lambda \mathbf{a}' \otimes \mathbf{n}'$. For each λ there exists a rotation R'_λ such that

$$R'_\lambda(U_1 + \lambda \mathbf{a}' \otimes \mathbf{n}') = (U_1 + \lambda \mathbf{a} \otimes \mathbf{n}) + \mathbf{b}_\lambda \otimes \mathbf{m}_\lambda,$$

and thus the two twinning systems are macroscopically compatible with a fully coherent interface of normal $\mathbf{m}_\lambda$ between them (cf. the lower part of Figure 7.3). The elements R'_λ , $\mathbf{b}_\lambda$ and $\mathbf{m}_\lambda$ can be calculated by Mallard's law (Lemma 2.4) applied to $U = U_1 + \lambda \mathbf{a} \otimes \mathbf{n}$ with $\mathbf{e} = [0 \ 1 \ 1]$, giving rise to a Type I and a Type II solution. Unlike in the single shear theory, these twins are not compound and therefore we distinguish these two solutions by the superscript α , where $\alpha = 1, 2$ stands for Type I and Type II respectively.

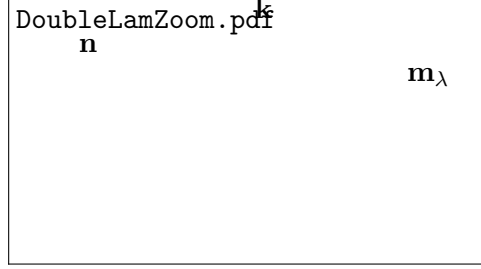


Fig. 7.3. A configuration of twins within twins, with macroscopic deformation gradient $U_1 + \lambda \mathbf{a} \otimes \mathbf{n} + \mu \mathbf{b}_\lambda^\alpha \otimes \mathbf{m}_\lambda^\alpha$, which (macroscopically) leaves the plane with normal $\mathbf{k}$ invariant.

The overall macroscopic deformations is then given by

$$U_1 + \lambda \mathbf{a} \otimes \mathbf{n} + \mu \mathbf{b}_\lambda^\alpha \otimes \mathbf{m}_\lambda^\alpha, \quad \lambda, \mu \in (0, 1). \quad (7.6)$$

As shown in Lemma 7.1, one can express (7.6) as $U_1 S_2^\alpha(\lambda, \mu) S_1(\lambda)$ where $S_1 \equiv S_1(\lambda) = \mathbb{I} + \lambda U_1^{-1} \mathbf{a} \otimes \mathbf{n}$ and $S_2 \equiv S_2^\alpha(\lambda, \mu) = \mathbb{I} + \mu U_1^{-1} \mathbf{b}_\lambda^\alpha \otimes S_1^{-T} \mathbf{m}_\lambda^\alpha$ and thus (7.6) is an instance of a double shear theory. We note that $\det S_1 = \det S_2 = 1$. By Proposition 2.1, in order to make the total shape deformation $F_{\lambda, \mu}^\alpha = R U_1 S_2^\alpha(\lambda, \mu) S_1(\lambda)$ an invariant plane strain, the volume fractions λ, μ need to be chosen such that the middle eigenvalue of $F_{\lambda, \mu}^{\alpha T} F_{\lambda, \mu}^\alpha$ is equal to one.

Determination of Admissible Volume Fractions

One possibility to determine if a matrix F has one as a singular value, is to solve $\det(F^T F - \mathbb{I}) = 0$. However, it turns out that for $\alpha = 1$ it is computationally easier

to consider a vector of the form $\mathbf{f} = (1, x, y)$ and solve the system of equations given by

$$F_{\lambda,\mu}^{\alpha T} F_{\lambda,\mu}^{\alpha} \mathbf{f} = \mathbf{f}$$

which is linear in x, y and quadratic in μ . For $\alpha = 2$ one considers a vector of the form $\mathbf{f} = (x, 1, y)$ instead. If one chooses the volume preserving Bain strain, i.e. $U_1 = \text{diag}(2^{-1/3}, 2^{1/6}, 2^{1/6})$, the solutions are approximately given by

$$\mu^{\alpha=1}(\lambda) \approx \frac{1}{2} \pm \frac{\sqrt{1.74\lambda^4 - 7.92\lambda^3 + 6.48\lambda^2 - 1.93\lambda + 0.196}}{2(\lambda - 1)\sqrt{2.78\lambda^2 - 7.56\lambda + 2.34}}$$

and

$$\mu^{\alpha=2}(\lambda) \approx \frac{1}{2} \pm \frac{\sqrt{-2.78\lambda^4 - 3.56\lambda^3 + 5.08\lambda^2 - 1.80\lambda + 0.20}}{2(\lambda - 1)\sqrt{-1.74\lambda^2 - 6.0\lambda + 2.34}}.$$

For general η_2, η_1 the expressions are lengthy and can be found in Appendix E. Figure 7.4 visualises the dependence $\mu^\alpha(\lambda)$ for the volume-preserving Bain strain. The endpoints of these curves correspond to the vanishing of one of the twinning systems (cf. (7.6)) and hence to the collapse of the system of twins within twins, to a simple twinning system with volume fractions given by (7.5). The figure remains qualitatively the same for typical lattice parameters. For each α and each

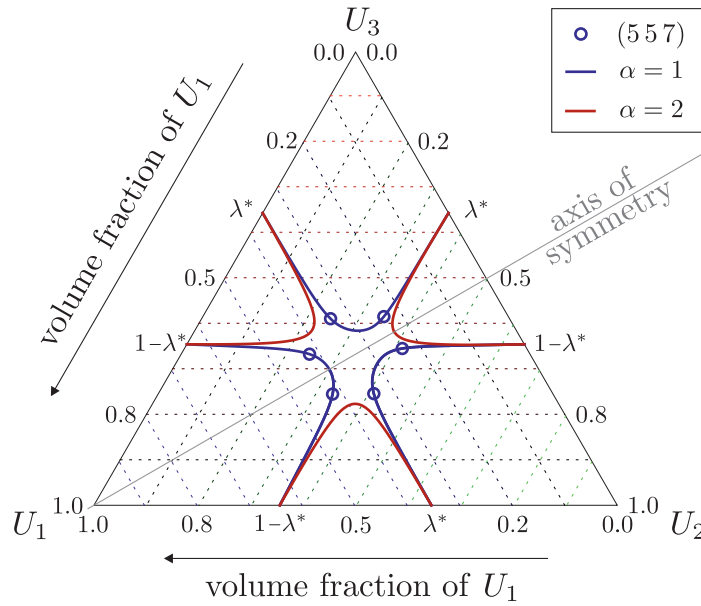


Fig. 7.4. Ternary plot of volume fractions $1 - \lambda$ of U_1 , $(1 - \mu^\alpha(\lambda))\lambda$ of U_2 and $\mu^\alpha(\lambda)\lambda$ of U_3 that make the twins within twins an invariant plane strain for $\eta_1 = 2^{1/6}$ and $\eta_2 = 2^{-1/3}$.

admissible pair $(\lambda, \mu^\alpha(\lambda))$ with corresponding strain $F_{\lambda, \mu^\alpha(\lambda)}^\alpha$, we can calculate two one-parameter families of habit plane normals through Proposition 2.1.⁵ By considering all possible combinations of twinning systems in our construction, we then obtain all crystallographically equivalent normals. For the volume-preserving Bain strain, the habit plane normals that can arise from the families $F_{\lambda, \mu^i(\lambda)}^i$, $i = 1, 2$ are visualised in Figure 7.5.

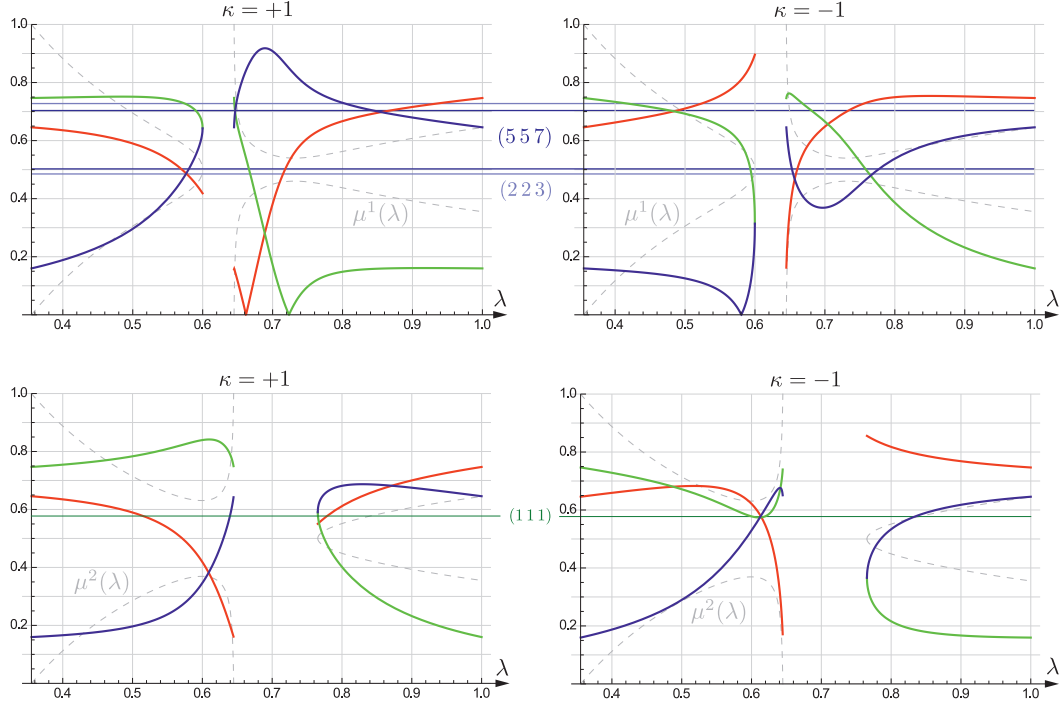


Fig. 7.5. Coordinates of the habit plane normals (blue, red, green) for the macroscopic strains $F_{\lambda, \mu^1(\lambda)}^1$ (top) and $F_{\lambda, \mu^2(\lambda)}^2$ (bottom) for $\kappa \in \{-1, 1\}$ (cf. Proposition 2.1). The lattice parameters are $\eta_1 = 2^{1/6}$ and $\eta_2 = 2^{-1/3}$, corresponding to the volume-preserving Bain strain.

Why Twins Within Twins?

It is natural to assume that the observed total shape deformation F requires small overall atomic movement (cf. Chapter 1) relative to the parent phase of austenite. By Example 1.2, a measure of this distance is the *strain energy*⁶ given by

$$d_2(F, \mathbb{I}) = |F^T F - \mathbb{I}|^2 = \sum_{i=1}^3 (\nu_i^2(F) - 1)^2.$$

⁵Even though in principal this can still be done explicitly, all attempts to obtain an explicit expression for the habit planes as functions of η_1, η_2, λ were unsuccessful.

⁶Alternatively, one may use $d_1(F, \mathbb{I}) = \sum_{i=1}^3 (\nu_i(F) - 1)^2$ which yields the same results.

By Chapter 4 we know that any microstructure with small strain energy (i.e. close to self-accommodation) must necessarily involve all three Bain variants in roughly similar volume fractions. In particular, this cannot be the case for an array of simply twinned martensitic variants and we ought to consider at least twins within twins (see also Fig. 7.7). Although, introducing even further levels of twinning can reduce the strain energy, one could argue that interfacial energy contributions, which are not accounted for in this model, may inhibit such behaviour.

A New Theory for the $\{5\ 5\ 7\}$ Lath Transformation

Combining the fact that $\{5\ 5\ 7\}$ cannot result from simple twinning (cf. Fig. 7.1) and that twins within twins are preferable in terms of strain energy, we now build a theory that predicts $\{5\ 5\ 7\}$ habit plane normals solely based on energy minimisation and geometric compatibility.

