On $V_{II}$ junctions: non stress-free junctions between martensitic plates

FRANCESCO DELLA PORTA*

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Abstract

The analytical understanding of microstructures arising in martensitic phase transitions relies usually on the study of stress-free interfaces between different variants of martensite. However, in the literature there are experimental observations of non stress-free junctions between martensitic plates, where the compatibility theory fails to be predictive. In this work, we focus on $V_{II}$ junctions, which are non stress-free interfaces between different martensitic variants experimentally observed in Ti$_{74}$Nb$_{23}$Al$_3$. We first motivate the formation of some non stress-free junctions by studying the boundary conditions for the two well problem. We then give a mathematical characterisation of $V_{II}$ junctions involving the theory of elasto-plasticity, and show that for deformation gradients as in Ti$_{74}$Nb$_{23}$Al$_3$ our characterisation can predict experimental results. Furthermore, we are able to prove that $V_{II}$ junctions are strict weak local minimisers of a simplified energy functional for martensitic transformations in the context of elasto-plasticity.

1 Introduction

Martensitic phase transitions are abrupt changes occurring in the crystalline structure of certain alloys or ceramics when the temperature is moved across a critical threshold. The high temperature phase is called austenite or parent phase, and usually enjoys cubic symmetry, while the low temperature phase is called martensite, and has lower symmetry (e.g., tetragonal, orthorhombic, monoclinic [12]). For this reason, martensite has usually more variants, which are symmetry related, and which in experiments often appear finely mixed. Martensitic phase transitions are important because they are the physical motivation of shape memory, the ability of certain materials to recover on heat deformations which are apparently plastic.

*Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany. francesco.dellaporta@mis.mpg.de

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After the seminal work of Ball and James [4] modelling martensitic phase transitions in the context of nonlinear elasticity (see Section 2), a vast literature has been developed to study energy minimisers, and energy minimising sequences representing microstructures, that is finely mixed martensitic variants, with zero energy (see e.g., [6,12,24] and references therein). A key tool to understand and predict martensico microstructures is the Hadamard jump condition (see e.g., [4, Prop. 1]) stating that if a continuous function $y$ is such that

$$\nabla y(x) = F_1 \quad \text{a.e. in } \{x \cdot m < 0\}, \quad \text{and} \quad \nabla y(x) = F_2 \quad \text{a.e. in } \{x \cdot m > 0\},$$

for some unit vector $m \in S^2$ and two matrices $F_1, F_2 \in \mathbb{R}^{3 \times 3}$, then

$$F_1 - F_2 = b \otimes m, \quad \text{for some } b \in \mathbb{R}^3.$$  \hspace{1cm} (1.1)

This condition imposes some necessary compatibility between two martensitic variants, or between two average martensitic deformation gradients representing different homogeneous microstructures, in order to have stress-free junctions. If (1.1) holds, then we say that $F_1, F_2$ are compatible across the plane $\{x \cdot m = 0\}$. Compatibility is a key ingredient not only to understand microstructures (see e.g., [4,12]) but also to understand hysteresis of the phase transformation [31] and recently to construct materials undergoing ultra-reversible phase transformations [14,30]. Nonetheless, in the literature experiments are reported where the above compatibility is not observed right off the phase interface, and where the phase junctions are not stress free. More precisely, martensite is elastically or plastically deformed to achieve compatibility between variants/phases. For example, in Figure 1a we show the situation of $V_I$ junctions observed in a cubic to orthorhombic transformation in Ti$_{74}$Nb$_{23}$Al$_3$ [22]. We have two different deformation gradients $F_1, F_2 \in \mathbb{R}^{3 \times 3}$ corresponding to two different martensitic variants, and the identity matrix $I$, deformation gradient in the austenite region. In the case of $V_I$ junctions we have

$$\text{rank}(F_1 - F_2) = 1, \quad \text{rank}(F_1 - I) > 1, \quad \text{rank}(F_2 - I) > 1,$$

and therefore the interfaces between austenite and martensite are not stress-free close to the junction between $F_1$ with $F_2$. Similarly, in the case of $V_{II}$ junctions (see Figure 1b), also observed in Ti$_{74}$Nb$_{23}$Al$_3$ [22], we have

$$\text{rank}(F_1 - F_2) > 1, \quad \text{rank}(F_1 - I) = 1, \quad \text{rank}(F_2 - I) = 1,$$  \hspace{1cm} (1.2)

and therefore $F_1$ and $F_2$ are not compatible. In Figure 1c we show an incompatible junction between the two average deformation gradients $F_1, F_2 \in \mathbb{R}^{3 \times 3}$ representing the average of the martensitic microstructures on the left and on the right of the red line [9,13]. In this case, as for the $V_{II}$ junctions, (1.2) holds. Non stress-free phase interfaces have also been observed in the X–interface configuration (Figure 1d) for which we refer the reader to [10,29].

The following approach to measure the incompatibility between non-stress free junctions has been proposed in [9]. Assuming that $F_1, F_2 \in \mathbb{R}^{3 \times 3}$ are such that $\text{rank}(F_1 - F_2) > 1$, and that
Figure 1: Examples of non stress free junctions (in red in the picture) experimentally observed in martensitic transformations: 1a–1b show respectively a $V_I$ and a $V_{II}$ junction, observed for example in [22, 23, 25]. The case 1c is a generalisation of $V_{II}$ junctions, where instead of two single variants of martensite we have two martensitic laminates, both compatible on average with austenite but not with each other (see [9, 13]). In Figure 1d an example of an X–interface, experimentally observed in [10], and studied in [29]. In Figure 1a and in Figure 1b, at the non stress-free junctions (red lines in the pictures) defects are observed in experiments.
\( F_2^{-T} F_2^T F_1 F_2^{-1} \) has middle eigenvalue one. \([4, \text{Prop. 4}]\) guarantees the existence of two rotations \( R_1, R_2 \in SO(3) \) such that \( \text{rank}(F_i - R_i F_2) = 1 \) for \( i = 1, 2 \). The incompatibility of \( F_1, F_2 \) can hence be measured by taking the minimum between the rotation angle of \( R_1 \), and the rotation angle of \( R_2 \). This is in agreement with the experimental results in \([9, 22]\) where the observed non stress-free junctions are the ones where \( \min\{\text{angle}(R_1), \text{angle}(R_2)\} \) is small. Another way to measure how far three deformations gradient, say \( F_1, F_2, I \) are to form a triple junction, that is to be all pairwise rank one connected, can be found in \([18]\). However, in the case for example of \( Ti_{74}Nb_{23}Al_3 \) \([22]\) these approaches do not allow to predict when two martensitic variants will form a \( V_I \) or a \( V_{II} \) junction. Indeed, experiments show that some martensitic variants strongly prefer to form \( V_I \) junctions, while others prefer \( V_{II} \) junctions.

The aim of this work is to study \( V_{II} \) junctions and their stability in the context of elasto-plasticity. The paper is organised as follows: in Section \( 2 \) we recall the nonlinear elasticity theory for martensitic phase transitions, and we introduce a simplified energy functional \( I \) to describe the physical phenomenon when plastic shears occur. This energy functional is nonetheless very general as it includes all possible martensitic variants and all possible slip systems for body centred cubic austenite (as in \( Ti_{74}Nb_{23}Al_3 \)). In Section \( 3 \) we give a partial explanation of why we observe non stress-free junctions of \( V_{II} \) type or like the ones in Figure \( 1c \). Our explanation is the following: these type of junctions usually form when two different plates of martensite, with deformation gradients \( F_1, F_2 \), nucleate at different points in the domain, and expand until they meet (see Figure \( 2a \) and Figure \( 2b \)). We hence consider a bounded domain \( \Omega \subset \mathbb{R}^3 \) as in Figure \( 3 \) and we prove that, under some further geometric hypotheses which are verified by the non stress-free junctions in \( Ti_{74}Nb_{23}Al_3 \) \([22]\) and in \( Ni_{65}Al_{35} \) \([9]\), there exists a one-to-one map \( y \in W^{1,\infty}(\Omega; \mathbb{R}^3) \) satisfying

\[
\begin{cases}
\nabla y(x) \in (SO(3)U_1 \cup SO(3)U_2)^{qc}, & \text{a.e. } x \in \Omega, \\
y(x) = F_1 x, & \text{on } \Gamma_1, \\
y(x) = F_2 x, & \text{on } \Gamma_2,
\end{cases}
\tag{1.3}
\]

with \( F_1, F_2 \in (SO(3)U_1 \cup SO(3)U_2)^{qc} \) if and only if \( \text{rank}(F_1 - F_2) \leq 1 \). Therefore, no stress-free microstructure built with the two martensitic variants \( U_1, U_2 \in \mathbb{R}^{3\times3}_{\text{Sym}} \) can fill the domain \( \Omega \) and match the previously nucleated plates \( F_1, F_2 \). In Section \( 4 \) we study when two simple shears \( S_1, S_2 \in \mathbb{R}^{3\times3} \) are such that

\[
\text{rank}(F_1 S_1 - F_2 S_2) \leq 1, \tag{1.4}
\]

given \( F_1, F_2 \) with \( \text{rank}(F_1 - F_2) = 2 \). In Section \( 5 \) we give a mathematical characterisation of \( V_{II} \) junctions as junctions reflecting \( (1.2) \), where the compatibility between \( F_1, F_2 \) is achieved thanks to single slips (and hence thanks to plastic effects), and which are strict weak local minimisers for the simplified energy \( I \) introduced in Section \( 2 \). In Section \( 6 \) we study the possibility to form \( V_{II} \) junctions in a one parameter family of deformation gradients, which approximates well the deformation gradient in \( Ti_{74}Nb_{23}Al_3 \). The obtained results are discussed at the end of the section, and seem to be in good agreement with experimental observations. Finally, in Section \( 7 \) we give some concluding remarks and possible directions to extend the present work.
Figure 2: Formation of $V_{II}$ junctions in Ti$_{74}$Nb$_{23}$Al$_3$ and of non stress-free junctions in Ni$_{65}$Al$_{35}$, respectively represented in Figure 2a and Figure 2b. In the former, it is experimentally observed that two different plates of martensite $F_1, F_2$ nucleate in an austenite domain and propagate until they meet. When the thickness of the two martensite plates increases, a $V_{II}$ junction is formed. In the latter, two different laminates of martensite nucleate at two different points of the sample and expand until they coalesce. Further expansion leads to a non stress-free junction. In both cases the average deformation gradient in the martensite regions is very close to be rank one connected to the identity matrix, coherently with the moving mask approximation in [16]. In the pictures, the arrows represent the directions of expansion of the phase boundaries.

Figure 3: Representation of $\Omega, \Gamma_1$ and $\Gamma_2$ as defined in (3.7) (on the left), and their projection on the plane spanned by $n_1, n_2$ (on the right).
2 A model for martensitic transformations with plastic shears

The most successful mathematical theory to describe martensitic phase transitions at a continuum level is the nonlinear elasticity theory, first introduced in [4], and successfully used to understand laminates and other microstructures (see [4,12]), as much as the shape-memory effect (see [11]), and, more recently, hysteresis (see [31]).