Firstly, the one-parameter families of habit plane normals obtained from twins within twins (see Section 7.3), contain normals very close to any $\{5\ 5\ 7\}$. This is at least the case for lattice parameters close to $\eta_1 = 2^{1/6} \approx 1.12$, $\eta_2 = 2^{-1/3} \approx 0.79$ corresponding to a volume-preserving transformation from fcc to bcc. This regime of parameters is suitable since $\{5\ 5\ 7\}$ habit planes are observed in low-carbon steels where the transformation is very nearly fcc-to-bcc. The resulting one-parameter families of habit plane normals, along with their crystallographically equivalent ones, are shown in Figure 7.6. We stress that the only free parameter in the generation of these normals is λ which fixes the choice of the shearing systems, based only on the energy minimising property of the microstructure. Secondly, out of these one-parameter families of normals, our theory can identify the $\{5\ 5\ 7\}$ habit plane normals as those satisfying a criterion of maximal compatibility. To this end, revisiting our construction of twins within twins there is a choice (cf. (7.6)) of using either $F_{\lambda, \mu^1(\lambda)}^1$ as an average strain, corresponding to the Type I solution from Mallard's law, or $F_{\lambda, \mu^2(\lambda)}^2$ corresponding to Type II. Figure 7.7 shows the strain energy associated with

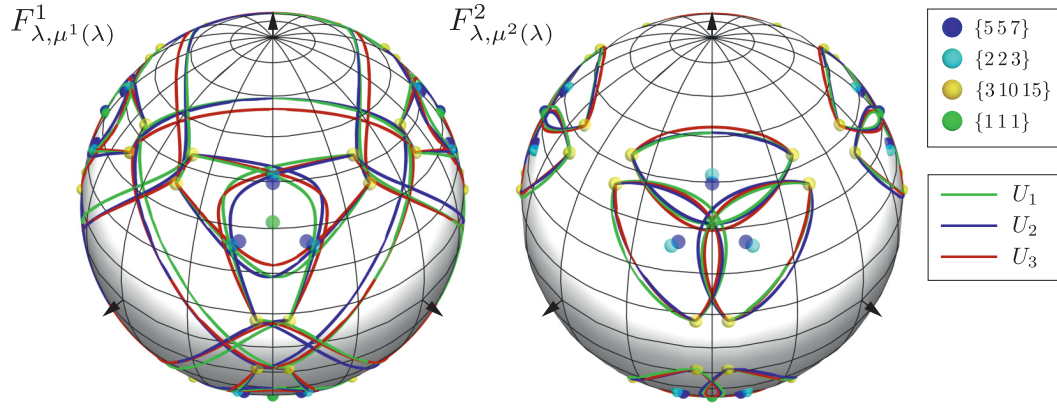


Fig. 7.6. Possible habit plane normals for $F^1_{\lambda, \mu^1(\lambda)}$ and $F^2_{\lambda, \mu^2(\lambda)}$ with $\eta_1 = 2^{1/6}$ and $\eta_2 = 2^{-1/3}$. Yellow points correspond to habit plane normals arising from simple twinning.

the two macroscopic strains as a function of λ . It is clear that the strain energy of $F^1_{\lambda, \mu^1(\lambda)}$ is significantly smaller than that of $F^2_{\lambda, \mu^2(\lambda)}$ and is thus preferable. We also note that the strain energies of both F^1 and F^2 increase rapidly as the volume fraction of U_1 approaches 0, λ^* or $1 - \lambda^*$, that is as the microstructure reduces to a single twinning system. Further, we remark that the $F^2_{\lambda, \mu^2(\lambda)}$ with minimal strain energy result in habit plane normals which are very nearly $\{1\ 1\ 1\}$ (see also Fig. 7.6). Nevertheless, the strain energies of any of the $F^1_{\lambda, \mu^1(\lambda)}$ that give rise to $\{5\ 5\ 7\}$ normals are lower (cf. Fig. 7.7). Even though, the strains resulting in $\{5\ 5\ 7\}$

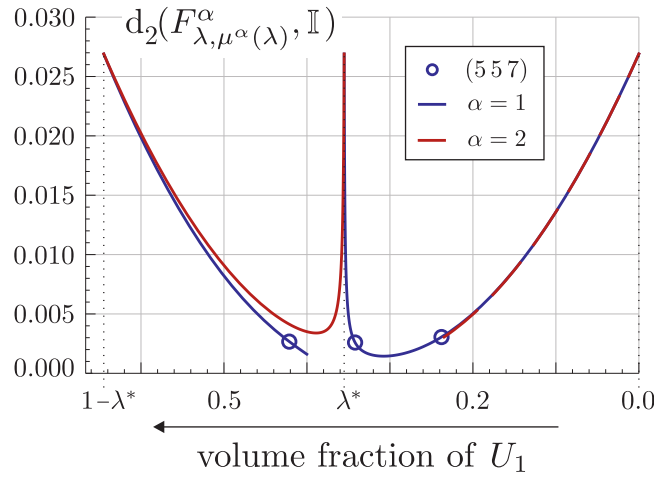


Fig. 7.7. The strain energies $d_2(F, \mathbb{I})$ for the double laminates $F = F^i_{\lambda, \mu^i(\lambda)}$, $i = 1, 2$ with $\eta_1 = 2^{1/6}$ and $\eta_2 = 2^{-1/3}$ as a function of the volume fraction λ of U_1 .

habit plane normals do not minimise the strain energy, they satisfy a strong criterion of compatibility. To understand this one must think in terms of the dynamic process of nucleation. As austenite is rapidly quenched, the martensite phase nucleates

at various sites. The strain in a given nucleation site may need to be an invariant plane strain but otherwise, has no reason to be the same as the strain in any other site. Nevertheless, there are essentially only three distinct families of systems of twins within twins and these can be classified by the Bain variant which is present in both of the simple twinning systems that comprise the overall microstructure. In Figure 7.6, these three families are distinguished by colour. As the nuclei grow and approach other nuclei, they need to remain compatible with each other. Remarkably, the only habit plane normals that arise from deformations with low strain energy and can be reached by all three families are $\{5\ 5\ 7\}$. In Figure 7.6, this can be seen from the fact that all differently coloured curves intersect close to $\{5\ 5\ 7\}$. For any two such regions of twins within twins with corresponding average strains $\mathbb{I} + \mathbf{b}_1 \otimes (5\ 5\ 7)$ and $\mathbb{I} + \mathbf{b}_2 \otimes (5\ 5\ 7)$, one can see that

$$(\mathbb{I} + \mathbf{b}_1 \otimes (5\ 5\ 7)) - (\mathbb{I} + \mathbf{b}_2 \otimes (5\ 5\ 7)) = (\mathbf{b}_1 - \mathbf{b}_2) \otimes (5\ 5\ 7),$$

implying that they can meet along a fully coherent planar interface of normal $(5\ 5\ 7)$. Of course, any nucleus interacts with its neighbours faster than it does with distant nuclei. As a result, blocks of similarly oriented regions of twins within twins (laths) may form whose overall orientation may differ from that of other blocks.

Interpretation of the Results

The proposed theory for the prediction of $(5\ 5\ 7)$ habit plane normals in lath martensite has two possible interpretations. On the one hand, it can be seen as a purely macroscopic theory. In particular, it is an instance of a double shear theory with a precise algorithm to produce the required shears based on energy minimisation, without the need for any further assumptions. All possible habit plane normals that can arise from the one parameter family (indexed by λ) of macroscopic deformations $F_{\lambda, \mu^{-1}(\lambda)}^1$ are shown in Figure 7.5 (top). Table 7.5 then lists the elements of the twinning systems for the values of λ that produce a near $(5\ 5\ 7)$ habit plane. With

the help of (7.6) it is easy to convert between the twinning and shearing systems and thus compute the elements S_1 and S_2 required in a double shear theory. At this macroscopic level it is not possible to distinguish between twins within twins, a single twin and one slip system, and a single variant and two slip systems.

Tab. 7.5. Elements of the twinning system (7.6) leading to $\{5\ 5\ 7\}$ habit plane normals. The remaining $\{5\ 5\ 7\}$ normals can be obtained from the crystallographically equivalent systems.

λ	0.576	0.659	0.762
a	$[\cdot374, -\cdot529, 0]$	$[\cdot374, -\cdot529, 0]$	$[\cdot374, -\cdot529, 0]$
n	$\frac{1}{\sqrt{2}}(1, 1, 0)$	$\frac{1}{\sqrt{2}}(1, 1, 0)$	$\frac{1}{\sqrt{2}}(1, 1, 0)$
$\mu^1(\lambda)$	0.581	0.621	0.546
b_{λ}	$[\cdot130, \cdot234, \cdot315]$	$[\cdot135, \cdot260, \cdot359]$	$[\cdot137, \cdot289, \cdot412]$
m	$\frac{1}{\sqrt{2}}(0, 1, -1)$	$\frac{1}{\sqrt{2}}(0, 1, -1)$	$\frac{1}{\sqrt{2}}(0, 1, -1)$

On the other hand, a physical mechanism for the formation of $(5\ 5\ 7)$ habit plane normals is proposed and thus a specific morphology on a microscopic level. According to this interpretation, each lath may itself be a region of twins within twins with a corresponding lath boundary of normal $(5\ 5\ 7)$. This type of morphology is depicted in Figure 7.3 with **k** being a $\{5\ 5\ 7\}$ normal and the other elements are as in Table 7.5. This morphology is a direct consequence of the underlying theory and it would be very interesting if it could be put to experimental scrutiny. A first step in this direction has been undertaken in recent independent experiments by [Zha+16]. The authors summarise that *“based on conventional belief, the lath martensites in low carbon steels are with high density dislocations as the substructure, in contrast to twin substructure in lenticular high carbon martensite. In the present work [...] it was found that lots of lath martensites consist of twin [sic] as their substructure, rather than high density dislocations.”*

Summary, Concluding Remarks and Outlook

This thesis concerned different aspects of the mathematical modelling of martensitic phase transformations with particular emphasis on its possible applications to steels. We summarise each chapter and highlight the most important results as well as addressing possibilities for future research.

In Chapter 1, we provided a rigorous proof for the existence of an optimal lattice transformation between any two given Bravais lattices with respect to a large number of optimality criteria. Furthermore, a precise algorithm and a GUI to determine this optimal transformation was given in Appendix B. As possible applications, the optimal transformation in steels, that is the transformation from fcc to bcc/bct, and in terephthalic acid were determined. Through Theorem 1.1 and with the help of the provided algorithm/programme we were able to rigorously determine the optimal phase transformation in any material undergoing a displacive phase transformation from one Bravais lattice to another. If the parent or product phases are multilattices, the proposed framework is not *a priori* applicable. Nevertheless, one may still consider Bravais sublattices of these multilattices and proceed as before. The choice of these sublattices may come from physical consideration. However, in order to rigorously determine the optimal transformation between two given multilattices one would need to measure the movement of *all* atoms consistently, that is one would need to take into account both the overall periodic deformation of the unit cell and the shuffle movement of atoms within the unit cell. The establishment of such a criterion would be of great interest and can hopefully be tackled in the future.

In Chapter 2, we reviewed the Ball-James model and related concepts such as quasiconvexity and gradient Young measures. We provided an alternative approach to derive some classical results on habit planes and volume fractions.

In Chapter 3, we presented a new approach to the three-well problem, which among other things, showed that the boundaries of K^{lc} (the inner bound) and K^{pc} (the outer bound) coincide in some (relatively) open sets. These open sets were given as level sets of functions of the form $|A(\pm 1, \pm 1, \pm 1)|^2$ and $|\text{cof } A(\pm 1, \pm 1, \pm 1)|^2$. We also gave a conjecture for the entire quasiconvex hull and established the outline for a possible future (numerical) proof.

In Chapter 4, we investigated the special case when the martensite can fit within austenite without introducing any strain - called self-accommodation. We provided bounds on their minimum complexity and showed that in self-accommodating microstructures all martensitic variants need to be present in roughly equal volume fractions. In the case of cubic-to-tetragonal we also provided results on the attainment of these bounds. As these results are purely theoretical it would be of interest to put them to experimental scrutiny. Furthermore, based on numerical simulations we conjectured that $\mathbb{I} \notin K^{(3)}$ and it would be very interesting to verify (or falsify) this claim analytically.

In Chapter 5, we investigated the contrary situation when a material cannot form self-accommodating microstructures and derived energy estimates for interior nucleation. Without making any a priori assumptions, apart from cylindrical symmetry, we concluded that the shape of an inclusion of martensite within austenite is minimised (within that set) for a flat and thin shape as observed in experiments. We showed that $W^{\text{qc}}(\mathbb{I})$ is always negative, so that within the model, it is always energetically preferable to nucleate martensite within austenite. Further, by comparing two different types of nucleation in Theorem 5.1 and Theorem 5.2, we concluded that for materials that almost fulfil the criteria for self-accommodation, i.e. $\det U_1 \approx 1$, it

is energetically preferable to form a self-accommodating inclusion rather than an inclusion with a core of a simple laminate.

In Chapter 6, we presented a unified approach to derive transformation strains and orientation relationship models in steels. An important aspect was the identification of strains with orientation relationships. This unified approach was used to derive the NW, KS and other models and to extend them to the situation of a tetragonal α' -phase. The obtained dependence on the ratio of tetragonality seemed to be in good qualitative agreement with previous experiments. It would be of interest to perform more targeted experiments over a range of ratios of tetragonality to be compared with our predictions.

In Chapter 7, we compared the (phenomenological) crystallographic theory of martensite with the Ball-James model. We provided a dictionary that translates between both theories and illustrated them in the setting of the $(3\ 10\ 15)_\gamma$ transformation. We also reviewed common extensions of the original crystallographic theory and emphasised that they require a large number of fitted input parameters. In the setting of the $(5\ 5\ 7)_\gamma$ transformations, we proposed a new theory, that on the one hand, naturally provides all input parameters but on the other hand also suggests a new morphology of the material. A first indication for the existence of this new morphology has recently been provided in [Zha+16] and it would be interesting to conduct further similar experiments.

Appendix

A Step by Step Construction of the Original Kurdjumov-Sachs Variants

We will show how the mechanism proposed by Kurdjumov & Sachs is equivalent to applying the Bain strain followed by a rotation. To spare the reader the possible burden of translating from German to English, we follow the description in [Gui96, Ch. 3] which is based on [KS30]. The construction by Kurdjumov & Sachs involves three major steps

1. Shearing $(111)_\gamma$ planes (Figure A.3),
2. Shear along $[01\bar{1}]_\gamma$ (Figure A.4) and
3. Final adjustment stretches (Figure A.5).

Most of the complexity of their derivation stems from considering a non-standard unit cell of the fcc lattice (cf. [Gui96, Fig. III.2 (a)]) which is depicted in Figure A.1. In particular, by considering a non-standard fcc unit cell, the resulting bcc unit cell, depicted in Figure A.2, is also non-standard.

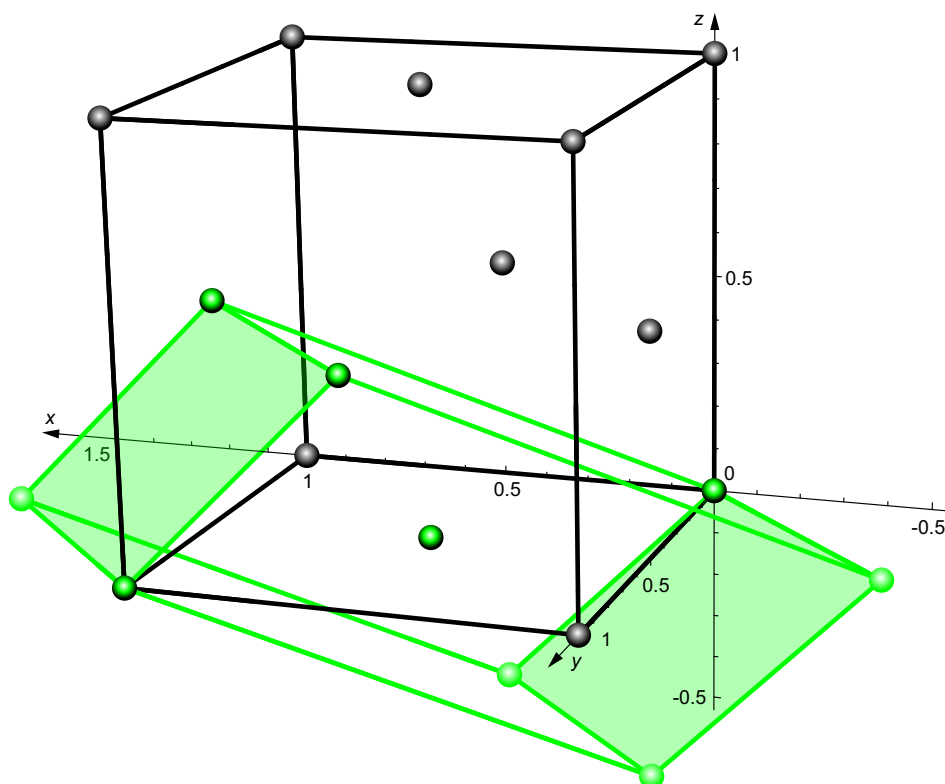


Fig. A.1. The transformation mechanism proposed by Kurdjumov & Sachs starts from a non-standard fcc unit cell. This non-standard unit cell (in green) is shown with respect to the standard fcc unit cell (in black) in a coordinate systems with axes $\{\mathbf{e}_{1,\gamma}, \mathbf{e}_{2,\gamma}, \mathbf{e}_{3,\gamma}\}$ along the standard fcc lattice vectors. An important feature of this non-standard cell is that the top and bottom faces (shaded green) are planes with normal $(1\ 1\ 1)_\gamma$. Atoms with two colours indicate that they are common to *both* unit cells. Of course, since both are unit cells of the same lattice, the generated lattices are identical.

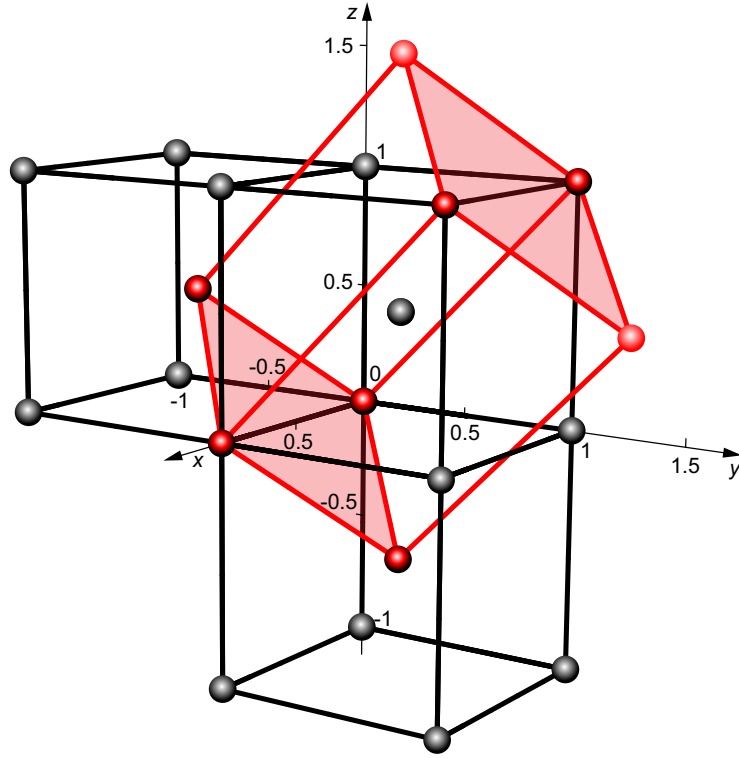


Fig. A.2. The resulting non-standard bcc unit cell (in red) with respect to a standard bcc lattice in a coordinate systems with axes $\{\mathbf{e}_{1,\alpha}, \mathbf{e}_{2,\alpha}, \mathbf{e}_{3,\alpha}\}$ along the standard bcc lattice vectors. An important feature of this non-standard cell is that the top and bottom faces (shaded red) are planes with normal $(0\ 1\ 1)_\alpha$. Atoms with two colours indicate that they are common to *both* the non-standard bcc unit cell (in red) and the three standard bcc unit cells (in black). Of course, since both are unit cells of the same lattice, the generated lattices are identical.

1. Shearing $(1\ 1\ 1)_\gamma$ Planes (Figure A.3)

The first step in the construction of Kurdjumov and Sachs is to shear the non-standard fcc unit cell (in green) along the $(1\ 1\ 1)_\gamma$ plane such that it matches the blue cell. That is, we apply the transformation

$$T_1 := \frac{1}{12} \begin{pmatrix} 10 & -2 & -2 \\ 1 & 13 & 1 \\ 1 & 1 & 13 \end{pmatrix} \approx \begin{pmatrix} 0.833 & -0.167 & -0.167 \\ 0.0833 & 1.08 & 0.0833 \\ 0.0833 & 0.0833 & 1.08 \end{pmatrix}.$$

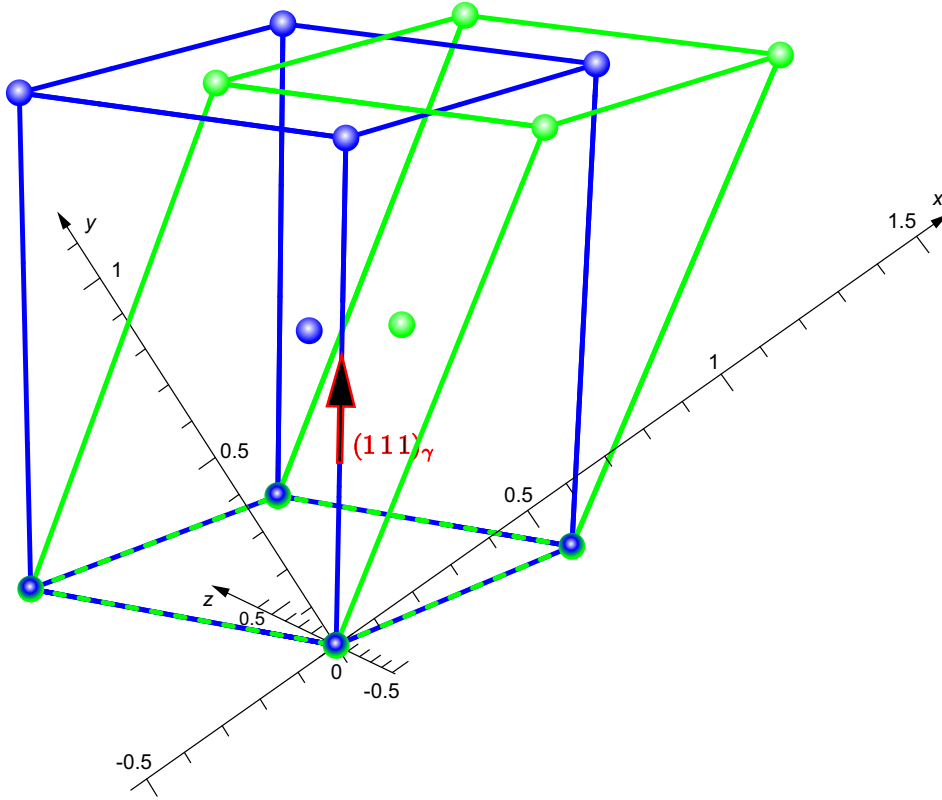


Fig. A.3. The transformation T_1 shears the non-standard fcc unit cell (in green) along the $(111)_\gamma$ plane to match the blue cell. Atoms and lines with two colours indicate that they are common to both cells. The red and black arrow indicates the direction $(111)_\gamma$, in particular $(111)_\gamma$ planes are orthogonal to this direction.

2. Shearing Along $[01\bar{1}]_\gamma$ Directions (Figure A.4)

The second step is to shear the blue cell along the $[01\bar{1}]_\gamma$ direction, such that the two base vectors enclose an angle of $\arccos(-\frac{1}{3})$ and thus enclose the same angle as the $[1\bar{1}1]_\alpha$ and $[11\bar{1}]_\alpha$ vectors in a bcc lattice. That is, we apply the transformation

$$T_2 := \frac{1}{3} \begin{pmatrix} -7 + 4\sqrt{6} & 5 - 2\sqrt{6} & 5 - 2\sqrt{6} \\ 5 - 2\sqrt{6} & 8 - 2\sqrt{6} & -10 + 4\sqrt{6} \\ 5 - 2\sqrt{6} & -10 + 4\sqrt{6} & 8 - 2\sqrt{6} \end{pmatrix} \approx \begin{pmatrix} 0.93 & 0.04 & 0.04 \\ 0.04 & 1.04 & -0.07 \\ 0.04 & -0.07 & 1.04 \end{pmatrix}.$$

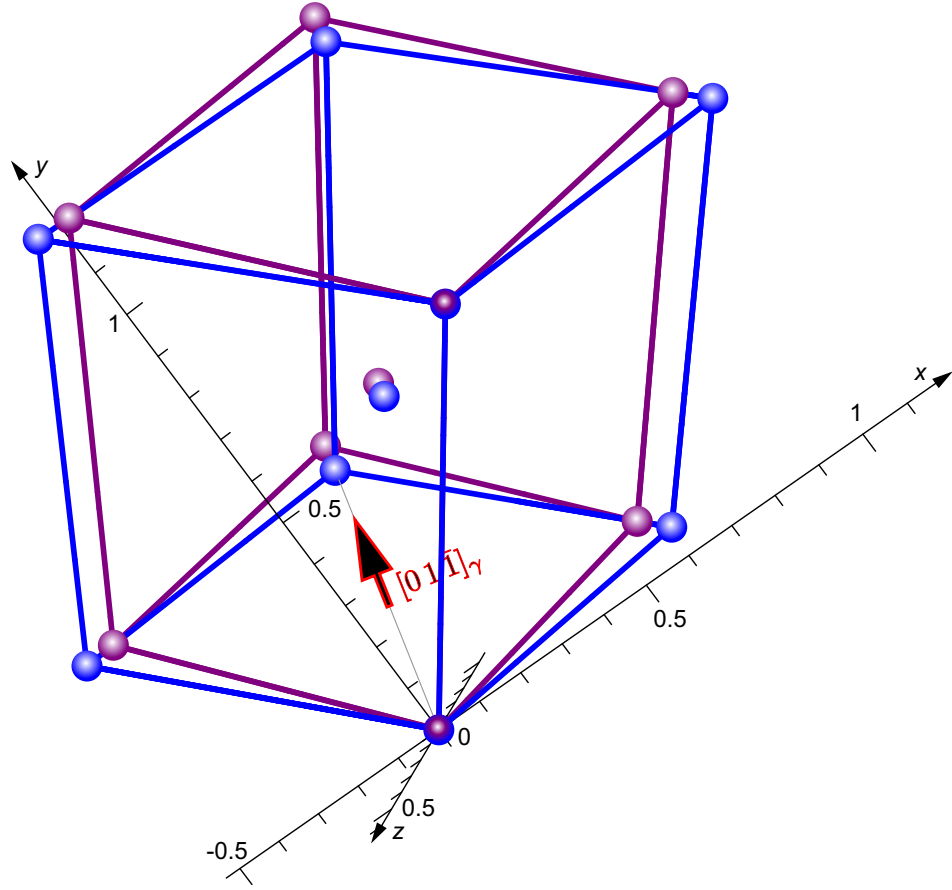


Fig. A.4. The transformation T_2 shears the blue cell to the purple cell such that the two base vectors enclose an angle of $\arccos(-\frac{1}{3})$. This angle coincides with the angle that the two bcc vectors $[1 \bar{1} 1]_\alpha$ and $[1 \bar{1} \bar{1}]_\alpha$ enclose. Atoms with two colours indicate that they are common to both cells. The red and black arrow indicates the direction $[0 1 \bar{1}]_\gamma$.

3. Final Adjustment Stretches (Figure A.5)

The final step is to perform a pure stretch along the edges of the purple cell to change the aspect ratio of the right parallelogram prism to $\sqrt{2} : \frac{\sqrt{3}}{2}$, so that it coincides with the aspect ratio of the non-standard bcc unit cell as depicted in Figure A.2. That is, we apply the transformation

$$T_3(\lambda) \approx \lambda \begin{pmatrix} 0.98 & -0.015 & -0.015 \\ -0.015 & 0.98 & -0.015 \\ -0.015 & -0.015 & 0.98 \end{pmatrix},$$

where $\lambda \in [1, \frac{\sqrt{2}}{3(\sqrt{6}-2)}] \approx [1, 1.049]$ and the extremal values of λ correspond to only decreasing the height and only increasing the width respectively. We may

choose $\lambda^* = \frac{5\sqrt{6}-12}{6(\sqrt{6}-2)(-3920\sqrt{3}+4801\sqrt{2})^{1/3}} \approx 1.027$ such that the overall deformation is volume preserving.