In the nonlinear elasticity model, changes in the crystal lattice are interpreted as elastic deformations in the continuum mechanics framework, and legitimised by the Cauchy-Born hypothesis. The deformations minimize hence a free energy

\[ E(y, \theta) = \int_\Omega W_e(\nabla y(x), \theta) \, dx. \]  

(2.5)

Here, \( \theta \) denotes the temperature of the crystal, the domain (open and connected) \( \Omega \) stands for the region occupied by a single crystal in the undistorted defect-free austenite phase at the transition temperature \( \theta = \theta_T \), while \( y(x) \) denotes the position of the particle \( x \in \Omega \) after the deformation of the lattice has occurred. By \( W_e \) we denote the free-energy density, depending on the temperature \( \theta \) and the deformation gradient \( \nabla y \). The behaviour of \( W_e \) on \( \theta \) must reflect the phase transition, that is when \( \theta < \theta_T \) and \( \theta > \theta_T \), the energy is respectively minimised by martensite and austenite. At \( \theta = \theta_T \) all phases are energetically equivalent.

Below, we assume \( \theta < \theta_T \) to be fixed, and we consider \( W_e \) to be defined by (omitting for ease of notation the dependence on \( \theta \))

\[ W_e(F) = \begin{cases} 
0, & \text{if } F \in \bigcup_{i=1}^N SO(3) U_i, \\
+\infty, & \text{otherwise,}
\end{cases} \]

where \( U_i = U_i(\theta) \in \mathbb{R}^{3 \times 3}_{\text{Sym}^+} \) are the \( N \) positive definite symmetric matrices corresponding to the transformation from austenite to the \( N \) variants of martensite at temperature \( \theta \). Here and below \( \mathbb{R}^{3 \times 3}_{\text{Sym}^+} \) represents the set of \( 3 \times 3 \) symmetric and positive definite matrices. We remark that \( N = \#P_a \#P_m \), where \( P_a, P_m \) are respectively the point groups of austenite and of martensite, and where we denoted by \# their cardinality. For each \( U_i, U_j \) there exists \( R \in P_a \) such that \( R^T U_j R = U_i \), so that \( U_i, U_j \) share the same eigenvalues. We remark that this energy satisfies frame indifference. That is, for all \( F \in \mathbb{R}^{3 \times 3} \) and all rotations \( R \in SO(3) \), \( W_e(RF) = W_e(F) \), reflecting the invariance of the free-energy density under rotations. Furthermore, \( W_e \) respects lattice symmetries, i.e., \( W_e(FQ) = W_e(F) \) for all \( F \in \mathbb{R}^{3 \times 3} \) and all rotations \( Q \in P_a \). Such a \( W_e \) has been already considered for example in [3,4,7,17] and corresponds to the physical situation where the elastic constants are infinity, which, as remarked in [3], is usually a reasonable approximation when studying martensitic phase transitions with no external (or at least small) load. Considering \( W_e \) to be \(+\infty\) out of the energy wells is also known as elastically rigid approximation, and is often used in the context of elasto-plasticity since elastic effects in metals are usually much smaller than plastic ones (see e.g., [26]).
We now want to keep in account the presence of plastic effects in the nonlinear elasticity model. Following [27] and references therein, we use the multiplicative decomposition of the deformation gradient
\[ \nabla y = F^e F^p, \]
where \( F^e, F^p \) respectively represent the elastic and the plastic component of the deformation gradient. The former describes the part of the deformation gradient which is reversible, while the latter captures the irreversible deformations given by the slip of atoms along planes. In solid crystals, atoms can slip just in particular directions on particular planes. For this reason, \( F^p \) must be of the form
\[ F^p = 1 + s \phi \otimes \psi \]
where \( s \in \mathbb{R}, \phi \in \mathbb{R}^3, \psi \in \mathcal{S}, \phi \cdot \psi = 0, \) and \( \phi \otimes \psi \in \mathcal{S} \subset \mathbb{R}^{3 \times 3}. \) Here, \( \phi \) is called slip direction and \( \psi \) is called the slip plane, while \( s \) is the amount of shear. The set \( \mathcal{S} \) is the set of all possible slip systems. For body centred cubic austenite, which is the case of Ti\(_{74}\)Nb\(_{23}\)Al\(_3\), there are six planes of type \( \{1,1,0\} \) each with two orthogonal \( \langle \bar{1}, 1, 1 \rangle \) \( \langle \bar{1}, 1, -1 \rangle \) directions, twenty-four planes \( \{1,2,3\} \) and twelve planes \( \{1,1,2\} \) each with one orthogonal \( \langle \bar{1}, 1, 1 \rangle \) direction.

Following the approach of [2, 15, 19] and references therein, we adopt the time discrete variational approach to elasto-plasticity [26], restricting ourselves to the first time step where most of the plastic events take place. We further assume cross hardening [2], which means that activity in one slip system suppresses the activity in all other slip systems at the same point. For this reason, we choose a plastic energy density \( W^p \) of the type
\[ W^p := \begin{cases} f(|s|), & \text{if } F^p = 1 + s \phi \otimes \psi, \text{ and } \phi \otimes \psi \in \mathcal{S}, \\ +\infty, & \text{otherwise}, \end{cases} \]
where \( f: [0, \infty) \to [0, \infty) \) is assumed to be continuous, strictly monotone and to satisfy \( f(0) = 0. \) Here, as for \( W^e, W^p \) could be finite and continuous. This approximation however simplifies the analytical study of the energy and allows to neglect any dependence of the results on the shape of the energy density out of its minima. We are now ready introduce an elasto-plastic energy density \( W \) defined as
\[ W(F) := \min \{ W^e(F^e) + W^p(F^p) : F^e F^p = F \}, \]
and an energy functional \( I \) for the system
\[ I(y, \Omega) = \int_{\Omega} W(\nabla y) \, dx. \quad (2.6) \]
We remark that the energy \( I \) is not quasiconvex and in general minimisers do not exist.

### 3 A rigidity result for the two well problem

In this section, we study the resolvability of Problem (1.3). As explained in the introduction, this gives a way to justify the formation of non stress-free junctions between martensitic plates.
Let \( n_1, n_2 \in S^2 \), \( n_1 \times n_2 \neq 0 \) and let us set \( n_\perp := \frac{n_1 \times n_2}{|n_1 \times n_2|} \). For \( R > 0 \), we define (see Figure 3)

\[
\Omega := \{ x \in \mathbb{R}^3 : \min\{ x \cdot n_1, x \cdot n_2 \} < 0, x \cdot n_\perp \in (0, 1) \text{ and } |x - n_\perp (n_\perp \cdot x)| < R \},
\]

\[
\Gamma_1 := \{ x \in \partial \Omega : x \cdot n_1 = 0 \text{ and } x \cdot n_2 > 0 \},
\]

\[
\Gamma_2 := \{ x \in \partial \Omega : x \cdot n_2 = 0 \text{ and } x \cdot n_1 > 0 \}.
\]

(3.7)

We can prove the following theorem:

**Theorem 3.1.** Let \( U_1, U_2 \in \mathbb{R}^{3\times 3} \) such that there exist \( \hat{e} \in S^2 \) satisfying

\[
U_1 = (2\hat{e} \otimes \hat{e} - 1)U_2(2\hat{e} \otimes \hat{e} - 1).
\]

(3.8)

Suppose further that \( u_* := \hat{e} \times U_1^T \hat{e} \) is such that \( u_* \times n_\perp \neq 0 \). Then there exist \( y \in W^{1,\infty}(\Omega; \mathbb{R}^3) \) such that \( y \) is \( 1 - 1 \) in \( \Omega \),

\[
\nabla y(x) \in K^{qc} := (SO(3) U_1 \cup SO(3) U_2)^{qc}, \quad \text{a.e. } x \in \Omega,
\]

and

\[
y(x) = \begin{cases} F_1 x, & \text{on } \Gamma_1, \\ F_2 x, & \text{on } \Gamma_2, \end{cases}
\]

for some \( F_1, F_2 \in K^{qc} \), if and only if there exist \( d \in \mathbb{R}^3 \) such that

\[
F_1 - F_2 = d \otimes (u_* \times n_\perp).
\]

(3.10)

**Proof. Necessity.** We first notice that \( \Omega \) is Lipschitz, and therefore by Morrey’s imbeddings \( y \in C^{0,1}(\Omega; \mathbb{R}^3) \) (see e.g., [1]). Therefore, \( y \) is continuous on the line \( n_\perp \), that is

\[
(F_1 - F_2)n_\perp = 0.
\]

(3.11)

Now, given (3.8), [14, Prop. 12] guarantees the existence of \( R \in SO(3), b \in \mathbb{R}^3, m \in S^2 \) such that

\[
RU_2 = U_1 + b \otimes m.
\]

(3.12)

Without loss of generality, we can take from standard twinning theory (see e.g., [12]) \( m = \hat{e}, b = 2\left( \frac{U_1^{-1} \hat{e}}{|U_1^{-1} \hat{e}|} - U_1 \hat{e} \right) \). The same results can be achieved by taking the only other solution of (3.12), that is \( b = U_1 \hat{e}, m = 2\left( \hat{e} - \frac{U_1 \hat{e}}{|U_1 \hat{e}|} \right) \). Following the strategy of [6], let us define the orthonormal system of coordinates

\[
u_1 := \frac{U_1^{-1} m}{|U_1^{-1} m|}, \quad u_3 := \frac{b}{|b|}, \quad u_2 := u_3 \times u_1,
\]

and let

\[
L := U_1^{-1} (1 - \delta u_3 \otimes u_1), \quad \delta \frac{1}{2} |U_1^{-1} m||b|.
\]

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Therefore, setting \(z(x) := y(Lx)\) the problem becomes equivalent to finding a \(1-1\) map \(z \in W^{1,\infty}(L^{-1} \Omega; \mathbb{R}^3)\) such that

\[
\nabla z(x) \in (SO(3)S^- \cup SO(3)S^+)^c, \quad \text{a.e. } x \in \Omega^L,
\]

with \(S^\pm = 1 \pm \delta u_3 \otimes u_1\), and

\[
z(x) = \begin{cases}
F_1 Lx, & \text{for every } x \in \Gamma_1^L, \\
F_2 Lx, & \text{for every } x \in \Gamma_2^L.
\end{cases}
\]

Here,

\[
\Omega^L := \{x \in \mathbb{R}^3 : Lx \in \Omega\}, \quad \Gamma_1^L := \{x \in \mathbb{R}^3 : Lx \in \Gamma_1\}, \quad \Gamma_2^L := \{x \in \mathbb{R}^3 : Lx \in \Gamma_2\}.
\]