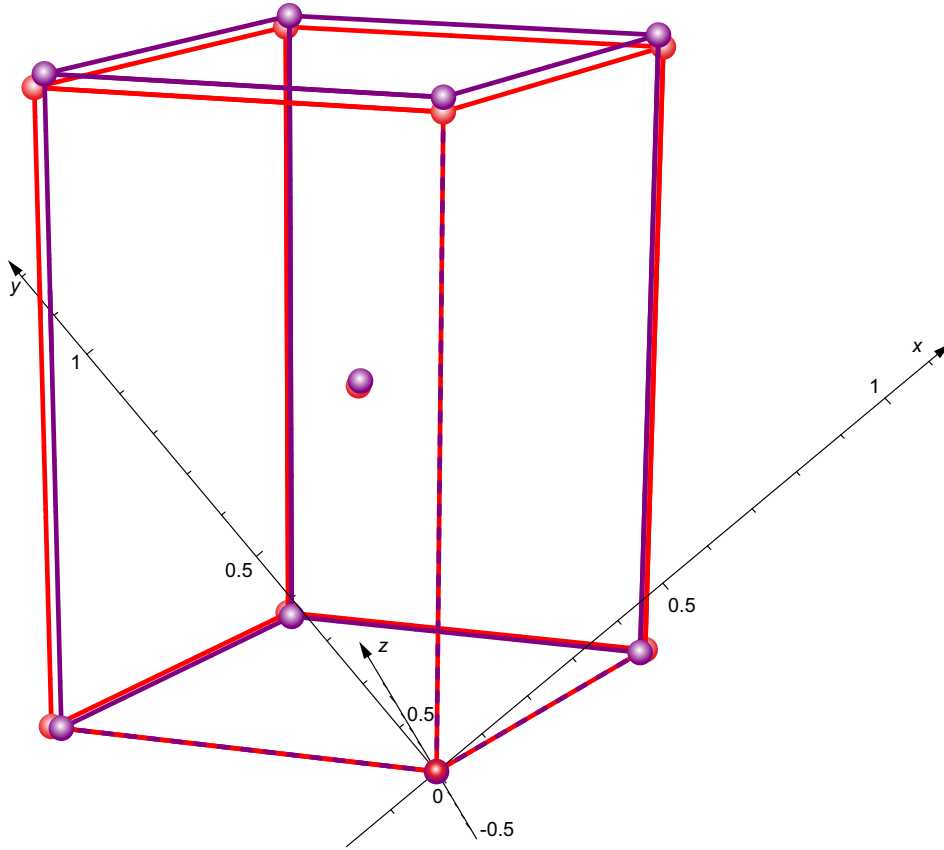


Fig. A.5. The transformation $T_3(\lambda^*)$ stretches the purple cell to the red cell such that the aspect ratio of the right parallelogram prism becomes $\sqrt{2} : \frac{\sqrt{3}}{2}$ and thus coincides with the aspect ratio of the non-standard bcc unit cell.

The Overall Transformation (Figure A.6)

Combining the previous three transformation, we obtain the overall deformation

T_{total} given by

$$T_{\text{total}} = T_3(\lambda^*)T_2T_1 \approx \begin{pmatrix} 0.788 & -0.135 & -0.135 \\ 0.0956 & 1.12 & -0.00814 \\ 0.0956 & -0.00814 & 1.12 \end{pmatrix}.$$

A polar decomposition $T_{\text{total}} = QP$ reveals

$$Q = R[9.728567590^\circ, [0\bar{1}1]] = \begin{pmatrix} 0.986 & -0.120 & -0.120 \\ 0.120 & 0.993 & -0.00720 \\ 0.120 & -0.00720 & 0.993 \end{pmatrix} \in \text{SO}(3),$$

$$P = U_1 = \text{diag}(2^{-1/3}, 2^{1/6}, 2^{1/6}) \approx \text{diag}(0.79, 1.12, 1.12).$$

Thus, the overall transformation is the Bain strain followed by a rotation as claimed. By construction, the close packed $(111)_\gamma$ (fcc) plane is parallel to the closest pack $(011)_\alpha$ (bcc) plane.¹

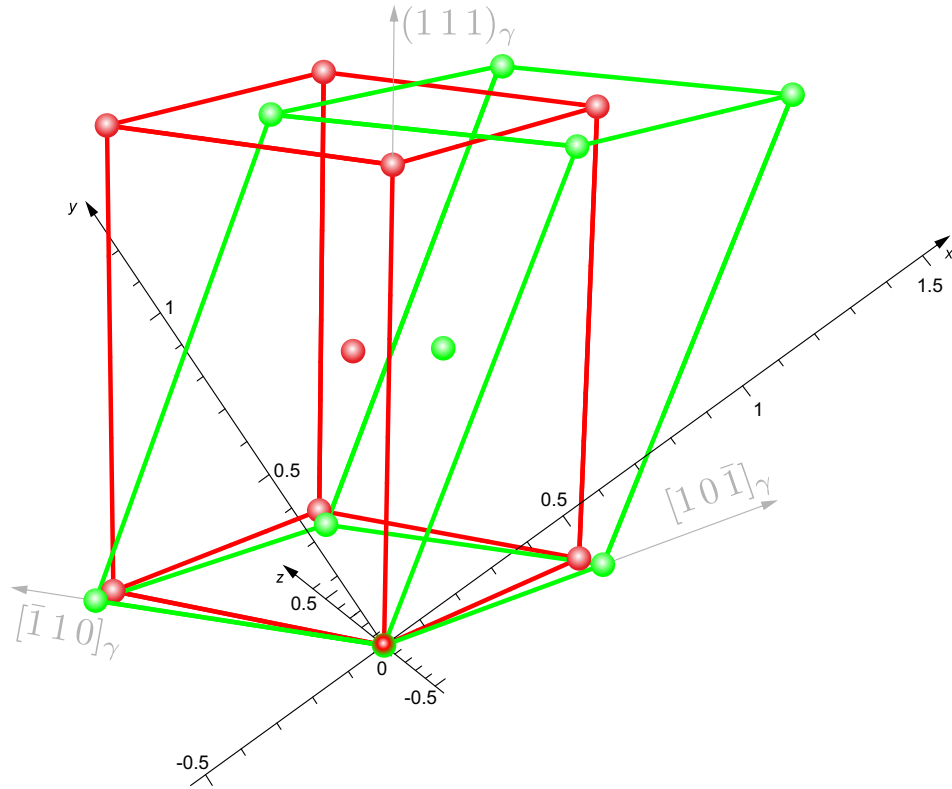


Fig. A.6. The overall transformation T_{total} applied to the non-standard fcc unit cell (in green, cf. Figure A.1) yields a non-standard bcc unit cell (in red, cf. Figure A.2) such that the close packed $(111)_\gamma$ (fcc) plane is parallel to the closest pack $(011)_\alpha$ (bcc) plane.

¹After having read Chapter 6, the reader will have realised that our construction yields the Nishiyama-Wassermann variant NW1 (cf. Table D1) and not a KS variant. In order to obtain a KS variant a further rotation about $(111)_\gamma$ is necessary (cf. Table D2). In Figure A.6, this rotation is such that it matches either the right or the left edge of the base of the green cell to either the right or the left edge of the base of the red cell - yielding either KS2 or KS3. Of course, this additional rotation does not contradict our original claim that the KS variant is just the Bain strain followed by a rotation.

The Action of the Pure Bain Strain (Figure A.7)

For comparison, Figure A.7 depicts the action of the pure Bain strain on the non-standard fcc unit cell. In particular, there is no parallelism between a close packed fcc plane and a closest packed bcc plane.

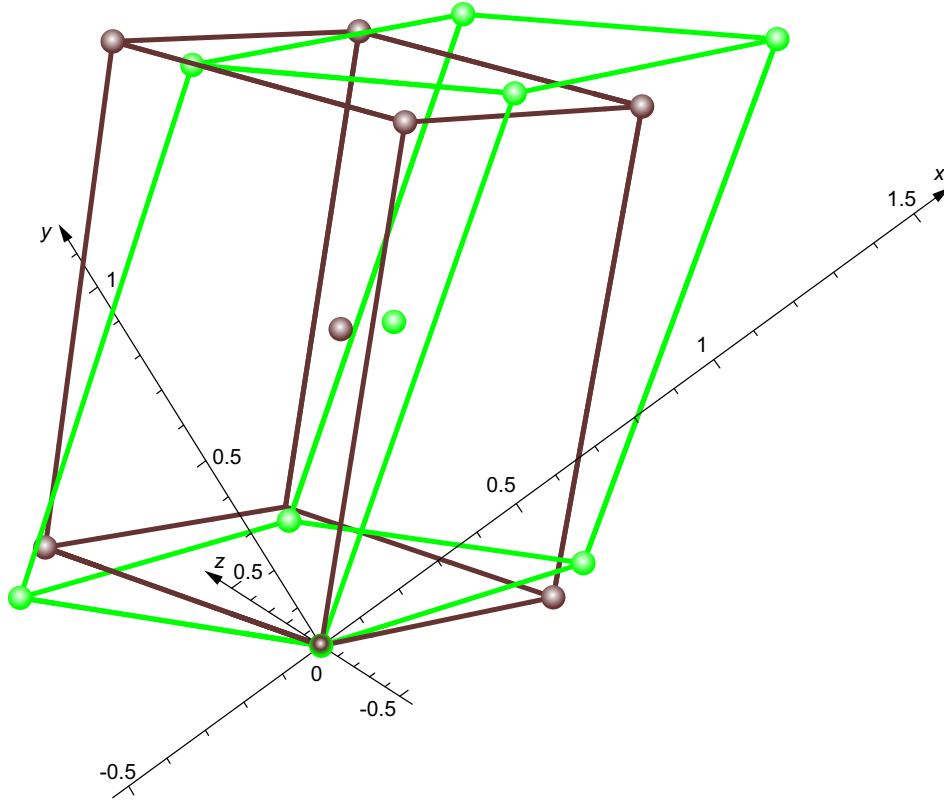


Fig. A.7. The action of the pure Bain strain $P = U_1 = \text{diag}(2^{-1/3}, 2^{1/6}, 2^{1/6})$ on the non-standard fcc unit cell (in green, cf. Figure A.1) resulting in a non-standard bcc unit cell (in brown, cf. Figure A.2).

Implementations to Determine the Optimal Lattice Transformations

B.1 Mathematica

The following Mathematica code¹ determines, for a given $k \in \mathbb{N}$, the optimal lattice transformation $H : \mathcal{L}(F) \rightarrow \mathcal{L}(G)$ within the set $\{H_\mu = G\mu F^{-1} : \mu \in \text{SL}^k(3, \mathbb{Z})\}$ for any given $F, G \in \text{GL}^+(3, \mathbb{R})$ and for any distance measure $d_r(H, \mathbb{I})$, $r > 0$. The case $r < 0$ is analogous.

For the transformation from fcc to bcc, F and G would be given by (1.10) and for the transformation from terephthalic acid I to II, F and G would be given by (1.23).

Firstly, we generate the set $\text{SL}^k(3, \mathbb{Z})$ ($=\text{SL}$):

```
SL = Select[Flatten[Table[{a, b, c, d, e, f, g, h, i},
    {a, -k, k}, {b, -k, k}, {c, -k, k}, {d, -k, k}, {e, -k, k}, {f, -k, k},
    {g, -k, k}, {h, -k, k}, {i, -k, k}], 8], Det[Partition[#, 3]] == 1 &];
```

Next we generate a list ($=\text{distlist}$) of all values of $d_r(H_\mu, \mathbb{I})$ for $\mu \in \text{SL}^k(3, \mathbb{Z})$:

```
Hmu = Function[mu, G.Partition[mu, 3].Inverse[F]];
distr = Function[mu, Norm[SingularValueList[Hmu[mu]]^r - {1, 1, 1}]];
distlist = distr/@SL;
```

¹The original .nb file can be found online under <http://solids.maths.ox.ac.uk/programs/OptLat.nb>

Then we generate a list (=poslist) of all the positions of μ 's in $SL^k(3, \mathbb{Z})$ that give rise to the minimal deformation distance:

```
poslist = Flatten[Position[distlist, RankedMin[distlist, 1]], 1];
```

Further we calculate the minimal deformation distance m_0 , the second to minimal deformation distance m_1 and return their numerical difference $\Delta = m_1 - m_0$ (=delta):

```
m0 = distlist[[poslist[[1]]]];
m1 = Sort[distlist][[Length[poslist]+1]];
delta = N[m1-m0]
```

Finally we return a list of all μ 's that give rise to an optimal deformation H_μ and a list of all optimal H_μ 's:

```
SL[[poslist]]
Hmu/@SL[[poslist]]
```

B.2 MATLAB

A Graphical User Interface (GUI) called 'OptLat' can either be found on MATLAB File Exchange² (requires MATLAB) or downloaded directly as a standalone Windows application³.

²<http://uk.mathworks.com/matlabcentral/fileexchange/55554-optlat>

³<http://solids.maths.ox.ac.uk/programs/OptLat.exe>

Remarks on Preliminary Numerical Implementations of the Three-Well Problem

We list some of the preliminary numerical results and give a more detailed explanation of the methods used.

The Mesh Method

The numerical determination of the set $\mathcal{L}$ of third order laminates was performed with the methods proposed in Chapter 3. That is, use Mallard's law twice to obtain second order laminates, calculate the correct $\mu_2 = \mu_2(\lambda_1, \lambda_2, \mu_1)$ and then use Lemma 3.11 to calculate the final rank-one connection. This third order laminate function was evaluated at its four independent parameters and each of them was sampled uniformly on $[0, 1]$. The most complex implementation was performed with a spacing of $\frac{1}{40}$ giving rise to a 40^4 mesh points in $\mathcal{L}$. In the final step, all elements from $\mathcal{P}^{24}$ that leave $(1 \ 1 \ 1)$ invariant were applied to $\mathcal{L}$ from the right and all elements were brought into upper triangular form.