Following [6], we can characterise the set \(K_L := (SO(3)S^- \cup SO(3)S^+)^c\) as

\[
K_L = \left\{ F \in \mathbb{R}^{3 \times 3} \left| \begin{array}{l}
F^T F = \alpha u_1 \otimes u_1 + u_2 \otimes u_2 + \gamma u_3 \otimes u_3 + \beta u_2 \otimes u_3, \\
0 < \alpha \leq 1 + \delta^2, 0 < \gamma \leq 1, \alpha \gamma - \beta^2 = 1
\end{array} \right. \right\},
\]

and where we denoted \(u_1 \otimes u_3 = u_1 \otimes u_3 + u_3 \otimes u_1\). Let us now define

\[
s_i := x \cdot u_i, \quad \alpha_i = L^T n_1 \cdot u_i, \quad \beta_i = L^T n_2 \cdot u_i,
\]

and remark that [5] together with the definition of \(K_L\) yield

\[
z = Q \begin{bmatrix} z_1(s_1, s_3) \\ s_2 \\ z_3(s_1, s_3) \end{bmatrix},
\]

for some Lipschitz scalar functions \(z_1, z_2\). Assume now that \(\alpha_i \neq 0\) for \(i = 1, 2, 3\), the other cases can be treated similarly to deduce (3.17) below. In this case

\[
u_2^T Q^T z = s_2 = u_2^T Q^T F_1 L \left( s_1 u_1 + s_2 u_2 - \frac{u_3}{\alpha_3} (\alpha_1 s_1 + \alpha_2 s_2) \right),
\]

for every

\[
(s_1, s_2) \in \{(t_1, t_2) \in \mathbb{R}^2 : t_1 = u_1 \cdot x, t_2 = u_2 \cdot x, x \in \Gamma_1^L\}\]

Therefore, varying \(s_1\) and \(s_3\) in an open interval we deduce that

\[
u_2^T Q^T F_1 L \left( u_1 - u_3 \frac{\alpha_1}{\alpha_3} \right) = 0,
\]

\[
u_2^T Q^T F_1 L \left( u_2 - u_3 \frac{\alpha_2}{\alpha_3} \right) = 1.
\]

There exist hence \(\lambda \in \mathbb{R}\) such that

\[
(L^T F_1^T Q - 1) u_2 = -\frac{\lambda}{\alpha_2} (\alpha_2 u_1 - \alpha_1 u_2) \times (\alpha_2 u_3 - \alpha_3 u_2) = \lambda L^T n_1,
\]
that is
\[ Q\mathbf{u}_2 = F_1^T L^{-T}(\mathbf{u}_2 + \lambda L^T \mathbf{n}_1). \] (3.17)

Taking the norm on both sides, we deduce that \( \lambda \) must satisfy
\[ 1 = |F_1^T L^{-T} \mathbf{u}_2|^2 + \lambda^2 |F_1^T \mathbf{n}_1|^2 + 2\lambda (L^{-1} F_1^T L^{-T} \mathbf{u}_2) \cdot L^T \mathbf{n}_1. \] (3.18)
We notice that \( F_1 \in K^{qc} \) implies that \( F_1 L \in K_L \) and hence \( L^T F_1^T F_1 L \mathbf{u}_2 = \mathbf{u}_2 \). This yields
\[ (L^T F_1^T F_1 L)^{-1} \mathbf{u}_2 = L^{-1} F_1^T L^{-T} \mathbf{u}_2 = \mathbf{u}_2. \]

Therefore, (3.18) simplifies to
\[ 0 = \lambda^2 |F_1^T \mathbf{n}_1|^2 + 2\beta_2 \lambda, \]
that is \( \lambda = 0 \) or \( \lambda = -\frac{2\beta_2}{|F_1^T \mathbf{n}_1|^2} \). In the same way, we can show that
\[ Q\mathbf{u}_2 = F_2^T L^{-T}(\mathbf{u}_2 + \mu L^T \mathbf{n}_2), \] (3.19)
with \( \mu = 0 \) or \( \mu = -\frac{2\beta_2}{|F_2^T \mathbf{n}_2|^2} \). We now claim that, even if \( \alpha_2, \beta_2 \neq 0 \), the only possible solution is \( \lambda = \mu = 0 \). Indeed, let \( \alpha_2 \neq 0 \) (the case \( \beta_2 \neq 0 \) can be treated similarly), and let us notice that
\[ z_1(s_1, s_3) = u_1 Q^T F_1 L \left( s_1 u_1 + s_3 u_3 - \frac{u_2}{\alpha_2} (\alpha_1 s_1 + \alpha_3 s_3) \right), \]
\[ z_3(s_1, s_3) = u_3 Q^T F_1 L \left( s_1 u_1 + s_3 u_3 - \frac{u_2}{\alpha_2} (\alpha_1 s_1 + \alpha_3 s_3) \right), \]
for every \( s_1, s_3 \) as in (3.16). As a consequence, \( z_1, z_3 \) are linear on the boundary, and hence are linear on the set
\[ \Omega_1 := \left\{ \mathbf{x} \in \mathbb{R}^3 : \mathbf{x} \cdot L^T \mathbf{n}_1 \leq 0, \frac{((L \mathbf{n}_1 \times L \mathbf{n}_2) \times \mathbf{u}_2) \cdot \mathbf{x}}{\text{sign} \alpha_2} \leq 0 \right\}. \]
This is the subset of \( \Omega_L \) where the boundary condition is propagated along the characteristic lines in direction \( \mathbf{u}_2 \). Therefore, given (3.13), we deduce the existence of \( G \in K_L \) such that \( z(\mathbf{x}) = G \mathbf{x} \) in \( \Omega_1 \). A version of the Hadamard jump condition (see e.g., [4, Prop. 1]) yields
\[ G - F_1 L = c \otimes L^T \mathbf{n}_1, \] (3.20)
for some \( c \in \mathbb{R}^3 \). The fact that \( G \in K_L \) together with (3.15) imply
\[ Q^T G \mathbf{u}_2 = \mathbf{u}_2. \]
Exploiting (3.17) and (3.20) we deduce
\[ F_1^{-T} L^{-T}(\mathbf{u}_2 + \lambda L^T \mathbf{n}_1) = F_1 L \mathbf{u}_2 + \alpha_2 c. \] (3.21)
Now, polar decomposition implies $F_1 L = R_1 V_1$, for some $R_1 \in SO(3)$, $V_1 \in \mathbb{R}^{3 \times 3}_{\text{sym}+}$. As $F_1 L \in K_L$ we also have $V_1 u_2 = u_2$ and $V_1^{-1} u_2 = u_2$, as much as $(F_1 L)^{-T} u_2 = R_1 u_2$. Thus, (3.21) becomes

$$c = \frac{\lambda}{\alpha_2} F_1^{-T} n_1.$$  

(3.22)

At the same time, the fact that $G, F_1 L \in K_L$ implies that $\det G = \det(F_1 L) = 1$. But (3.20) entails,

$$\det G = \det(F_1 L)(1 + L^{-1} F_1^{-1} c \cdot L^T n_1) = \det(F_1 L) \left(1 + \frac{\lambda}{\alpha_2} |F_1^{-T} n_1|^2\right),$$

which implies that $\lambda = 0$. The same argument can be applied to prove $\mu = 0$. Therefore, (3.17) and (3.19) simplify to

$$Qu_2 = F_1^{-T} L^{-T} u_2 = R_1 u_2 = F_1 L u_2, \quad \text{and} \quad Qu_2 = F_2^{-T} L^{-T} u_2 = R_2 u_2 = F_2 L u_2$$

from which we deduce

$$(F_1 - F_2) L u_2 = 0.$$  

(3.23)

Here $R_2 \in SO(3)$ is given by the polar decomposition of $F_2 L$, and is such that $F_2 L = R_2 V_2$ for some $V_2 \in \mathbb{R}^{3 \times 3}_{\text{sym}+}$. Now, as $u_s \parallel L u_2$, the hypothesis that $u_s \times n_\perp \neq 0$ implies that $u_2$ and $n_\perp$ are linearly independent. As a consequence, (3.11) and (3.23) imply

$$\text{rank}(F_1 - F_2) \leq 1,$$

and (3.10). Sufficiency. Let us define

$$z(x) = \begin{cases} F_1 L x, & \text{in } \Omega_1, \\ F_2 L x, & \text{in } \Omega \setminus \Omega_1. \end{cases}$$

It is easy to check that $z$ satisfies (3.13)–(3.14), proving the statement. \hfill \square

Remark 3.1. Let $F_1, F_2$ be the deformation gradients measured experimentally in Ti$_{74}$Nb$_{23}$Al$_3$ or in Ni$_{63}$Al$_{35}$. By (1.2) we have $F_1 = 1 + b_1 \otimes m_1$, $F_2 = 1 + b_2 \otimes m_2$ for some $b_1, b_2 \in \mathbb{R}^3$ and $m_1, m_2 \in S^2$ such that $\text{rank}(F_1 - F_2) = 2$. Taking $n_1 = m_1$ and $n_2 = m_2$ we have that $u_s \times n_\perp \neq 0$ is verified, and therefore Theorem 3.1 implies that no stress-free junction involving just two martensitic variants can be observed.

Remark 3.2. The result is independent of the shape of $\partial \Omega \setminus (\Gamma_1 \cup \Gamma_2)$.

Remark 3.3. By [14, Prop. 12], (3.8) is equivalent to the existence of $R \in SO(3), b, m \in \mathbb{R}^3$ satisfying (3.12). If (3.8) fails, then, under some further physically relevant restrictions on the parameters of $U_1, U_2$, [27] implies that $K = K^{qc}$, and that $y$ is affine.

Remark 3.4. A similar result holds if we replace $\Omega$ with

$$\Omega' := \{ x \in \mathbb{R}^3 : x \in \Omega^\circ, \, x \cdot n_\perp \in (0, 1) \text{ and } |x - n_\perp (n_\perp \cdot x)| < R \} \setminus \overline{\Omega},$$

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Figure 4: Representation of the domain considered in Remark 3.4. This domain corresponds to the formation of incompatible junctions as in Figure 2b.

for which we refer to Figure 4. In this case, however, necessary and sufficient conditions are (3.10) and, if $d \neq 0$,

$$(u_\ast \cdot n_1)(u_\ast \cdot n_2) \geq 0.$$  

This latter condition is to guarantee that the information carried by the characteristic lines in direction $u_\ast$ from the boundary conditions do not overlap.