The set $\mathcal{M}$ of polyconvex boundary points was calculated by defining a function

$$(a, b, d, f) \mapsto \begin{pmatrix} a & d & e(a, b, d, f) \\ 0 & b & f \\ 0 & 0 & \det(U_1)/(ab) \end{pmatrix},$$

where $e(a, b, d, f)$ is such that the polyconvex bound $A \mapsto |A(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2 \leq |U(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2$ is satisfied with equality. The range of the four parameters was chosen with the help of the remaining polyconvex bounds.¹ Finally all points that violate any of the other polyconvex conditions were deleted. All operations are elementary and thus there was no limit in the number of points that can be calculated. However, if $\mathcal{M}$ is too big the comparison with $\mathcal{L}$ becomes very time consuming.

To generate the datapoints of distances the built-in MATLAB function `pdist2` was used with the arguments `pdist2(L, m, 'chebychev', 'Smallest', 1)` within a `parfor` loop running through all elements $m \in \mathcal{M}$. Figure C.1 shows a histogram of the l^∞ -distances for $|\mathcal{M}| \approx 10^5$, $|\mathcal{L}| \approx 10^8$ and $U_1 = \text{diag}(3/4, 1, 1)$. Additional performance improvements were achieved by sorting both $\mathcal{M}$ and $\mathcal{L}$ alphabetically prior to the comparison. The run-time of this computation was 25 hours on a high-end desktop computer.

Discussion

If the conjecture was true and if $\mathcal{L}$ would contain *all* third order laminates, we would expect that the histogram is a delta function centred at 0. However, Figure C.1 shows a peak around $\text{dist}(m, \mathcal{L}) = 0.0075$. Due to the *ad hoc* nature of the implementation, this shift is only an indication that the conjecture may not be true as it stands. In particular errors due to the discreteness of the mesh have not been calculated and thus it is not clear whether this discrepancy is within the expected margin. Further possible reasons for this mismatch include rounding errors, a possibly inefficient choice of points in $\mathcal{L}$, a mesh that is generally too coarse or even the failure of capturing all third order laminates that stay on the boundary.

¹Roughly the two diagonal elements were between the maximal and minimal singular values of U_1 and the two off-diagonal elements were significantly smaller.

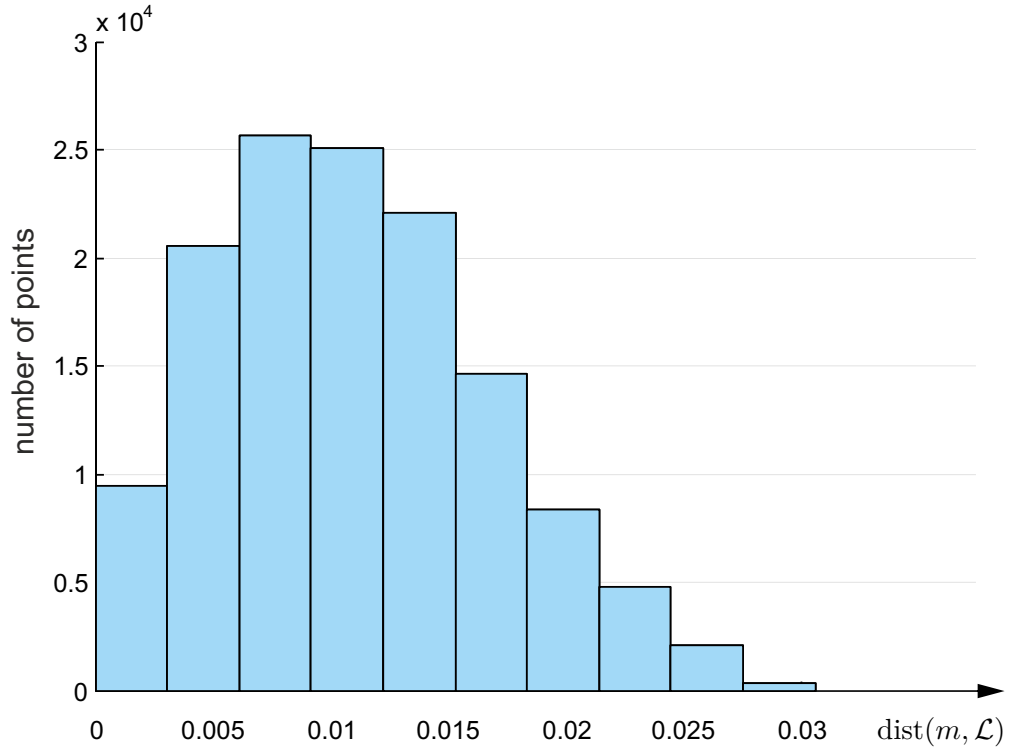


Fig. C.1. Histogram of the l^∞ -distances between points $m \in \mathcal{M}$ in the (conjectured) polyconvex boundary and the mesh of third order laminates $\mathcal{L}$. The sizes of the respective sets were $|\mathcal{M}| \approx 10^5$, $|\mathcal{L}| \approx 10^8$ and the transformation strain was assumed to be $U_1 = \text{diag}(3/4, 1, 1)$.

The Minimisation Method

A preliminary implementation of the minimisation method has been carried out in Mathematica. As for the mesh method, the approach was to construct a third order laminate function with the help of the proposed methods. Since every step is explicit, it was possible to obtain a rational function $l : \mathbb{R}^4 \rightarrow \text{GL}^+(3, \mathbb{R})$ such that $f([0, 1]^4)$ is contained in the set of third order laminates that satisfy the polyconvex bound $A \mapsto |A(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2 \leq |U(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)|^2$ with equality. However, the complexity of this rational function exceeded the capacities of Mathematica (the closed form expression was on the order of 100 printed pages) and it was not possible to carry out the minimisation.

Discussion

The construction of a rational closed form expression for the third order laminates seems too complex to carry out. It would be beneficial to perform the minimisation over a set of nested functions that return the third order laminates (e.g. the sequence of functions described in the mesh method).

General Simplifications

The following general simplifications have proven useful. Without loss of generality we can rescale $U_1 = \text{diag}(\eta_2, \eta_1, \eta_1)$ such that $U_1 = \text{diag}(l, 1, 1)$ and we can assume $l < 1$. Further, we can use the $\text{SO}(3)$ invariance from the left (cf. Lemma 3.1) and only consider for example symmetric or upper triangular matrices which are cheaper to store and better behaved numerically. The following lemma shows how, up to a rotation from the left, each element in a simple laminate can be expressed as a symmetric matrix.

Lemma C.1. *(Symmetric parametrisation of elements in ∂K_2^{qc})*

Given a simple laminate $A'(\lambda) \subset K_2^{\text{qc}}$ (particularly $A'(\lambda) \subset \partial K_2^{\text{qc}}$), we can find a re-parametrisation by a single parameter $\varphi \in [\arctan l, \arctan l^{-1}]$ such that $A(\varphi(\lambda)) \in \text{SO}(3)A'(\lambda)$ for all $\lambda \in [0, 1]$ and $A(\varphi(\lambda))$ is symmetric. It is given by

$$A(\varphi) = \begin{pmatrix} \beta(\varphi) & 0 & \pm\gamma(\varphi) \\ 0 & 1 & 0 \\ \pm\gamma(\varphi) & 0 & \alpha(\varphi) \end{pmatrix} \in \partial K_2^{\text{qc}},$$

where

$$\begin{aligned}\alpha(\varphi) &= \frac{\cos^2 \varphi (1 + l^2) + l}{\sqrt{1 + l^2} (\cos \varphi + \sin \varphi)}, \\ \beta(\varphi) &= \frac{\sin^2 \varphi (1 + l^2) + l}{\sqrt{1 + l^2} (\cos \varphi + \sin \varphi)}, \\ \gamma(\varphi) &= \frac{(1 + l^2) \cos \varphi \sin \varphi - l}{\sqrt{1 + l^2} (\cos \varphi + \sin \varphi)}.\end{aligned}$$

Further, we can avoid using trigonometric functions by substituting $q = \arctan \varphi \in [l, l^{-1}]$. In this case, we obtain

$$A(q) = \begin{pmatrix} \frac{(1+l+l^2)q^2+l}{\sqrt{1+l^2}(1+q)\sqrt{1+q^2}} & 0 & \pm \frac{l(l^{-1}-q)(q-l)}{\sqrt{1+l^2}(1+q)\sqrt{1+q^2}} \\ 0 & 1 & 0 \\ \pm \frac{l(l^{-1}-q)(q-l)}{\sqrt{1+l^2}(1+q)\sqrt{1+q^2}} & 0 & \frac{1+l^2+l(1+q^2)}{\sqrt{1+l^2}(1+q)\sqrt{1+q^2}} \end{pmatrix}.$$

Proof. Recall that by Lemma 3.5, for one of the simple laminates we have $\gamma > 0$ and

$$\begin{aligned}i. \quad f_1(A) &= (\alpha + \gamma)^2 + (\beta + \gamma)^2 = 1 + l^2 =: r^2, \\ ii. \quad \det(A) &= \alpha\beta - \gamma^2 = l.\end{aligned}$$

Thus let us set $(\alpha, \beta) := (r \cos \varphi - \gamma, r \sin \varphi - \gamma)$ so that *i.* is satisfied. Using this Ansatz in *ii.* gives

$$r^2 \cos \varphi \sin \varphi - \gamma r (\cos \varphi + \sin \varphi) + \gamma^2 - \gamma^2 = l$$

and thus

$$\gamma = \frac{r^2 \cos \varphi \sin \varphi - l}{r(\cos \varphi + \sin \varphi)} = \frac{(1 + l^2) \cos \varphi \sin \varphi - l}{2\sqrt{2}r \sin(\varphi + \pi/4)} \stackrel{!}{\geq} 0.$$

It suffices to consider $\varphi \in (-\pi/4, 3\pi/4)$, so that the denominator has positive sign.

With the substitution $\varphi = \arctan x$, the condition $\gamma > 0$ reads

$$(1 + l^2) \frac{1}{\sqrt{1 + x^2}} \frac{x}{\sqrt{1 + x^2}} - l = (1 + l^2) \frac{x}{1 + x^2} - l \geq 0$$

which is equivalent to solving $x^2 - (l^{-1} + l)x + 1 \leq 0$ and thus $x \in [l, l^{-1}]$. Hence

$$\varphi \in [\arctan l, \arctan l^{-1}].$$

The case $\gamma < 0$ can be shown analogously with f_1 replaced by f_2 . □

Overview of Orientation

Relationship Models

D.1 Nishiyama-Wassermann (NW)

The transformation T_{NW1} is uniquely defined through our unified approach (cf. Section 6.1) as the transformation that:

- leaves the normal $\mathbf{n} = (1\ 1\ 1)_\gamma$ and the direction $\mathbf{v} = [1\ 0\ \bar{1}]_\gamma$ unrotated,
- has pure stretch component U_2 .

The resulting transformation strain is

$$T_{\text{NW1}} = R_2 U_2 = R[\phi(r), [1\ 0\ \bar{1}]] U_2,$$

where $\phi(r) = \arccos\left(\frac{1+\sqrt{2}r}{\sqrt{3}\sqrt{1+r^2}}\right)$. The corresponding OR matrix is

$$O_{\text{NW1}} = R[-45^\circ, \mathbf{e}_2] R[-\phi(r), [1\ 0\ \bar{1}]]$$

which yields the OR

$$(1\ 1\ 1)_\gamma \parallel (0\ 1\ r)_{\alpha'} \text{ and } [1\ 0\ \bar{1}]_\gamma \parallel [1\ 0\ 0]_{\alpha'}.$$

The application of $\mathcal{P}^{24}$ yields the remaining eleven NW ORs (cf. Table D1). Note that, unlike Table 6.1, Table D1 takes the tetragonality of the bct lattice into account

and the bct vectors are given in a way that is consistent with the transformation strains and not only up to crystallographic equivalence.

Tab. D1. The NW orientation relationships. The corresponding transformation strain in each row is given by $T_{\text{NW}j} = R[\phi(r), P_{2j-1}[1\ 0\ \bar{1}]] U_j$.

OR ^a	fcc plane ^b	bcc plane ^c	fcc direction ^d	bcc direction ^e	Bain Variant ^f
NW1	$(1\ 1\ 1)_\gamma$	$(0\ 1\ r)_{\alpha'}$	$[1\ 0\ \bar{1}]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_2
NW2	$(1\ 1\ 1)_\gamma$	$(r\ 0\ 1)_{\alpha'}$	$[\bar{1}\ 1\ 0]_\gamma$	$[0\ 1\ 0]_{\alpha'}$	U_3
NW3	$(1\ 1\ 1)_\gamma$	$(1\ r\ 0)_{\alpha'}$	$[0\ \bar{1}\ 1]_\gamma$	$[0\ 0\ 1]_{\alpha'}$	U_1
NW4	$(\bar{1}\ 1\ 1)_\gamma$	$(\bar{r}\ 1\ 0)_{\alpha'}$	$[1\ 0\ 1]_\gamma$	$[0\ 0\ 1]_{\alpha'}$	U_2
NW5	$(\bar{1}\ 1\ 1)_\gamma$	$(0\ r\ 1)_{\alpha'}$	$[\bar{1}\ \bar{1}\ 0]_\gamma$	$[\bar{1}\ 0\ 0]_{\alpha'}$	U_3
NW6	$(\bar{1}\ 1\ 1)_\gamma$	$(\bar{1}\ 0\ r)_{\alpha'}$	$[0\ 1\ \bar{1}]_\gamma$	$[0\ 1\ 0]_{\alpha'}$	U_1
NW7	$(1\ \bar{1}\ 1)_\gamma$	$(r\ \bar{1}\ 0)_{\alpha'}$	$[\bar{1}\ 0\ 1]_\gamma$	$[0\ 0\ 1]_{\alpha'}$	U_2
NW8	$(1\ \bar{1}\ 1)_\gamma$	$(0\ \bar{r}\ 1)_{\alpha'}$	$[1\ 1\ 0]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_3
NW9	$(1\ \bar{1}\ 1)_\gamma$	$(1\ 0\ \bar{r})_{\alpha'}$	$[0\ \bar{1}\ \bar{1}]_\gamma$	$[0\ \bar{1}\ 0]_{\alpha'}$	U_1
NW10	$(1\ 1\ \bar{1})_\gamma$	$(r\ 1\ 0)_{\alpha'}$	$[\bar{1}\ 0\ \bar{1}]_\gamma$	$[0\ 0\ \bar{1}]_{\alpha'}$	U_2
NW11	$(1\ 1\ \bar{1})_\gamma$	$(0\ r\ \bar{1})_{\alpha'}$	$[1\ \bar{1}\ 0]_\gamma$	$[1\ 0\ 0]_{\alpha'}$	U_3
NW12	$(1\ 1\ \bar{1})_\gamma$	$(1\ 0\ \bar{r})_{\alpha'}$	$[0\ 1\ 1]_\gamma$	$[0\ 1\ 0]_{\alpha'}$	U_1
^a NWj ^b $P_{2j-1}(1\ 1\ 1)_\gamma$ ^c $P_{2j-1}(0\ 1\ r)_{\alpha'}$ ^d $P_{2j-1}[1\ 0\ \bar{1}]_\gamma$ ^e $P_{2j-1}(1\ 0\ 0)_{\alpha'}$ ^f $U_j = P_{2j-1}U_2P_{2j-1}^T$					

D.2 Kurdjumov-Sachs (KS)

The transformation T_{KS1} is uniquely defined through our unified approach (cf. Section 6.1) as the transformation that:

- leaves the normal $\mathbf{n} = (1\ 1\ 1)_\gamma$ and the direction $\mathbf{v} = [1\ 0\ \bar{1}]_\gamma$ unrotated,
- has pure stretch component U_3 .

The resulting transformation strain is

$$T_{\text{KS1}} = R[\theta(r), [1\ 1\ 1]] R[\phi(r), [\bar{1}\ 1\ 0]] U_3,$$

where $\theta(r) = \arccos\left(\frac{\sqrt{3}\sqrt{r^2+1}+1}{2\sqrt{r^2+2}}\right)$, The corresponding OR matrix is

$$O_{\text{KS1}} = R[45^\circ, \mathbf{e}_3] R[-\phi(r), [\bar{1}\ 1\ 0]] R[-\theta(r), [1\ 1\ 1]]$$

which yields the OR

$$(1\ 1\ 1)_\gamma \parallel (0\ r\ 1)_{\alpha'} \text{ and } [1\ 0\ \bar{1}]_\gamma \parallel [1\ 1\ \bar{r}]_{\alpha'}.$$

The application of $\mathcal{P}^{24}$ yields the remaining 23 KS ORs (cf. Table D2). Note that, unlike Table 6.2, Table D2 takes the tetragonality of the bct lattice into account and the bct vectors are given in a way that is consistent with the transformation strains and not only up to crystallographic equivalence.

Tab. D2. The KS orientation relationships. The corresponding transformation strain in each row is given by $T_{KSj} = R[\theta(r), P_j[111]] R[\phi(r), P_j[\bar{1}10]] U_j$.

OR ^a	fcc plane ^b	bcc plane ^c	fcc direction ^d	bcc direction ^e	Bain Variant ^f
KS1	$(111)_\gamma$	$(0r1)_{\alpha'}$	$[10\bar{1}]_\gamma$	$[11\bar{r}]_{\alpha'}$	U_3
KS2	$(\bar{1}\bar{1}\bar{1})_\gamma$	$(\bar{1}\bar{r}0)_{\alpha'}$	$[10\bar{1}]_\gamma$	$[r\bar{1}\bar{1}]_{\alpha'}$	U_1
KS3	$(111)_\gamma$	$(10r)_{\alpha'}$	$[\bar{1}10]_\gamma$	$[\bar{r}11]_{\alpha'}$	U_1
KS4	$(\bar{1}\bar{1}\bar{1})_\gamma$	$(0\bar{1}\bar{r})_{\alpha'}$	$[\bar{1}10]_\gamma$	$[\bar{1}r\bar{1}]_{\alpha'}$	U_2
KS5	$(111)_\gamma$	$(r10)_{\alpha'}$	$[0\bar{1}1]_\gamma$	$[1\bar{r}1]_{\alpha'}$	U_2
KS6	$(\bar{1}\bar{1}\bar{1})_\gamma$	$(\bar{r}0\bar{1})_{\alpha'}$	$[0\bar{1}1]_\gamma$	$[\bar{1}\bar{1}r]_{\alpha'}$	U_3
KS7	$(\bar{1}11)_\gamma$	$(\bar{1}r0)_{\alpha'}$	$[101]_\gamma$	$[r11]_{\alpha'}$	U_1
KS8	$(1\bar{1}\bar{1})_\gamma$	$(0\bar{r}\bar{1})_{\alpha'}$	$[101]_\gamma$	$[1\bar{1}r]_{\alpha'}$	U_3
KS9	$(\bar{1}11)_\gamma$	$(01r)_{\alpha'}$	$[\bar{1}\bar{1}0]_\gamma$	$[\bar{1}\bar{r}1]_{\alpha'}$	U_2
KS10	$(1\bar{1}\bar{1})_\gamma$	$(10\bar{r})_{\alpha'}$	$[\bar{1}\bar{1}0]_\gamma$	$[\bar{r}\bar{1}\bar{1}]_{\alpha'}$	U_1
KS11	$(\bar{1}11)_\gamma$	$(\bar{r}01)_{\alpha'}$	$[01\bar{1}]_\gamma$	$[\bar{1}1\bar{r}]_{\alpha'}$	U_3
KS12	$(1\bar{1}\bar{1})_\gamma$	$(r\bar{1}0)_{\alpha'}$	$[01\bar{1}]_\gamma$	$[1r\bar{1}]_{\alpha'}$	U_2
KS13	$(1\bar{1}1)_\gamma$	$(1\bar{r}0)_{\alpha'}$	$[\bar{1}01]_\gamma$	$[\bar{r}\bar{1}1]_{\alpha'}$	U_1
KS14	$(\bar{1}\bar{1}\bar{1})_\gamma$	$(0r\bar{1})_{\alpha'}$	$[\bar{1}01]_\gamma$	$[\bar{1}1r]_{\alpha'}$	U_3
KS15	$(1\bar{1}1)_\gamma$	$(0\bar{1}r)_{\alpha'}$	$[110]_\gamma$	$[1r1]_{\alpha'}$	U_2
KS16	$(\bar{1}\bar{1}\bar{1})_\gamma$	$(\bar{1}0r)_{\alpha'}$	$[110]_\gamma$	$[r1\bar{1}]_{\alpha'}$	U_1
KS17	$(1\bar{1}1)_\gamma$	$(r01)_{\alpha'}$	$[0\bar{1}\bar{1}]_\gamma$	$[1\bar{1}\bar{r}]_{\alpha'}$	U_3
KS18	$(\bar{1}\bar{1}\bar{1})_\gamma$	$(\bar{r}10)_{\alpha'}$	$[0\bar{1}\bar{1}]_\gamma$	$[\bar{1}\bar{r}\bar{1}]_{\alpha'}$	U_2
KS19	$(11\bar{1})_\gamma$	$(1r0)_{\alpha'}$	$[\bar{1}0\bar{1}]_\gamma$	$[\bar{r}1\bar{1}]_{\alpha'}$	U_1
KS20	$(\bar{1}\bar{1}1)_\gamma$	$(0\bar{r}1)_{\alpha'}$	$[\bar{1}0\bar{1}]_\gamma$	$[\bar{1}\bar{1}\bar{r}]_{\alpha'}$	U_3
KS21	$(11\bar{1})_\gamma$	$(01\bar{r})_{\alpha'}$	$[1\bar{1}0]_\gamma$	$[1\bar{r}\bar{1}]_{\alpha'}$	U_2
KS22	$(\bar{1}\bar{1}1)_\gamma$	$(\bar{1}0r)_{\alpha'}$	$[1\bar{1}0]_\gamma$	$[r\bar{1}1]_{\alpha'}$	U_1
KS23	$(11\bar{1})_\gamma$	$(r0\bar{1})_{\alpha'}$	$[011]_\gamma$	$[11r]_{\alpha'}$	U_3
KS24	$(\bar{1}\bar{1}1)_\gamma$	$(\bar{r}\bar{1}0)_{\alpha'}$	$[011]_\gamma$	$[\bar{1}r1]_{\alpha'}$	U_2
^a KSj ^b $P_j(111)_\gamma$ ^c $P_j(0r1)_{\alpha'}$ ^d $P_j[10\bar{1}]_\gamma$ ^e $P_j[11\bar{r}]_{\alpha'}$ ^f $U_j = P_j U_3 P_j^T$					

D.3 Pitsch (PT)

The transformation T_{P1} is uniquely defined through our unified approach (cf. Section 6.1) as the transformation that:

- leaves the normal $\mathbf{n} = (1\ 1\ 0)_\gamma$ and the direction $\mathbf{v} = [0\ 0\ 1]_\gamma$ unrotated,
- has pure stretch component U_2 .

The resulting transformation strain is

$$T_{P1} = R[\psi(r), [1\ 0\ 0]] U_2,$$

where $\psi(r) = -\arccos\left(\frac{\sqrt{2}+r}{\sqrt{2+r^2}}\right)$. The corresponding OR matrix is

$$O_{P1} = R[45^\circ, \mathbf{e}_2] R[-\psi(r), [1\ 0\ 0]]$$

which yields the OR

$$(0\ 1\ \bar{1})_\gamma \parallel (\bar{r}\ 2\ \bar{r})_{\alpha'} \text{ and } [1\ 0\ 0]_\gamma \parallel [1\ 0\ \bar{1}]_{\alpha'}$$

The application of $\mathcal{P}^{24}$ yields the remaining eleven P ORs (cf. Table D3).

Remark. O_{P1} also yields the parallelism $[0\ 1\ 1]_\gamma \parallel [1\ r\ 1]_{\alpha'}$ stated in [Pit59] (for $r = 1$).

Tab. D3. The Pitsch orientation relationships. The corresponding transformation strain in each row is given by $T_{Pj} = R[\psi(r), P_{2j-1}[1\ 0\ 0]] U_j$.

OR ^a	fcc plane ^b	bcc plane ^c	fcc direction ^d	bcc direction ^e	Bain Variant ^f
P1	$(0\ 1\ \bar{1})_\gamma$	$(\bar{r}\ 2\ \bar{r})_{\alpha'}$	$[1\ 0\ 0]_\gamma$	$[1\ 0\ \bar{1}]_{\alpha'}$	U_2
P2	$(\bar{1}\ 0\ 1)_\gamma$	$(\bar{r}\ \bar{r}\ 2)_{\alpha'}$	$[0\ 1\ 0]_\gamma$	$[\bar{1}\ 1\ 0]_{\alpha'}$	U_3
P3	$(1\ \bar{1}\ 0)_\gamma$	$(2\ \bar{r}\ \bar{r})_{\alpha'}$	$[0\ 0\ 1]_\gamma$	$[0\ \bar{1}\ 1]_{\alpha'}$	U_1
P4	$(1\ 1\ 0)_\gamma$	$(r\ 2\ \bar{r})_{\alpha'}$	$[0\ 0\ 1]_\gamma$	$[1\ 0\ 1]_{\alpha'}$	U_2
P5	$(0\ \bar{1}\ 1)_\gamma$	$(r\ \bar{r}\ 2)_{\alpha'}$	$[\bar{1}\ 0\ 0]_\gamma$	$[\bar{1}\ \bar{1}\ 0]_{\alpha'}$	U_3
P6	$(\bar{1}\ 0\ \bar{1})_\gamma$	$(\bar{2}\ \bar{r}\ \bar{r})_{\alpha'}$	$[0\ 1\ 0]_\gamma$	$[0\ 1\ \bar{1}]_{\alpha'}$	U_1
P7	$(\bar{1}\ \bar{1}\ 0)_\gamma$	$(\bar{r}\ \bar{2}\ \bar{r})_{\alpha'}$	$[0\ 0\ 1]_\gamma$	$[\bar{1}\ 0\ 1]_{\alpha'}$	U_2
P8	$(0\ 1\ 1)_\gamma$	$(\bar{r}\ r\ 2)_{\alpha'}$	$[1\ 0\ 0]_\gamma$	$[1\ 1\ 0]_{\alpha'}$	U_3
P9	$(1\ 0\ \bar{1})_\gamma$	$(2\ r\ \bar{r})_{\alpha'}$	$[0\ \bar{1}\ 0]_\gamma$	$[0\ \bar{1}\ \bar{1}]_{\alpha'}$	U_1
P10	$(\bar{1}\ 1\ 0)_\gamma$	$(\bar{r}\ 2\ r)_{\alpha'}$	$[0\ 0\ \bar{1}]_\gamma$	$[\bar{1}\ 0\ \bar{1}]_{\alpha'}$	U_2
P11	$(0\ \bar{1}\ \bar{1})_\gamma$	$(\bar{r}\ \bar{r}\ \bar{2})_{\alpha'}$	$[1\ 0\ 0]_\gamma$	$[1\ \bar{1}\ 0]_{\alpha'}$	U_3
P12	$(1\ 0\ 1)_\gamma$	$(2\ \bar{r}\ r)_{\alpha'}$	$[0\ 1\ 0]_\gamma$	$[0\ 1\ 1]_{\alpha'}$	U_1

^a P_j ^b $P_{2j-1}(0\ 1\ \bar{1})_\gamma$ ^c $P_{2j-1}(\bar{r}\ 2\ \bar{r})_{\alpha'}$ ^d $P_{2j-1}[1\ 0\ 0]_\gamma$ ^e $P_{2j-1}(1\ 0\ \bar{1})_{\alpha'}$

^f $U_j = P_{2j-1}U_2P_{2j-1}^T$

D.4 Greninger-Troiano (GT)

The transformation T_{GT1} is uniquely defined through our unified approach (cf. Section 6.1) as the transformation that:

- leaves the normal $\mathbf{n} = (1\ 1\ 1)_\gamma$ and the direction $\mathbf{v} = [\bar{5}\ 17\ \bar{1}2]_\gamma$ unrotated,
- has pure stretch component U_3 .