**Remark 3.5.** In general, the statement of Theorem 3.1 does not hold when $u_\ast \times n_\perp = 0$. Consider for example

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

for some $\eta_1, \eta_2 > 0$. Let further $F_1 = U_1$, $F_2 = U_2$. Let further

$$e_1 := [100]^T, \quad e_2 := [010]^T, \quad e_3 := [001]^T,$$

and

$$b_1 = \frac{\sqrt{2}(\eta_1 - \eta_2)}{\eta_1 + \eta_2}(-\eta_1 e_1 + \eta_2 e_2), \quad b_2 = \frac{\sqrt{\eta_1^2 + \eta_2^2}(\eta_1 - \eta_2)}{\eta_1 + \eta_2}(e_1 + e_2),$$

$$m_1 = \frac{1}{\sqrt{2}}(e_1 + e_2), \quad m_2 = \frac{1}{\sqrt{\eta_1^2 + \eta_2^2}}(\eta_2 e_1 - \eta_1 e_2).$$

We choose $n_1, n_2 \in \mathbb{S}^2$ such that

$$n_1 \cdot e_3 = n_2 \cdot e_3 = 0, \quad (e_2 - e_1) \cdot n_1 \leq 0, \quad (\eta_2 e_1 - \eta_1 e_2) \cdot n_2 \leq 0,$$

so that the situation becomes fully two-dimensional (cf. Figure 5). Indeed, $u_\ast = n_\perp = e_3$. Then, we can construct $y \in W^{1,\infty}(\Omega; \mathbb{R}^3)$ as

$$y(x) = \begin{cases} F_1 x, & \text{if } x \cdot m_1 \leq 0, \\ (F_1 + b_1 \otimes m_1)x, & \text{if } 0 < x \cdot m_1, 0 < x \cdot m_2, \\ F_2 x, & \text{if } x \cdot m_1 \leq 0, \end{cases}$$

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where continuity is guaranteed by the fact that $F_1 + b_1 \otimes m_1 - F_2 = b_2 \otimes m_2$. In this case, following [20], $\nabla y \in K^{qc}$ if and only if $B := F_1 + b_1 \otimes m_1$ satisfies
$$\det B = \det U_1, \quad |B(e_1 \pm e_2)|^2 \leq \eta_1^2 + \eta_2^2.$$ It can be checked that both the first and the second property are satisfied for every $\eta_1, \eta_2 > 0$. Therefore, if $u_\ast \times n = 0$, (3.10) can fail.

4 Plastic junctions

In this section we want to investigate when, given two matrices $F_1, F_2 \in \mathbb{R}^{3 \times 3}$, with $\text{rank}(F_1 - F_2) = 2$, there exist two simple shears $S_i = 1 + s_i \phi_i \otimes \psi_i, \phi_i \otimes \psi_i \in S, i = 1, 2$, such that $\text{rank}(F_1 S_1 - F_2 S_2) \leq 1$. These results are useful for the mathematical characterisation of $V_{II}$ junctions given in the next section. Here and below, we denote by $S$ the set of admissible slip systems (or a suitable subset of it), and by $M$ the set of martensitic variants $\bigcup_{i=1}^N U_i$ (or a suitable subset of it).

Under our hypotheses on $F_1, F_2$, there exist $b_1, b_2 \in \mathbb{R}^3$ and $m_1, m_2 \in S^2$ such that
$$F_2 = F_1 + b_1 \otimes m_1 + b_2 \otimes m_2.$$ Therefore, our problem becomes equivalent to find $\phi_1 \otimes \psi_1, \phi_2 \otimes \psi_2 \in S$ and $s_1, s_2 \in \mathbb{R}$ such that
$$\text{rank}(s_1 F_1 \phi_1 \otimes \psi_1 - b_1 \otimes m_1 - b_2 \otimes m_2 - s_2 F_2 \phi_2 \otimes \psi_2) \leq 1. \quad (4.24)$$ The following proposition gives necessary conditions for the existence of solutions to (4.24):

**Lemma 4.1.** Let $a_1, a_2, \phi_1, \phi_2, n_1, n_2, \psi_1, \psi_2 \in \mathbb{R}^3$ and $\text{rank}(a_1 \otimes n_1 - a_2 \otimes n_2) = 2$. Then, necessary condition for the existence of $s_1, s_2 \in \mathbb{R}$ such that
$$\text{rank}(a_1 \otimes n_1 - a_2 \otimes n_2 + s_1 \phi_1 \otimes \psi_1 - s_2 \phi_2 \otimes \psi_2) \leq 1 \quad (4.25)$$
is that at least one of the following four conditions hold:

\[
\begin{align*}
\phi_1 \cdot (a_1 \times a_2) &= \phi_2 \cdot (a_1 \times a_2) = 0, & \phi_1 \cdot (a_1 \times a_2) &= \psi_1 \cdot (n_1 \times n_2) = 0, \\
\phi_2 \cdot (a_1 \times a_2) &= \psi_2 \cdot (n_1 \times n_2) = 0, & \psi_1 \cdot (n_1 \times n_2) &= \psi_2 \cdot (n_1 \times n_2) = 0.
\end{align*}
\]

**Proof.** Since \(\text{cof}(F) = 0\) if and only if \(\text{rank}(F) \leq 1\), (4.25) is equivalent to

\[
0 = -(a_1 \times a_2) \otimes (n_1 \times n_2) + s_1(a_1 \times \phi_1) \otimes (n_1 \times \psi_1)
- s_2(a_1 \times \phi_2) \otimes (n_1 \times \psi_2) - s_1(a_2 \times \phi_1) \otimes (n_2 \times \psi_1)
+ s_2(a_2 \times \phi_2) \otimes (n_2 \times \psi_2) - s_1 s_2(\phi_1 \times \phi_2) \otimes (\psi_1 \times \psi_2).
\]

(4.26)

Taking now the scalar product of (4.26) with \(\phi_1 \otimes \psi_2\) and \(\phi_2 \otimes \psi_1\) we respectively obtain

\[
[(a_1 \times a_2) \cdot \phi_1][ (n_1 \times n_2) \cdot \psi_2] = 0, & [(a_1 \times a_2) \cdot \phi_2][ (n_1 \times n_2) \cdot \psi_1] = 0.
\]

(4.27)

Recalling that \(\text{rank}(a_1 \otimes n_1 - a_2 \otimes n_2) = 2\) implies that \(a_1 \times a_2 \neq 0\) and \(n_1 \times n_2 \neq 0\), from (4.27) we deduce the claim. \(\square\)

In general, the necessary conditions provided by Lemma 4.1 are not sufficient. In other cases, infinitely solutions \(s_1, s_2\) may exist given two slip systems \(\phi_1 \otimes \psi_1, \phi_2 \otimes \psi_2 \in S\). In Proposition 4.1 we prove that, under certain hypotheses on the shear systems which are relevant in the following section, there exists a unique couple \((s_1, s_2)\) such that (4.25) is satisfied.

**Proposition 4.1.** Let \(a_1, a_2, \phi_1, \phi_2, n_1, n_2, \psi_1, \psi_2 \in \mathbb{R}^3\). Suppose further that \(\text{rank}(a_1 \otimes n_1 - a_2 \otimes n_2) = 2\). Then,

- if \(\psi_1 = \alpha_1 n_1 + \alpha_2 n_2, \psi_2 = \beta_1 n_1 + \beta_2 n_2\) for some \(\alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{R}\), and if \((\alpha_2 a_1 + \alpha_1 a_2) \cdot (\phi_1 \times \phi_2), (\beta_2 a_1 + \beta_1 a_2) \cdot (\phi_1 \times \phi_2) \neq 0\), then \(s_1, s_2 \in \mathbb{R}\) are such that (4.25) is satisfied if and only if they satisfy

\[
\begin{align*}
(a_1 \times a_2) \cdot \phi_2 &= s_1(\alpha_2 a_1 + \alpha_1 a_2) \cdot (\phi_1 \times \phi_2), \\
(a_1 \times a_2) \cdot \phi_1 &= s_2(\beta_2 a_1 + \beta_1 a_2) \cdot (\phi_1 \times \phi_2);
\end{align*}
\]

(4.28)

- if \(\phi_1 = \gamma_1 a_1 + \gamma_2 a_2, \phi_2 = \delta_1 a_1 + \delta_2 a_2\) for some \(\gamma_1, \gamma_2, \delta_1, \delta_2 \in \mathbb{R}\), and if \((\gamma_2 n_1 + \gamma_1 n_2) \cdot (\psi_1 \times \psi_2), (\delta_2 n_1 + \delta_1 n_2) \cdot (\psi_1 \times \psi_2) \neq 0\), then \(s_1, s_2 \in \mathbb{R}\) are such that (4.25) is satisfied if and only if they satisfy

\[
\begin{align*}
(n_1 \times n_2) \cdot \psi_2 &= s_1(\gamma_2 n_1 + \gamma_1 n_2) \cdot (\psi_1 \times \psi_2), \\
(n_1 \times n_2) \cdot \psi_1 &= s_2(\delta_2 n_1 + \delta_1 n_2) \cdot (\psi_1 \times \psi_2).
\end{align*}
\]

(4.29)

- if \(\phi_1 = \gamma_1 a_1 + \gamma_2 a_2, \phi_2 = \delta_1 a_1 + \delta_2 a_2\) and \(\psi_1 = \alpha_1 n_1 + \alpha_2 n_2, \psi_2 = \beta_1 n_1 + \beta_2 n_2\) for some \(\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1, \gamma_2, \delta_1, \delta_2 \in \mathbb{R}\), then \(s_1, s_2 \in \mathbb{R}\) are such that (4.25) is satisfied if and only if they satisfy

\[
|a_1 \times a_2| = s_1(\alpha_2 \gamma_2 - \alpha_1 \gamma_1) - s_2(\beta_2 \delta_2 - \beta_1 \delta_1) - s_1 s_2(\alpha_1 \beta_2 - \alpha_2 \beta_1)(\gamma_1 \delta_2 - \gamma_2 \delta_1).
\]

(4.30)

In particular, there may be a one parameter family of solutions.
Proof. We just prove the first case, as the second case can be proved in a similar way, and the third is a direct consequence of (4.31) below. Assuming \( \psi_1 = \alpha_1 n_1 + \alpha_2 n_2 \) and \( \psi_2 = \beta_1 n_1 + \beta_2 n_2 \), solving (4.26) is equivalent to solve

\[
0 = -a_1 \times a_2 + s_1 (\alpha_2 a_1 + \alpha_1 a_2) \times \phi_1 - s_2 (\beta_2 a_1 + \beta_1 a_2) \times \phi_2 - s_1 s_2 (\alpha_1 \beta_2 - \alpha_2 \beta_1) \phi_1 \times \phi_2. \tag{4.31}
\]

By testing this equation by \( \phi_1 \) and \( \phi_2 \) we obtain the necessity of (4.28). Now, let us show that, under our assumptions, (4.28) are also sufficient conditions. In order to do this, it is sufficient to show that, for \( s_1, s_2 \) as in (4.28), the equality in (4.31) tested with \( \rho \), for some \( \rho \in \mathbb{R}^3 \) such that \( \rho \cdot (\phi_1 \times \phi_2) \neq 0 \), holds. Under our assumptions, at least one out of \( a_1 \cdot (\phi_1 \times \phi_2) \neq 0 \) and \( a_2 \cdot (\phi_1 \times \phi_2) \neq 0 \) holds. Suppose without loss of generality the first one, as the other case can be deduced similarly. We can thus multiply

\[
-a_1 \times a_2 + s_1 (\alpha_2 a_1 + \alpha_1 a_2) \times \phi_1 - s_2 (\beta_2 a_1 + \beta_1 a_2) \times \phi_2 - s_1 s_2 (\alpha_1 \beta_2 - \alpha_2 \beta_1) \phi_1 \times \phi_2
\]

by \( a_1 [ (\alpha_2 a_1 + \alpha_1 a_2) \cdot (\phi_1 \times \phi_2) ] [ (\beta_2 a_1 + \beta_1 a_2) \cdot (\phi_1 \times \phi_2) ] \) and deduce that the resulting number is zero, which concludes the proof of the first statement.

The results above motivate Definition 4.1 below.

**Definition 4.1.** Let \( R_1, R_2 \in SO(3) \) and \( V_1, V_2 \in M \) such that \( \text{rank}(R_1 V_1 - R_2 V_2) = 2 \). Let also \( \bar{t}_1, \bar{t}_2 \in \mathbb{R} \setminus \{0\} \) and \( \phi_1 \otimes \psi_1, \phi_2 \otimes \psi_2 \in S \) be such that

\[
F_i(t) = R_i V_i \left( 1 + s \phi_i \otimes \psi_i \right)
\]

satisfies

\[
F_1(\bar{t}_1) - F_2(\bar{t}_2) = \hat{b} \otimes m,
\]

for some \( \hat{b} \in \mathbb{R}^3, m \in S^2 \). Then, we say that \( F_1 \) and \( F_2 \) form a plastic junction at \((\bar{t}_1, \bar{t}_2)\) for \( R_1 V_1, R_2 V_2 \).

We say that the plastic junction formed by \( F_1 \) and \( F_2 \) at \((\bar{t}_1, \bar{t}_2)\) is locally rigid if there exists \( \delta > 0 \) such that, for every \( R \in SO(3) \setminus \{1\} \) with \( |R - 1| \leq \delta \), and every \( t_1, t_2 \in \mathbb{R} \) satisfying \( |t_1 - \bar{t}_1| + |t_2 - \bar{t}_2| \leq \delta \), there exists no \( b \in \mathbb{R}^3 \) such that

\[
RF_1(t_1) - F_2(t_2) = b \otimes m. \tag{4.32}
\]

The following result gives sufficient conditions for a plastic junctions to be locally rigid. The notation below refers to the notation of Definition 4.1.

**Proposition 4.2.** Let \( F_1 \) and \( F_2 \) form a plastic junction at \((\bar{t}_1, \bar{t}_2)\) as defined in Definition 4.1. Let further \( \psi_1, \psi_2 \parallel m \), \( \text{cof}(R_1 V_1 - R_2 V_2) = b \otimes \hat{m} \) for some \( b \in \mathbb{R}^3 \setminus \{0\} \), \( \hat{m} \in S^2 \) such that \( \hat{m} \cdot m = \hat{m} \cdot \psi_1 = \hat{m} \cdot \psi_2 = 0 \), and

\[
\left( R_1 V_1 \hat{m} \times R_1 V_1 (v + \bar{t}_1 \phi_1 (\psi_1 \cdot v)) \right) \cdot \left( R_1 V_1 \phi_1 \times R_2 V_2 \phi_2 \right) \neq 0,
\]

where \( v := m \times \hat{m} \). \tag{4.33}

Then the plastic junction formed by \( F_1 \) and \( F_2 \) at \((\bar{t}_1, \bar{t}_2)\) is locally rigid.
Proof. Let us first notice that, (4.32) can be written as

\[ RR_1V_1(1 + t_1 φ_1 ⊗ ψ_1) − (R_1V_1 + b_1 ⊗ m_1 + b_2 ⊗ m_2)(1 + t_2 φ_2 ⊗ ψ_2) = b ⊗ m, \]

(4.34)

for some \( b_1, b_2 ∈ \mathbb{R}^3 \setminus \{0\} \), \( m_1, m_2 ∈ S^2 \) such that \( \frac{m_1 × m_2}{|m_1 × m_2|} = \frac{m × ψ_1}{|m × ψ_1|} = \hat{m} \). Testing (4.34) by \( \hat{m} \), we deduce that necessary condition for \( R ∈ SO(3) \) to satisfy (4.32), is that the rotation axis of \( R \) is \( R_1V_1\hat{m} \). Furthermore, letting \( v := m × \hat{m} \), necessary condition for the existence of \( R ∈ SO(3) \) such that (4.32) hold is that

\[ RR_1V_1(1 + t_1 φ_1 ⊗ ψ_1)v − (R_1V_1 + b_1 ⊗ m_1 + b_2 ⊗ m_2)(1 + t_2 φ_2 ⊗ ψ_2)v = 0, \]

which is (4.34) tested by \( v \). Let hence \( R(θ) : [0, 2π] → SO(3) \) be the rotation of axis \( R_1V_1\hat{m} \) and angle \( θ \). Let us also define the smooth function

\[ f(θ, t_1, t_2) := RR_1V_1(1 + t_1 φ_1 ⊗ ψ_1)v − (R_1V_1 + b_1 ⊗ m_1 + b_2 ⊗ m_2)(1 + t_2 φ_2 ⊗ ψ_2)v. \]

Necessary and sufficient condition to have local rigidity if \( R \) has axis \( \hat{m} \) is that \( f = 0 \) in a neighbourhood of \((0, \bar{t}_1, \bar{t}_2)\). But

\[ \frac{∂}{∂θ} f(0, \bar{t}_1, \bar{t}_2) = \frac{R_1V_1\hat{m}}{|R_1V_1\hat{m}|} × (R_1V_1(v + \bar{t}_1 φ_1(ψ_1 • v))), \]

\[ \frac{∂}{∂t_1} f(0, \bar{t}_1, \bar{t}_2) = (ψ_1 • v)R_1V_1 φ_1, \]

\[ \frac{∂}{∂t_2} f(0, \bar{t}_1, \bar{t}_2) = (ψ_2 • v)R_2V_2 φ_2. \]

Therefore, if condition (4.33) is satisfied, rank \( \nabla f(0, \bar{t}_1, \bar{t}_2) = 3 \), and hence there exists a neighbourhood of \((0, \bar{t}_1, \bar{t}_2)\) such that for every \( w := (θ, t_1 − \bar{t}_1, t_2 − \bar{t}_2) \) with \( 0 < |w| ≤ δ \)

\[ f(θ, t_1, t_2) = \nabla f(0, \bar{t}_1, \bar{t}_2)w + o(|w| δ) ≠ 0, \]

which is the claim. \( \square \)

5 Stability of plastic junctions

In this section we give sufficient conditions for plastic junctions to be weak local minimisers of the energy functional \( I \). We recall that any Lipschitz continuous map \( y \) is a weak local minimiser if there exists \( ε > 0 \) such that \( I(ρ) > I(y) \) for any Lipschitz continuous map \( ρ \) satisfying \( \|y − ρ\|_{W^{1,∞}} ≤ ε \). At the end of the section we give a mathematical characterisation of \( V_{II} \) junctions as plastic junctions which are weak local minimisers, and reflect Figure 1b.

Before stating the main result let us introduce the following definition:

**Definition 5.1.** Let \( s ∈ \mathbb{R} \), \( R_φ ∈ SO(3) \), \( U ∈ M \) and \( φ_φ ⊗ ψ_φ ∈ S \). We say that \( F = R_φU(1 + sφ_φ ⊗ ψ_φ) \) enjoys the separation property if there exists \( ρ > 0 \) such that \( |F − G| > ρ \) for every \( G = R_φV(1 + tφ_φ ⊗ ψ_φ) \), with \( t ∈ \mathbb{R} \), \( R_φ ∈ SO(3) \), \( V ∈ M \), \( φ_φ ⊗ ψ_φ ∈ S \) and where at least one out of \( U ≠ V \) and \( φ_φ ⊗ ψ_φ ≠ φ_φ ⊗ ψ_φ \) holds.
Remark 5.1. If $F$ enjoys the separation property, then in a neighbourhood of $F$ there exists a unique decomposition $F = F^c F^p$ of finite energy.

We are now ready to prove the following theorem:

Theorem 5.1. Let $R_1V_1, R_2V_2$ be as in Definition 4.1 and $\tilde{F}_1, \tilde{F}_2 \in \mathbb{R}^{3 \times 3}$ form a plastic junction at $(\tilde{t}_1, \tilde{t}_2)$ for $R_1V_1, R_2V_2$ which is locally rigid. Assume further:

1. $F_1 := \tilde{F}_1(\tilde{t}_1), F_2 := \tilde{F}_2(\tilde{t}_2)$ enjoy the separation property;

2. $F_1 - F_2 = b \otimes m$ and $\text{cof}(R_1V_1 - R_2V_2) = \hat{b} \otimes \hat{m}$ for some $b, \hat{b} \in \mathbb{R}^3 \setminus \{0\}$, $m, \hat{m} \in S^2$;

3. (Domain) The domain $\omega$ is defined as $\omega := \{x \in \mathbb{R}^3 : \min\{x \cdot n_1, x \cdot n_2\} < 0\}$ for some $n_1, n_2 \in S^2$. We also define $\gamma_i := \{x \in \partial \omega \in \mathbb{R}^3 : x \cdot n_i = 0\}$ for $i = 1, 2$;

4. (Geometry) $n_1, n_2, \psi_1, \psi_2, m \perp \hat{m}$. Also, (cf. Figure 6) there exist $\theta_m, \theta_{\psi_1}, \theta_{\psi_2}, \theta_{n_2} \in (0, 2\pi)$ (or in $(-2\pi, 0)$) such that $|\theta_{\psi_1}| < |\theta_m| < |\theta_{\psi_2}| < |\theta_{n_2}|$, and

$$R_m(\theta_{\psi_1}) \gamma_1 \subset \{x : x \cdot \psi_1 = 0\}, \quad R_m(\theta_m) \gamma_1 \subset \{x : x \cdot m = 0\},$$

$$R_m(\theta_{\psi_2}) \gamma_1 \subset \{x : x \cdot \psi_2 = 0\}, \quad R_m(\theta_{n_2}) \gamma_1 = \gamma_2,$$

where $R_m(\theta) \gamma_1$ is the rotation of angle $\theta$ and axis $\hat{m}$ of the half-plane $\gamma_1$. Furthermore, $R_m(\theta) \gamma_1 \subset \omega$ for any $\theta \in (0, \theta_{n_2})$ (resp. $(\theta_{n_2}, 0)$).

5. (Local minimiser) $y \in W^{1,\infty}(\mathbb{R}^3; \mathbb{R}^3)$ is defined by

$$y(x) = \begin{cases} 
F_1x, & \text{if } x \in \Omega_1 := \{x \in \omega : \hat{x} \subset R_m(\theta) \gamma_1, x \in (\theta_{\psi_1}, 0) \} \}, \\
F_2x, & \text{if } x \in \Omega_2 := \{x \in \omega : \hat{x} \subset R_m(\theta) \gamma_1, x \in (0, \theta_{\psi_1}) \} \}, \\
R_1V_1x, & \text{if } x \in \Omega_3 := \{x \in \omega : \hat{x} \subset R_m(\theta) \gamma_1, x \in (\theta_{\psi_1}, \theta_m) \} \}, \\
R_2V_2x, & \text{if } x \in \Omega_4 := \{x \in \omega : \hat{x} \subset R_m(\theta) \gamma_1, x \in (\theta_{\psi_2}, \theta_{n_2}) \} \}. 
\end{cases}$$

Then, if $(\nabla^2 \phi_i \times \psi_i) \cdot m \neq 0$, for $i = 1, 2$, there exists $\varepsilon > 0$ such that

$$\int_{\omega} (W(\nabla \rho) - W(\nabla y)) \, dx > 0, \quad (5.36)$$

for every $\rho \in W^{1,\infty}_m(\omega; \mathbb{R}^3)$ such that $\rho \neq y$, $\rho = y$ on $\gamma_1 \cup \gamma_2$, $\rho$ is $1-1$, and $\|\nabla \rho - \nabla y\|_{L^\infty} \leq \varepsilon$.