The resulting transformation strain is

$$T_{\text{GT1}} = R[\xi(r), [1\ 1\ 1]] R[\phi(r), [\bar{1}\ 1\ 0]] U_3,$$

where $\xi(r) = \arccos\left(\frac{7^2+17^2\sqrt{3}\sqrt{1+r^2}}{\sqrt{2}\sqrt{5^2+12^2+17^2}\sqrt{7^2+17^2+17^2r^2}}\right)$. The corresponding OR matrix is

$$O_{\text{GT1}} = R[45^\circ, \mathbf{e}_3] R[-\phi(r), [\bar{1}\ 1\ 0]] R[-\xi(r), [1\ 1\ 1]]$$

which yields the OR

$$(1\ 1\ 1)_\gamma \parallel (0\ r\ 1)_{\alpha'} \text{ and } [\bar{1}2\ \bar{5}\ 17]_\gamma \parallel [\bar{7}\ \bar{1}7\ 17r]_{\alpha'}.$$

The application of $\mathcal{P}^{24}$ yields the remaining 23 GT ORs (cf. Table D4).

Example

Let $r = 1.045$ (as in [GT49]) then $(1\ 1\ 1)_\gamma : (0\ 1\ 1)_{\alpha'} \approx 1.26^\circ$, $[1\ 1\ \bar{2}]_\gamma : [0\ 1\ \bar{1}]_{\alpha'} \approx 2.82^\circ$, $[1\ 0\ \bar{1}]_\gamma : [1\ 1\ \bar{1}]_{\alpha'} \approx 2.94^\circ$ and $[0\ \bar{1}\ 1]_\gamma : [1\ \bar{1}\ 1]_{\alpha'} \approx 7.86^\circ$.

Tab. D4. The GT orientation relationships. The corresponding transformation strain in each row is given by $T_{GTj} = R[\xi(r), P_j[1\ 1\ 1]] R[\phi(r), P_j[\bar{1}\ 1\ 0]] U_j$.

OR ^a	fcc plane ^b	bcc plane ^c	fcc direction ^d	bcc direction ^e	Bain Variant ^f
GT1	$(1\ 1\ 1)_\gamma$	$(0\ r\ 1)_{\alpha'}$	$[\bar{1}2\ \bar{5}\ 17]_\gamma$	$[\bar{7}\ \bar{1}7\ 17r]_{\alpha'}$	U_3
GT2	$(\bar{1}\ \bar{1}\ \bar{1})_\gamma$	$(\bar{1}\ \bar{r}\ 0)_{\alpha'}$	$[\bar{1}7\ 5\ 12]_\gamma$	$[17r\ 17\ 7]_{\alpha'}$	U_1
GT3	$(1\ 1\ 1)_\gamma$	$(1\ 0\ r)_{\alpha'}$	$[17\ \bar{1}2\ \bar{5}]_\gamma$	$[17r\ \bar{7}\ \bar{1}7]_{\alpha'}$	U_1
GT4	$(\bar{1}\ \bar{1}\ \bar{1})_\gamma$	$(0\ \bar{1}\ \bar{r})_{\alpha'}$	$[12\ \bar{1}7\ 5]_\gamma$	$[7\ \bar{1}7r\ 17]_{\alpha'}$	U_2
GT5	$(1\ 1\ 1)_\gamma$	$(r\ 1\ 0)_{\alpha'}$	$[\bar{5}\ 17\ 12]_\gamma$	$[\bar{1}7\ 17r\ \bar{7}]_{\alpha'}$	U_2
GT6	$(\bar{1}\ \bar{1}\ \bar{1})_\gamma$	$(\bar{r}\ 0\ \bar{1})_{\alpha'}$	$[5\ 12\ \bar{1}7]_\gamma$	$[17\ 7\ \bar{1}7r]_{\alpha'}$	U_3
GT7	$(\bar{1}\ 1\ 1)_\gamma$	$(\bar{1}\ r\ 0)_{\alpha'}$	$[\bar{1}7\ \bar{5}\ 12]_\gamma$	$[17r\ \bar{1}7\ \bar{7}]_{\alpha'}$	U_1
GT8	$(1\ \bar{1}\ \bar{1})_\gamma$	$(0\ \bar{r}\ \bar{1})_{\alpha'}$	$[\bar{1}2\ 5\ \bar{1}7]_\gamma$	$[\bar{7}\ 17\ \bar{1}7r]_{\alpha'}$	U_3
GT9	$(\bar{1}\ 1\ 1)_\gamma$	$(0\ 1\ r)_{\alpha'}$	$[12\ 17\ \bar{5}]_\gamma$	$[7\ 17r\ \bar{1}7]_{\alpha'}$	U_2
GT10	$(1\ \bar{1}\ \bar{1})_\gamma$	$(1\ 0\ \bar{r})_{\alpha'}$	$[17\ 12\ 5]_\gamma$	$[17r\ 7\ 17]_{\alpha'}$	U_1
GT11	$(\bar{1}\ 1\ 1)_\gamma$	$(\bar{r}\ 0\ 1)_{\alpha'}$	$[\bar{5}\ 12\ \bar{1}7]_\gamma$	$[17\ \bar{7}\ 17r]_{\alpha'}$	U_3
GT12	$(1\ \bar{1}\ \bar{1})_\gamma$	$(r\ \bar{1}\ 0)_{\alpha'}$	$[5\ 17\ 12]_\gamma$	$[\bar{1}7\ \bar{1}7r\ 7]_{\alpha'}$	U_2
GT13	$(1\ \bar{1}\ 1)_\gamma$	$(1\ \bar{r}\ 0)_{\alpha'}$	$[17\ 5\ \bar{1}2]_\gamma$	$[17r\ 17\ \bar{7}]_{\alpha'}$	U_1
GT14	$(\bar{1}\ 1\ \bar{1})_\gamma$	$(0\ r\ \bar{1})_{\alpha'}$	$[\bar{1}2\ \bar{5}\ \bar{1}7]_\gamma$	$[7\ \bar{1}7\ \bar{1}7r]_{\alpha'}$	U_3
GT15	$(1\ \bar{1}\ 1)_\gamma$	$(0\ \bar{1}\ r)_{\alpha'}$	$[\bar{1}2\ \bar{1}7\ 5]_\gamma$	$[\bar{7}\ \bar{1}7r\ \bar{1}7]_{\alpha'}$	U_2
GT16	$(\bar{1}\ 1\ \bar{1})_\gamma$	$(\bar{1}\ 0\ r)_{\alpha'}$	$[\bar{1}7\ \bar{1}2\ 5]_\gamma$	$[17r\ \bar{7}\ 17]_{\alpha'}$	U_1
GT17	$(1\ \bar{1}\ 1)_\gamma$	$(r\ 0\ 1)_{\alpha'}$	$[\bar{5}\ 12\ 17]_\gamma$	$[\bar{1}7\ 7\ 17r]_{\alpha'}$	U_3
GT18	$(\bar{1}\ 1\ \bar{1})_\gamma$	$(\bar{r}\ 1\ 0)_{\alpha'}$	$[5\ 17\ 12]_\gamma$	$[17\ 17r\ 7]_{\alpha'}$	U_2
GT19	$(1\ 1\ \bar{1})_\gamma$	$(1\ r\ 0)_{\alpha'}$	$[17\ \bar{5}\ 12]_\gamma$	$[17r\ \bar{1}7\ 7]_{\alpha'}$	U_1
GT20	$(\bar{1}\ \bar{1}\ 1)_\gamma$	$(0\ \bar{r}\ 1)_{\alpha'}$	$[\bar{1}2\ 5\ 17]_\gamma$	$[7\ 17\ 17r]_{\alpha'}$	U_3
GT21	$(1\ 1\ \bar{1})_\gamma$	$(0\ 1\ \bar{r})_{\alpha'}$	$[\bar{1}2\ 17\ 5]_\gamma$	$[\bar{7}\ 17r\ 17]_{\alpha'}$	U_2
GT22	$(\bar{1}\ \bar{1}\ 1)_\gamma$	$(\bar{1}\ 0\ r)_{\alpha'}$	$[\bar{1}7\ 12\ 5]_\gamma$	$[17r\ 7\ \bar{1}7]_{\alpha'}$	U_1
GT23	$(1\ 1\ \bar{1})_\gamma$	$(r\ 0\ \bar{1})_{\alpha'}$	$[\bar{5}\ \bar{1}2\ \bar{1}7]_\gamma$	$[\bar{1}7\ \bar{7}\ \bar{1}7r]_{\alpha'}$	U_3
GT24	$(\bar{1}\ \bar{1}\ 1)_\gamma$	$(\bar{r}\ \bar{1}\ 0)_{\alpha'}$	$[5\ \bar{1}7\ \bar{1}2]_\gamma$	$[17\ \bar{1}7r\ \bar{7}]_{\alpha'}$	U_2
^a GT _j	^b $P_j(1\ 1\ 1)_\gamma$	^c $P_j(0\ r\ 1)_{\alpha'}$	^d $P_j[\bar{1}2\ \bar{5}\ 17]_\gamma$	^e $P_j[\bar{7}\ \bar{1}7\ \bar{1}7r]_{\alpha'}$	^f $U_j = P_j U_3 P_j^T$

D.5 Inverse Greninger-Troiano (GT')

The transformation $T_{GT'1}$ is uniquely defined through our unified approach (cf. Section 6.1) as the transformation that:

- leaves the normal $\mathbf{n} = (\bar{1}\bar{7}\bar{7}17)_\gamma$ and the direction $\mathbf{v} = [101]_\gamma$ unrotated,
- has pure stretch component U_3 .

The resulting transformation strain is

$$T_{GT'1} = R[\iota(r), [101]] R[-\psi(r), [010]] U_3 = R[\iota(r), [101]] R_{P2} U_3$$

where $\iota(r) = \arccos\left(\frac{17^2\sqrt{2}\sqrt{2+r^2}+7^2r}{\sqrt{17^2+17^2+7^2}\sqrt{2\cdot 17^2+7^2r^2+17^2r^2}}\right)$. The corresponding OR matrix is

$$O_{GT'1} = R[45^\circ, [001]] R[\psi(r), [010]] R[-\iota(r), [101]]$$

which yields the OR

$$(\bar{1}\bar{7}\bar{7}17)_\gamma \parallel (\bar{5}r\bar{12}r17)_{\alpha'} \text{ and } [101]_\gamma \parallel [11r]_{\alpha'}.$$

The application of $\mathcal{P}^{24}$ yields the remaining 23 GT' ORs (cf. Table D5).

Tab. D5. The GT' orientation relationships. The corresponding transformation strain in each row is given by $T_{GT'j} = R[\nu(r), P_j[1\ 0\ 1]] R[-\psi(r), P_j[0\ 1\ 0]] U_j$.

OR ^a	fcc plane ^b	bcc plane ^c	fcc direction ^d	bcc direction ^e	Bain Variant ^f
GT'1	$(\bar{1}\bar{7}\ \bar{7}\ 17)_\gamma$	$(\bar{5}r\ \bar{1}2r\ 17)_{\alpha'}$	$[1\ 0\ 1]_\gamma$	$[1\ 1\ r]_{\alpha'}$	U_3
GT'2	$(\bar{1}\bar{7}\ 7\ 17)_\gamma$	$(\bar{1}\bar{7}\ 12r\ 5r)_{\alpha'}$	$[\bar{1}\ 0\ \bar{1}]_\gamma$	$[\bar{r}\ \bar{1}\ \bar{1}]_{\alpha'}$	U_1
GT'3	$(17\ \bar{1}\bar{7}\ \bar{7})_\gamma$	$(17\ \bar{5}r\ \bar{1}2r)_{\alpha'}$	$[1\ 1\ 0]_\gamma$	$[r\ 1\ 1]_{\alpha'}$	U_1
GT'4	$(17\ \bar{1}\bar{7}\ 7)_\gamma$	$(5\ \bar{1}7r\ 12r)_{\alpha'}$	$[\bar{1}\ \bar{1}\ 0]_\gamma$	$[\bar{1}\ \bar{r}\ \bar{1}]_{\alpha'}$	U_2
GT'5	$(\bar{7}\ 17\ \bar{1}\bar{7})_\gamma$	$(\bar{1}2r\ 17\ 5r)_{\alpha'}$	$[0\ 1\ 1]_\gamma$	$[1\ r\ 1]_{\alpha'}$	U_2
GT'6	$(7\ 17\ \bar{1}\bar{7})_\gamma$	$(12r\ 5r\ \bar{1}\bar{7})_{\alpha'}$	$[0\ \bar{1}\ \bar{1}]_\gamma$	$[\bar{1}\ \bar{1}\ \bar{r}]_{\alpha'}$	U_3
GT'7	$(\bar{1}\bar{7}\ \bar{7}\ \bar{1}\bar{7})_\gamma$	$(\bar{1}\bar{7}\ \bar{1}2r\ 5r)_{\alpha'}$	$[\bar{1}\ 0\ 1]_\gamma$	$[\bar{r}\ 1\ 1]_{\alpha'}$	U_1
GT'8	$(\bar{1}\bar{7}\ 7\ \bar{1}\bar{7})_\gamma$	$(5r\ 12r\ \bar{1}\bar{7})_{\alpha'}$	$[1\ 0\ \bar{1}]_\gamma$	$[1\ \bar{1}\ r]_{\alpha'}$	U_3
GT'9	$(17\ 17\ \bar{7})_\gamma$	$(5r\ 17\ \bar{1}2r)_{\alpha'}$	$[\bar{1}\ 1\ 0]_\gamma$	$[\bar{1}\ r\ 1]_{\alpha'}$	U_2
GT'10	$(17\ 17\ 7)_\gamma$	$(17\ 5r\ 12r)_{\alpha'}$	$[1\ \bar{1}\ 0]_\gamma$	$[r\ \bar{1}\ \bar{1}]_{\alpha'}$	U_1
GT'11	$(\bar{7}\ \bar{1}\bar{7}\ 17)_\gamma$	$(12r\ 5r\ 17)_{\alpha'}$	$[0\ 1\ 1]_\gamma$	$[\bar{1}\ 1\ r]_{\alpha'}$	U_3
GT'12	$(\bar{7}\ \bar{1}\bar{7}\ 17)_\gamma$	$(\bar{1}2r\ \bar{1}\bar{7}\ 5r)_{\alpha'}$	$[0\ \bar{1}\ \bar{1}]_\gamma$	$[1\ \bar{r}\ \bar{1}]_{\alpha'}$	U_2
GT'13	$(17\ 7\ \bar{1}\bar{7})_\gamma$	$(17\ 12r\ 5r)_{\alpha'}$	$[1\ 0\ 1]_\gamma$	$[r\ \bar{1}\ 1]_{\alpha'}$	U_1
GT'14	$(17\ \bar{7}\ \bar{1}\bar{7})_\gamma$	$(5r\ \bar{1}2r\ \bar{1}\bar{7})_{\alpha'}$	$[\bar{1}\ 0\ \bar{1}]_\gamma$	$[\bar{1}\ 1\ \bar{r}]_{\alpha'}$	U_3
GT'15	$(\bar{1}\bar{7}\ \bar{1}\bar{7}\ \bar{7})_\gamma$	$(5r\ \bar{1}\bar{7}\ \bar{1}2r)_{\alpha'}$	$[1\ \bar{1}\ 0]_\gamma$	$[1\ \bar{r}\ 1]_{\alpha'}$	U_2
GT'16	$(\bar{1}\bar{7}\ \bar{1}\bar{7}\ 7)_\gamma$	$(\bar{1}\bar{7}\ 5r\ 12r)_{\alpha'}$	$[\bar{1}\ 1\ 0]_\gamma$	$[\bar{r}\ 1\ \bar{1}]_{\alpha'}$	U_1
GT'17	$(\bar{7}\ 17\ 17)_\gamma$	$(\bar{1}2r\ 5r\ 17)_{\alpha'}$	$[0\ \bar{1}\ 1]_\gamma$	$[1\ \bar{1}\ r]_{\alpha'}$	U_3
GT'18	$(7\ 17\ 17)_\gamma$	$(12r\ 17\ 5r)_{\alpha'}$	$[0\ 1\ \bar{1}]_\gamma$	$[\bar{1}\ r\ \bar{1}]_{\alpha'}$	U_2
GT'19	$(17\ \bar{7}\ 17)_\gamma$	$(17\ \bar{1}2r\ 5r)_{\alpha'}$	$[\bar{1}\ 0\ 1]_\gamma$	$[r\ 1\ \bar{1}]_{\alpha'}$	U_1
GT'20	$(17\ 7\ 17)_\gamma$	$(5r\ 12r\ 17)_{\alpha'}$	$[1\ 0\ \bar{1}]_\gamma$	$[\bar{1}\ \bar{1}\ r]_{\alpha'}$	U_3
GT'21	$(\bar{1}\bar{7}\ 17\ 7)_\gamma$	$(5r\ 17\ 12r)_{\alpha'}$	$[\bar{1}\ \bar{1}\ 0]_\gamma$	$[1\ r\ \bar{1}]_{\alpha'}$	U_2
GT'22	$(\bar{1}\bar{7}\ 17\ \bar{7})_\gamma$	$(\bar{1}\bar{7}\ 5r\ \bar{1}2r)_{\alpha'}$	$[1\ 1\ 0]_\gamma$	$[\bar{r}\ \bar{1}\ 1]_{\alpha'}$	U_1
GT'23	$(\bar{7}\ \bar{1}\bar{7}\ \bar{1}\bar{7})_\gamma$	$(\bar{1}2r\ 5r\ \bar{1}\bar{7})_{\alpha'}$	$[0\ \bar{1}\ 1]_\gamma$	$[1\ 1\ \bar{r}]_{\alpha'}$	U_3
GT'24	$(7\ \bar{1}\bar{7}\ \bar{1}\bar{7})_\gamma$	$(12r\ \bar{1}\bar{7}\ 5r)_{\alpha'}$	$[0\ 1\ \bar{1}]_\gamma$	$[\bar{1}\ \bar{1}\ 1]_{\alpha'}$	U_2
^a GT' $_j$	^b $P_j(\bar{1}\bar{7}\ \bar{7}\ 17)_\gamma$	^c $P_j(\bar{5}r\ \bar{1}2r\ 17)_{\alpha'}$	^d $P_j[1\ 0\ 1]_\gamma$	^e $P_j[1\ 1\ r]_{\alpha'}$	^f $U_j = P_j U_3 P_j^T$

Analytical Dependence of Volume Fractions for Double Laminates

Let F^α with $\alpha \in \{1, 2\}$ denote the two distinct double laminates corresponding to the Type I and Type II solutions of Mallard's law (Lemma 2.4) applied to a simple laminate, i.e. macroscopically

$$F^\alpha = U_1 + \lambda \mathbf{a} \otimes \mathbf{n} + \mu \mathbf{b}_\lambda^\alpha \otimes \mathbf{m}_\lambda^\alpha,$$

where $U_1 = \text{diag}(\eta_2, \eta_1, \eta_1)$ and $U_1 + \lambda \mathbf{a} \otimes \mathbf{n}$ is the macroscopic deformation gradient of a simple laminate. Then, in order to have an interface between a double laminate and austenite (i.e. $\nu_2(F^\alpha) = 1$), the dependence $\mu^\alpha(\lambda)$ is as follows.

For $\alpha = 1$ (Type I)

$$\mu^1(\lambda) = \frac{1}{2} \pm \frac{\sqrt{\alpha_4 \lambda^4 + \alpha_3 \lambda^3 + \alpha_2 \lambda^2 + \alpha_1 \lambda + \alpha_0}}{2(\lambda - 1)(\eta_2^2 - \eta_1^2) \sqrt{\beta_2 \lambda^2 + \beta_1 \lambda + \beta_0}}$$

where

$$\begin{aligned}
\alpha_4 &= (3 - \eta_1^2) (\eta_2 - \eta_1)^4 (\eta_2 + \eta_1)^4 \\
\alpha_3 &= -2 (2\eta_1^4 - 5\eta_1^2 + \eta_2^2) (\eta_2 - \eta_1)^3 (\eta_2 + \eta_1)^3 \\
\alpha_2 &= 2 (\eta_1^6 \eta_2^2 + \eta_1^4 \eta_2^4 - 3\eta_1^6 - 5\eta_1^4 \eta_2^2 - 4\eta_1^2 \eta_2^4 + 7\eta_1^4 + 3\eta_1^2 \eta_2^2 + 2\eta_2^4 - \eta_1^2 - \eta_2^2) \\
&\quad \times (\eta_2 - \eta_1)^2 (\eta_2 + \eta_1)^2 \\
\alpha_1 &= 2 (\eta_1^2 + \eta_2^2) (2\eta_1^6 \eta_2^2 - 2\eta_1^6 - 6\eta_1^4 \eta_2^2 + 2\eta_1^2 \eta_2^4 + 5\eta_1^4 + 2\eta_1^2 \eta_2^2 - \eta_2^4 - 2\eta_1^2) \\
&\quad \times (\eta_2 - \eta_1) (\eta_2 + \eta_1) \\
\alpha_0 &= (\eta_1 - 1) (\eta_1 + 1) (\eta_1^2 + \eta_2^2)^2 (2 - \eta_1^2 - \eta_2^2) (\eta_1^2 - 2\eta_1^2 \eta_2^2 + \eta_2^2) \\
\beta_2 &= (3\eta_1^2 - 1) (\eta_2 - \eta_1)^2 (\eta_2 + \eta_1)^2 \\
\beta_1 &= 2\eta_1^2 (\eta_2 - \eta_1) (\eta_2 + \eta_1) (\eta_1^2 + \eta_2^2) \\
\beta_0 &= (\eta_1 - 1) (\eta_1 + 1) (\eta_1^2 + \eta_2^2)^2.
\end{aligned}$$

For $\alpha = 2$ (Type II)

$$\mu^2(\lambda) = \frac{1}{2} \pm \frac{\sqrt{\alpha_4 \lambda^4 + \alpha_3 \lambda^3 + \alpha_2 \lambda^2 + \alpha_1 \lambda + \alpha_0}}{2(\lambda - 1)(\eta_2^2 - \eta_1^2) \sqrt{\beta_2 \lambda^2 + \beta_1 \lambda + \beta_0}},$$

where

$$\begin{aligned}
\alpha_4 &= -(3\eta_1^2 - 1) (\eta_1 - \eta_2)^4 (\eta_2 + \eta_1)^4 \\
\alpha_3 &= 2 (\eta_1^4 - 5\eta_2^2 \eta_1^2 + 2\eta_2^2) (\eta_1 - \eta_2)^3 (\eta_2 + \eta_1)^3 \\
\alpha_2 &= 2 (\eta_2^2 \eta_1^6 + \eta_2^4 \eta_1^4 - 2\eta_1^6 - 3\eta_2^2 \eta_1^4 - 7\eta_2^4 \eta_1^2 + 4\eta_1^4 + 5\eta_2^2 \eta_1^2 + 3\eta_2^4 - \eta_1^2 - \eta_2^2) (\eta_1 - \eta_2)^2 (\eta_2 + \eta_1)^2 \\
\alpha_1 &= 2 (\eta_1^2 + \eta_2^2) (\eta_1 - \eta_2) (\eta_2 + \eta_1) (2\eta_2^4 \eta_1^4 + \eta_1^6 - 2\eta_2^2 \eta_1^4 - 5\eta_2^4 \eta_1^2 - 2\eta_1^4 + 6\eta_2^2 \eta_1^2 + 2\eta_2^4 - 2\eta_2^2) \\
\alpha_0 &= (\eta_1 - 1) (\eta_1 + 1) (\eta_1^2 + \eta_2^2)^2 (2 - \eta_1^2 - \eta_2^2) (\eta_1^2 - 2\eta_2^2 \eta_1^2 + \eta_2^2) \\
\beta_2 &= (\eta_1^2 - 3) (\eta_1 - \eta_2)^2 (\eta_2 + \eta_1)^2 \\
\beta_1 &= -2 (\eta_1 - \eta_2) (\eta_2 + \eta_1) (\eta_1^2 + \eta_2^2) \\
\beta_0 &= (\eta_1 - 1) (\eta_1 + 1) (\eta_1^2 + \eta_2^2)^2.
\end{aligned}$$

The Group $\mathcal{P}^{24}$

The elements of $\mathcal{P}^{24}$ in the standard Euclidean basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are given by

$$\begin{aligned}
 P_1 = \mathbf{1} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & P_2 = R[180^\circ, \mathbf{e}_1 - \mathbf{e}_3] &= \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \\
 P_3 = R[120^\circ, \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, & P_4 = R[180^\circ, \mathbf{e}_2 - \mathbf{e}_3] &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \\
 P_5 = R[-120^\circ, \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, & P_6 = R[180^\circ, \mathbf{e}_1 - \mathbf{e}_2] &= \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\
 P_7 = R[-90^\circ, \mathbf{e}_2] &= \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & P_8 = R[180^\circ, \mathbf{e}_1] &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\
 P_9 = R[180^\circ, \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, & P_{10} = R[-120^\circ, \mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \\
 P_{11} = R[90^\circ, \mathbf{e}_3] &= \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & P_{12} = R[120^\circ, \mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3] &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}, \\
 P_{13} = R[180^\circ, \mathbf{e}_1 + \mathbf{e}_3] &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & P_{14} = R[180^\circ, \mathbf{e}_2] &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\
 P_{15} = R[90^\circ, \mathbf{e}_1] &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, & P_{16} = R[-120^\circ, \mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3] &= \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \\
 P_{17} = R[-90^\circ, \mathbf{e}_3] &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & P_{18} = R[120^\circ, -\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}, \\
 P_{19} = R[90^\circ, \mathbf{e}_2] &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, & P_{20} = R[180^\circ, \mathbf{e}_3] &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
 P_{21} = R[-90^\circ, \mathbf{e}_1] &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, & P_{22} = R[-120^\circ, -\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \\
 P_{23} = R[180^\circ, \mathbf{e}_1 + \mathbf{e}_2] &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, & P_{24} = R[120^\circ, \mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3] &= \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}.
 \end{aligned}$$

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For the convenience of the reader all references (excluding books) can be found under tinyurl.com/ThesisRef2016.

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Colophon

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