Definition 5.2. Let $y \in W^{1,\infty}_m(\omega; \mathbb{R}^3)$ be as in Theorem 5.1. Let further all the hypotheses in Theorem 5.1 be satisfied. Then we say that $y$ is a locally stable plastic junction between $R_1V_1$ and $R_2V_2$. If further $y \in W^{1,\infty}_m(\mathbb{R}^3; \mathbb{R}^3)$ and $y(x) = x$ in $\omega^c$, then we say that $y$ is a $V_{11}$ junction between $R_1V_1$ and $R_2V_2$. 

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Figure 6: Representation of $\omega$ as defined in Theorem 5.1. Here, $\psi_1$, $\psi_2$, $m$ and $\Omega_1$, $\Omega_2$, $\Omega_3$, $\Omega_4$ are as in Theorem 5.1.

Remark 5.2. In order to apply our theory to Ti$_{74}$Nb$_{23}$Al$_3$ the definition of $V_{II}$ junction could be weakened. Indeed, it would be sufficient to assume that $y \in W^{1,\infty}_{\text{loc}}(\mathbb{R}^3;\mathbb{R}^3)$ satisfies hypotheses 4 and 5 of Theorem 5.1 that the plastic junction between $R_1V_1$ and $R_2V_2$ is locally rigid, and that $y(x) = x$ in $\omega^c$. However, we prefer to endow the stability property in the notion of $V_{II}$ junction.

Remark 5.3. The Hadamard jump condition implies that a necessary condition in order to form a $V_{II}$ junction between $R_1V_1$ and $R_2V_2$ is that $\text{rank}(R_1V_1 - 1) \leq 1$ and $\text{rank}(R_2V_2 - 1) \leq 1$.

Remark 5.4. The hypothesis 4 requiring that $n_1$, $n_2$, $\psi_1$, $\psi_2$, $m \perp \hat{m}$ guarantees the continuity of $y$ along the line $s\hat{m}$ for $s \in \mathbb{R}$, and justifies the bi-dimensional representation of stable plastic junctions given in (6).

Remark 5.5. In the statement of Theorem 5.1 we replaced the Lipschitz bounded domain $\Omega$ with the unbounded $\omega$ in the inequality (5.36) for the energy $I$. This domain can be interpreted as a blow-up close to the line given by $\gamma_1 \cap \gamma_2$, where the incompatibility occurs. Mathematically, this choice is motivated by the argument in the proof, which relies on rigidity for plain strains. More precisely, this leads to the fact that the deformation gradient on the plane of compatibility $\{x \cdot m = 0\}$ is propagated in $\Omega_1$ along the characteristic lines in direction $(V_1^i\phi_i \times \psi_i)$, and in $\Omega_2$ along the lines in direction $(V_2^i\phi_i \times \psi_i)$. Therefore, in (5.36) the domain $\omega$ can be replaced by any Lipschitz domain $\Omega \in \omega$ with $\partial \Omega \cap \{x \cdot n_i = 0\}$ of strictly positive $H^2$ measure for both $i = 1, 2$, and such that for every $x \in \Omega \cap \Omega_i$, $i = 1, 2$, $x + s(V_i^i\phi_i \times \psi_i) \in \Omega$ for every $s \in [0, s^*_i]$, where $s^* \in \mathbb{R}$ is such that $(x + s_i^*(V_i^i\phi_i \times \psi_i)) \cdot m = 0$. This last condition guarantees that the information is transported by the characteristic lines $(V_i^i\phi_i \times \psi_i)$ from the plane of compatibility $\{x \cdot m = 0\}$ to every point in the domain.
Proof. Let $\delta_1, \delta_2 > 0$ be as in Definition 5.1 such that $F_1, F_2$ respectively enjoy the separation property. Let also $\delta_3 := \frac{1}{2} \min \{ \|RU - V\| : U \neq V \in \mathcal{M}, R \in SO(3) \}$, and let us take $\varepsilon_0 = \min \{\delta_1, \delta_2, \delta_3\}$. Therefore, by hypothesis (1), given any $p \in W_{loc}^{1,\infty}(\omega; \mathbb{R}^3)$ such that $\|\nabla p - \nabla y\|_{L^\infty} \leq \varepsilon_0$ it must satisfy

$$\nabla p(x) = \begin{cases} \nabla z^{(1)}, & \text{in } \Omega_1, \\ \nabla z^{(2)}, & \text{if } \Omega_2, \end{cases}$$

for some Lipschitz continuous $z^{(1)}, z^{(2)}$ such that

$$\nabla z^{(1)}(x) = \hat{R}_1(x)V_1(1 + t_1(x)\phi_1 \otimes \psi_1), \quad \nabla z^{(2)} = \hat{R}_2(x)V_2(1 + t_2(x)\phi_2 \otimes \psi_2), \quad (5.37)$$

for some measurable $t_i : \Omega_i \to \mathbb{R}$, and $\hat{R}_i : \Omega_i \to SO(3)$, $i = 1, 2$. Define now $\tilde{z}^{(i)}(x) := z^{(i)}(V_i^{-1}x)$. We notice that,

$$\det \nabla \tilde{z}^{(i)} = 1, \quad (\nabla \tilde{z}^{(i)})^T(\nabla \tilde{z}^{(i)}) = 1 + t_i(x)V_i\phi_i \otimes V_{i}^{-1}\psi_i + t_i^2(x)|V_i\phi_i|^2V_{i}^{-1}\psi_i \otimes V_{i}^{-1}\psi_i,$$

where $u \otimes v = u \otimes v + v \otimes u$ for any $u, v \in \mathbb{R}^3$. It follows then by [3] Thm. 3.1 that $\tilde{z}^{(i)}$ is a plain strain, and we can hence deduce the existence of $Q_1, Q_2 \in SO(3)$ such that

$$\tilde{z}^{(i)} = Q_i(\tilde{z}^{(i)}_1(s^{(i)}(s^{(i)}_1, s^{(i)}_3)u^{(i)}_1 + s^{(i)}_2u^{(i)}_2 + s^{(i)}_3(s^{(i)}_1, s^{(i)}_3)), u^{(i)}_3,$$

for some Lipschitz functions $\tilde{z}^{(i)}_1, \tilde{z}^{(i)}_3$, and where

$$u^{(i)}_1 := \frac{V_i^{-1}\psi_i}{|V_i^{-1}\psi_i|}, \quad u^{(i)}_3 := \frac{V_i\phi_i}{|V_i\phi_i|}, \quad u^{(i)}_2 = u^{(i)}_3 \times u^{(i)}_1, \quad s^{(i)}_j = x \cdot u^{(i)}_j.$$

Now, given the fact that the $\tilde{z}^{(i)}$ are Lipschitz continuous and that $(V_i^2\phi_i \otimes \psi_i) \cdot m \neq 0$, (and hence $u^{(i)}_2 \cdot V_i^{-1}m \neq 0$) the value of $\nabla \tilde{z}^{(i)}$ is well defined on the plane $\{x \cdot V_i^{-1}m = 0\}$. Indeed,

$$\nabla \tilde{z}^{(i)}(x) = \nabla \tilde{z}^{(i)}(x + ru^{(i)}_2) \quad (5.38)$$

for almost every $x \in \{x \cdot V_i^{-1}m = 0\}$ and for every $r$ such that $r \text{sign}(u^{(i)}_2 \cdot V_i^{-1}m) > 0$ for $i = 1$, and such that $r \text{sign}(u^{(i)}_2 \cdot V_i^{-1}m) < 0$ if $i = 2$. As a consequence, the value of $\nabla z^{(1)}, \nabla z^{(2)}$ on $\{x \cdot m = 0\}$ is well defined, and is respectively in $L^\infty(\gamma_1; \mathbb{R}^{3\times 3})$, $L^\infty(\gamma_2; \mathbb{R}^{3\times 3})$. By the continuity of $p$ and a weak version of the Hadamard jump condition (see [16] Remark 10]) we deduce that

$$\nabla z^{(1)}(x) - \nabla z^{(2)}(x) = \hat{b}(x) \otimes m, \quad \text{a.e. } x \in \{x \in \omega : \hat{x} \cdot m = 0\},$$

for some measurable $\hat{b} : \{\hat{x} \in \omega : \hat{x} \cdot m = 0\} \to \mathbb{R}^3$. We now claim that this implies the existence of $R_0 \in SO(3)$ such that $\nabla z^{(i)}(x) = R_0F_i, H^2$-a.e. in $x \in \{x : \hat{x} \cdot m = 0\}$, $i = 1, 2$. Indeed, since $z^{(i)}$ with $i = 1, 2$, are plain strains and $V_i^{-1}m \cdot u^{(i)}_2 \neq 0$ (see (5.38)), $|\nabla z^{(i)} - F_i| \leq \varepsilon_0$ for a.e. $x \in \{\hat{x} : \hat{x} \cdot m = 0\}$. Let us consider the smooth functions

$$f_i(R, t) = |RR_iV_i(1 + t\phi_i \otimes \psi_i) - R_iV_i(1 + \tilde{t}_i\phi_i \otimes \psi_i)|,$$

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and let $\delta^*$ be as in Definition 4.1. Since the $f_i$'s are continuous, $f_i \to \infty$ as $t \to \infty$ and $f_i = 0$ if and only if $R = 1$ and $t = t_i$, there exists $\varepsilon_1 > 0$ such that $f_i \leq \varepsilon_1$ implies $|R - 1| + |t - t_i| \leq \frac{1}{2}\delta^*$ for $i = 1, 2$. Let us hence fix $\varepsilon := \min\{\varepsilon_0, \varepsilon_1\}$. Therefore, if $|\nabla z^{(i)} - y| \leq \varepsilon$ a.e. in $\Omega_i$ with $i = 1, 2$, then $|R_1^T(x)R_2(x) - 1| + |t_1(x) - t_1| + |t_2(x) - t_2| \leq \delta^*$ a.e. in $x \in \{\hat{x} \in \omega: \hat{x} \cdot m = 0\}$. By the fact that $F_1, F_2$ form a plastic junction which is locally stable, it must hold $R_1^TR_2 = 1$, $t_1 = t_1$, $t_2 = t_2$, and therefore we deduce that there exists a measurable function $R_0: \{\hat{x} \in \omega: \hat{x} \cdot m = 0\} \to SO(3)$ such that $\nabla z^{(i)} = R_0(x)F_i$ a.e. on $\{\hat{x} \in \omega: \hat{x} \cdot m = 0\}$ and for $i = 1, 2$. Now, given any $x \in \Omega_i$, $i = 1, 2$, there exists $x_0 \in \{\hat{x} \in \omega: \hat{x} \cdot m = 0\}$ and $s_0 \in \mathbb{R}$ such that $x = x_0 + s_0 V_i^{-2} \psi$. Again, since $z^{(i)}$ are plain strains and $V_i^{-1}m \cdot u_2^{(i)} \neq 0$, (5.38) holds. But a result by Reshetnyak (see e.g., [4, 28]) implies that $R_0$ must be constant, concluding the proof of the claim. As a consequence, since $\tilde{z}^{(i)}$ is a plain strain and linear on $\{x \cdot V_i^{-1}m = 0\}$, $z^{(i)}$ must be linear in $\Omega_i$, with $i = 1, 2$, and of the form (5.37) with $\hat{R}_i = R_0R_i$, $\bar{R}_i = R_0R_i$ for some $R_0 \in SO(3)$. We remark that the energy of $\rho$ in $\Omega_2$ is independent of $R_0$. Suppose now that $\nabla \rho \neq R_iV_i$ in $\Omega_{2+i}$ for $i = 1$ or and $i = 2$. Then, since $\varepsilon \leq \delta_3$ there exist $\hat{\Omega}_{2+i} \subset \Omega_{2+i}$ of positive measure where $F^p \neq 0$ and hence the plastic energy is not zero. As a consequence (5.36) must hold. If instead $\rho = y$ on $\Omega_3 \cup \Omega_4$, then the Hadamard jump condition implies

$$R_iV_i - \hat{R}_0R_iV_i(1 + t_i\phi_t \otimes \psi) = \hat{b} \otimes \psi, \quad i = 1, 2,$$

(5.39)

for some $\hat{b} \in \mathbb{R}^3$. Following [4, Prop. 4], this is possible if and only if $\hat{R}_0 = 1$, and thus $\rho = y$, leading to the claimed result. \hfill \Box

## 6 \ $V_{II}$ junctions in Ti$_{74}$Nb$_{23}$Al$_3$

In this section we study the presence of $V_{II}$ junctions in cubic to orthorhombic transformations when the deformation gradients have both the middle eigenvalue and the determinant equal to one. This is done under the additional hypothesis that a parameter of the lattice deformation gradient $\lambda \in (1, \sqrt{2})$. A similar argument could be applied to study the case when $\lambda < 1$. As explained below, this situation is a good approximation of the martensitic transformation in Ti$_{74}$Nb$_{23}$Al$_3$ and similar materials. We remark that our results are obtained in the case where the energy has all the wells, that is where the elastic energy is null on $\bigcup_{i=1}^6 SO(3)U_i$, where $U_i$ are the six matrices transforming a cubic lattices into an orthorhombic one, and where we consider all possible slip system for body centred cubic austenite. However, the generality of the results leads to many long computations and, for this reason, in this section some of the hypotheses of Theorem 5.1 are verified numerically or with the aid of a plot. At the end of the section we compare the results obtained with experimental results.

The transformation in Ti$_{74}$Nb$_{23}$Al$_3$ is from a cubic to an orthorhombic lattice, and therefore
the deformation gradients \( \mathbf{U}_i \) describing the change of lattice vectors are given by

\[
\begin{align*}
\mathbf{U}_1 &= \begin{bmatrix} \frac{d}{2} & 0 & 0 \\ 0 & \frac{1 + \lambda}{2} & \frac{1 - \lambda}{2} \\ 0 & \frac{1}{2} & \frac{1 + \lambda}{2} \end{bmatrix}, & \mathbf{U}_2 &= \begin{bmatrix} \frac{d}{2} & 0 & 0 \\ 0 & \frac{1 + \lambda}{2} & -\frac{1 - \lambda}{2} \\ 0 & -\frac{1}{2} & \frac{1 + \lambda}{2} \end{bmatrix}, & \mathbf{U}_3 &= \begin{bmatrix} \frac{1 + \lambda}{2} & 0 & 0 \\ 0 & d & 0 \\ 0 & \frac{1 + \lambda}{2} & 0 \end{bmatrix}, \\
\mathbf{U}_4 &= \begin{bmatrix} \frac{1 + \lambda}{2} & 0 & -\frac{1 - \lambda}{2} \\ 0 & d & 0 \\ -\frac{1}{2} & 0 & \frac{1 + \lambda}{2} \end{bmatrix}, & \mathbf{U}_5 &= \begin{bmatrix} \frac{1 + \lambda}{2} & 0 & -\frac{1 - \lambda}{2} \\ 0 & d & 0 \\ 0 & 0 & d \end{bmatrix}, & \tilde{\mathbf{U}}_6 &= \begin{bmatrix} \frac{1 + \lambda}{2} & 0 & -\frac{1 - \lambda}{2} \\ 0 & -\frac{1}{2} & 0 \end{bmatrix}.
\end{align*}
\] (6.40)

Since in Ti_{74}Nb_{23}Al_{3} the middle eigenvalue of the transformation matrices \( \lambda_2 \) is such that \(|\lambda_2 - 1| < 4 \cdot 10^{-6} \) we implicitly assumed it to be equal to one in (6.40). Therefore, the eigenvalues of the \( \mathbf{U}_i \)'s are \( d, 1, \lambda \), and, coherently with the lattice deformation in Ti_{74}Nb_{23}Al_{3}, we assume also that \( 0 < d < 1 < \lambda \). A similar analysis could be worked out in the case where \( d > 1 > \lambda > 0 \). Under these assumptions, [4] Prop. 4] guarantees for every \( i = 1, \ldots, 6 \) the existence of two couples of vectors \((\mathbf{a}_i^-, \mathbf{n}_i^-)\) and \((\mathbf{a}_i^+, \mathbf{n}_i^+)\) such that

\[
\mathbf{R}_i^+ \mathbf{U}_i = 1 + \mathbf{a}_i^+ \otimes \mathbf{n}_i^+, \quad \mathbf{R}_i^- \mathbf{U}_i = 1 + \mathbf{a}_i^- \otimes \mathbf{n}_i^-,
\]
for some \( \mathbf{R}_i^+, \mathbf{R}_i^- \in SO(3) \). The different \( \mathbf{a}_i^+, \mathbf{n}_i^+ \) depending on \( \lambda, d \) are given by:

\[
\begin{align*}
\mathbf{a}_1^+ &= \alpha(-\gamma, 1, 1), & \mathbf{n}_1^+ &= (\beta, 1, 1), \\
\mathbf{a}_1^- &= \alpha(\gamma, 1, 1), & \mathbf{n}_1^- &= (-\beta, 1, 1), \\
\mathbf{a}_2^+ &= \alpha(-\gamma, -1, 1), & \mathbf{n}_2^+ &= (\beta, -1, 1), \\
\mathbf{a}_2^- &= \alpha(\gamma, -1, 1), & \mathbf{n}_2^- &= (-\beta, -1, 1), \\
\mathbf{a}_3^+ &= \alpha(1, -\gamma, 1), & \mathbf{n}_3^+ &= (1, \beta, 1), \\
\mathbf{a}_3^- &= \alpha(1, \gamma, 1), & \mathbf{n}_3^- &= (1, -\beta, 1),
\end{align*}
\)

\[
\begin{align*}
\mathbf{a}_4^+ &= \alpha(-1, -\gamma, 1), & \mathbf{n}_4^+ &= (-1, \beta, 1), \\
\mathbf{a}_4^- &= \alpha(-1, \gamma, 1), & \mathbf{n}_4^- &= (-1, -\beta, 1), \\
\mathbf{a}_5^+ &= \alpha(1, 1, -\gamma), & \mathbf{n}_5^+ &= (1, 1, \beta), \\
\mathbf{a}_5^- &= \alpha(1, 1, \gamma), & \mathbf{n}_5^- &= (1, 1, -\beta), \\
\mathbf{a}_6^+ &= \alpha(-1, 1, -\gamma), & \mathbf{n}_6^+ &= (-1, 1, \beta), \\
\mathbf{a}_6^- &= \alpha(-1, 1, \gamma), & \mathbf{n}_6^- &= (-1, 1, -\beta),
\end{align*}
\]

where

\[
\alpha = \frac{d(\lambda^2 - 1)}{2(d + \lambda)}, \quad \beta = -\frac{\sqrt{2(1 - d^2)}}{\sqrt{\lambda^2 - 1}}, \quad \gamma = -\frac{\lambda \sqrt{2(1 - d^2)}}{d \sqrt{\lambda^2 - 1}}.
\]

As explained in the introduction, in experiments for Ti_{74}Nb_{23}Al_{3} [22] one observes the nucleation of different plates of martensite \( \mathbf{F}_i \) with \( \mathbf{F}_i = 1 + \mathbf{a}_i^{\sigma_i} \otimes \mathbf{n}_i^{\sigma_i} \), where \( \sigma_i \in \{+,-\} \) and \( i \in \{1, \ldots, 6\} \), which expand until they encounter another plate of martensite \( \mathbf{F}_j \) with similar properties. Since the nucleation is happening at the interior, of the domain, we restrict ourselves to the case where \( \det \mathbf{U}_i = 1 \), and hence \( d = \lambda^{-1} \). The analysis below however, holds also in the case \( d = 0.9661, \lambda = 1.0331 \) (the lattice parameters for Ti_{74}Nb_{23}Al_{3} where \( |\det \mathbf{U}_i - 1| < 1.9 \cdot 10^{-3} \)) and for every \((d, \lambda) \in (0, 1) \times (1, \infty) \setminus \bigcup_{i=1}^{N} \text{Im}(c_i) \), where \( \text{Im}(c_i) \) is the image of \( c_i \), and \( c_i \) are a finite number \( N \in \mathbb{N} \) of polynomial curves \( c_i : (0, 1) \to (1, \infty) \). Furthermore we restrict ourselves to the physically relevant range \( \lambda \in (1, \sqrt{2}) \). It is worth noticing that when \( \lambda = \sqrt{2} \) the cofactor conditions are satisfied, and hence stress free triple junctions are possible (see e.g., [14]). We now want to find plastic junctions as Defined in 4.1 and where \( \mathbf{R}_1 \mathbf{V}_1 = 1 + \mathbf{a}_i^{\sigma_i} \otimes \mathbf{n}_i^{\sigma_i} \) and \( \mathbf{R}_2 \mathbf{V}_2 \) is of the form (cf. Remark 5.3)

\[
1 + \mathbf{a}_i^{\sigma_i} \otimes \mathbf{n}_i^{\sigma_i}
\]
(6.41)
for $\sigma_i \in \{+, -\}$ and some $i \in \{1, \ldots, 6\}$. The case where $R_1 V_1$ has the form (6.41) but $(i, \sigma_i) \neq (1, +)$ can be treated similarly, or simply deduced from our case by symmetry. We remark that, under our assumptions,

$$a_i^{\sigma_i} \times a_j^{\sigma_j} \neq 0, \quad n_i^{\sigma_i} \times n_j^{\sigma_j} \neq 0,$$

for any $(i, \sigma_i) \neq (j, \sigma_j) \in \{1, \ldots, 6\} \times \{+, -\}$. As a consequence $\text{rank}(R_1 V_1 - R_2 V_2) = 2$. The aim of this Section is to prove the following result:

**Theorem 6.1.** Let $\lambda \in (1, \sqrt{2})$. Let $\mathcal{M} = \bigcup_{i=1}^{6} U_i$ and $S$ be the set of all possible simple slips for body centred cubic lattices. Let us also define

$$\eta_1 = \frac{2\lambda^4 + 5\sqrt{2}\lambda^3 + 4\lambda^2 - 5\sqrt{2}\lambda - 6}{2(2\lambda^4 + 5\sqrt{2}\lambda^3 - 4\lambda^2 + 3\sqrt{2}\lambda + 2)}, \quad \eta_2 = \frac{2\lambda^4 + \sqrt{2}\lambda^3 - 4\lambda^2 - \sqrt{2}\lambda + 2}{2(2\lambda^4 + 5\sqrt{2}\lambda^3 - 4\lambda^2 + 3\sqrt{2}\lambda + 2)},$$

and

$$\xi_1 = \frac{-2\lambda^4 - 5\sqrt{2}\lambda^3 + 4\lambda^2 + 5\sqrt{2}\lambda - 6}{2(2\lambda^4 - 5\sqrt{2}\lambda^3 - 4\lambda^2 - 3\sqrt{2}\lambda + 2)}, \quad \xi_2 = \frac{2\lambda^4 - \sqrt{2}\lambda^3 - 4\lambda^2 + \sqrt{2}\lambda + 2}{2(2\lambda^4 - 5\sqrt{2}\lambda^3 - 4\lambda^2 - 3\sqrt{2}\lambda + 2)}.$$

Then, there exist a plastic junction (in the sense of Definition 5.2) for $1 + a_1^+ \otimes n_1^+$ and $1 + a_i^{\sigma_i} \otimes n_i^{\sigma_i}$ with $i \in \{2, \ldots, 6\}$, $\sigma_i \in \{+, -\}$ if and only if

(a) $(i, \sigma_i) = (3, +)$, $\psi_1 = \psi_2 = (-1, 1, 0)$ and

$$\phi_1 = -(1, 1, 1), \quad \phi_2 = (1, 1, -1), \quad (\bar{t}_1, \bar{t}_2) = (\eta_1, \eta_2), \quad \text{or} \quad \phi_1 = (1, 1, -1), \quad \phi_2 = -(1, 1, 1), \quad (\bar{t}_1, \bar{t}_2) = (-\eta_2, -\eta_1);$$

(b) $(i, \sigma_i) = (4, -)$, $\psi_1 = \psi_2 = (1, 1, 0)$ and

$$\phi_1 = (-1, 1, 1), \quad \phi_2 = (-1, 1, -1), \quad (\bar{t}_1, \bar{t}_2) = (\xi_1, \xi_2), \quad \text{or} \quad \phi_1 = (-1, 1, -1), \quad \phi_2 = (-1, 1, 1), \quad (\bar{t}_1, \bar{t}_2) = (-\xi_2, -\xi_1);$$

(c) $(i, \sigma_i) = (5, +)$, $\psi_1 = \psi_2 = (-1, 0, 1)$ and

$$\phi_1 = -(1, 1, 1), \quad \phi_2 = (1, -1, 1), \quad (\bar{t}_1, \bar{t}_2) = (\eta_1, \eta_2), \quad \text{or} \quad \phi_1 = (1, -1, 1), \quad \phi_2 = -(1, 1, 1), \quad (\bar{t}_1, \bar{t}_2) = (-\eta_2, -\eta_1);$$

(d) $(i, \sigma_i) = (6, -)$, $\psi_1 = \psi_2 = (1, 0, 1)$ and

$$\phi_1 = (-1, 1, 1), \quad \phi_2 = (-1, -1, 1), \quad (\bar{t}_1, \bar{t}_2) = (\xi_1, \xi_2), \quad \text{or} \quad \phi_1 = (-1, -1, 1), \quad \phi_2 = (-1, 1, 1), \quad (\bar{t}_1, \bar{t}_2) = (-\xi_2, -\xi_1);$$

All these plastic junctions are locally stable and can form $V_{II}$ junctions in the sense of Definition 5.2. There exists no $V_{II}$ junction (in the sense of Definition 5.2) between $1 + a_1^+ \otimes n_1^+$ and $1 + a_i^- \otimes n_i^-$. Figure 7 shows the dependence of $\eta_1, \eta_2$ and $\xi_1, \xi_2$ on $\lambda$. The results in Theorem 6.1 are compared with experimental observations at the end of the section.
Figure 7: Plotting the dependence of $\eta_1, \eta_2$ and $\xi_1, \xi_2$ on $\lambda$. In black $\eta_1$ (continuous line) and $\eta_2$ (dashed line). In blue $\xi_1$ (continuous line) and $\xi_2$ (dashed line). On the right hand side, the plot is a zoom of the plot on the left.

6.1 Proof of Theorem 6.1

We divide the proof into steps to simplify the presentation.

Existence of plastic junctions. By Lemma 4.1, and taking in consideration all the slip systems for body centred cubic lattices (see Section 2), we can see that necessary conditions to have plastic junctions for $1 + a_1^+ \otimes n_1^+$ and $1 + a_i^{\sigma_i} \otimes n_i^{\sigma_i}$ with $i \in \{2, \ldots, 6\}$, $\sigma_i \in \{+,-\}$ are given by each of the points (i)–(iii) below:

(i) $(i, \sigma_i) = (3, +)$ and $\psi = (-1, 1, 0)$; (iii) $(i, \sigma_i) = (5, +)$ and $\psi = (-1, 0, 1)$;

(ii) $(i, \sigma_i) = (4, -)$ and $\psi = (1, 1, 0)$; (iv) $(i, \sigma_i) = (6, -)$ and $\psi = (1, 0, 1)$.

In all the above cases $\psi_1 = \psi_2$ and we therefore simplified notation by writing simply $\psi$. We now show that this conditions are sufficient to have plastic junctions. Thanks to Proposition 4.1 we can find $t_1, t_2 \in \mathbb{R}$ such that

$$\text{rank}((1 + a_1^+ \otimes n_1^+)(1 + t_1 \phi_1 \otimes \psi) - (1 + a_i^{\sigma_i} \otimes n_i^{\sigma_i})(1 + t_2 \phi_2 \otimes \psi)) = 1. \quad (6.42)$$

Here, again, $\phi_1, \phi_2$ are the two different Burger’s vectors in the plane orthogonal to $\psi$, among the slip systems for body centred cubic lattices. We recall that, in these cases, for every $\psi$ there are exactly two (up to sign change) $\phi$ such that $(\phi, \psi)$ is a slip systems for body centred cubic lattices. By post-multiplying the above equation by $(1 + t_1 \phi_1 \otimes \psi)^{-1}(1 + t_2 \phi_2 \otimes \psi)^{-1}$ we get

$$\text{rank}((1 + a_1^+ \otimes n_1^+)(1 - t_2 \phi_2 \otimes \psi) - (1 + a_i^{\sigma_i} \otimes n_i^{\sigma_i})(1 - t_1 \phi_1 \otimes \psi)) = 1. \quad (6.43)$$

Therefore, if the solution of (6.43) is unique, it can be identified with the unique solutions of (6.42). An application of Proposition 4.1 leads to (a)–(d).
we have that for the first option in the cases (a)–(d) hypotheses, are locally rigid (in the sense of Definition 4.1) we make use of Proposition 4.2. Under our

in order to verify that the constructed plastic junctions are locally rigid (in the sense of Definition 4.1) we make use of Proposition 4.2. Under our hypotheses, \( \text{cof}(R_1 V_1 - R_2 V_2) = (a_1^+ \times a_2^\sigma) \otimes (n_1^+ \times n_2^\sigma) \), and, in the notation of Proposition 4.2, \( \hat{m} = \frac{n_1^+ \times n_2^\sigma}{|n_1^+ \times n_2^\sigma|} \) and \( \hat{b} = |n_1^+ \times n_2^\sigma| a_1^+ \times a_2^\sigma \). Furthermore, defined

\[
M_1^+ := -2\sqrt{2}\lambda^5 - 8\lambda^4 + 7\sqrt{2}\lambda^3 + 2\lambda^2 + 3\sqrt{2}\lambda - 2, \quad M_2^+ := 2\lambda^4 + 7\sqrt{2}\lambda^3 - 16\lambda^2 + \sqrt{2}\lambda + 6, \\
M_3^+ := -2\lambda(\sqrt{2}\lambda^4 + 5\lambda^3 - 2\sqrt{2}\lambda^2 + 3\lambda + \sqrt{2}), \quad M_1^- := -(2\lambda^4 - 7\sqrt{2}\lambda^3 + 16\lambda^2 - 2\sqrt{2}\lambda + 6), \\
M_2^- := 2\sqrt{2}\lambda^5 - 8\lambda^4 - 7\sqrt{2}\lambda^3 + 2\lambda^2 - 3\sqrt{2}\lambda - 2, \quad M_3^- := 2\lambda(\sqrt{2}\lambda^4 - 5\lambda^3 - 2\sqrt{2}\lambda^2 - 3\lambda + \sqrt{2}),
\]

we have that for the first option in the cases (a)–(d) \( \hat{m} \) is respectively parallel to

\[
(M_1^+, M_2^+, M_3^+), \quad (M_1^-, M_2^-, M_3^-), \quad (M_1^+ M_2^+, M_3^+), \quad (M_1^- M_2^-, M_3^-). \quad (6.44)
\]

For the second option in the cases (a)–(d), \( \hat{m} \) can be deduced by pre-multiplying the vectors in (6.44) by \((1 + t_2 \phi_2 \otimes \psi)^{-T}(1 + t_1 \phi_1 \otimes \psi)^{-T}\). We now have all the ingredients to show (see 4.33)

\[
f(\lambda) := \left( R_1 V_1 \hat{m} \times R_1 V_1 (v + \tilde{t}_1 \phi_1 (\psi \cdot v)) \right) \cdot \left( R_1 V_1 \phi_1 \times R_2 V_2 \phi_2 \right) \neq 0, \quad v = \hat{m} \times \hat{m}. \quad (6.45)
\]

The easiest way to show this is graphically by plotting in Figure 10 the function \( f \) for the cases (a)–(d).

**Separation property.** Let \( F_1 = (1 + a_1^+ \otimes n_1^+)(1 + \tilde{t}_1 \phi_1 \otimes \psi) \) and \( F_2 = (1 + a_i^\sigma \otimes n_i^\sigma)(1 + \tilde{t}_2 \phi_2 \otimes \psi) \), where \((i, \sigma)_i, \tilde{t}_1, \tilde{t}_2 \) and \( \phi_1, \phi_2, \psi \) are as in (a)–(d). We first claim that for each \( \lambda \in (1, \sqrt{2}) \) there exists \( \rho_0 > 0 \) such that

\[
g_1(t) := |F_1^T F_1 - (1 + t \psi_1 \otimes \phi_1) U_1^2 (1 + t \phi_1 \otimes \psi_1)|^2 \geq \rho_0^2, \quad (6.46)
\]

\[
g_2(t) := |F_2^T F_2 - (1 + t \psi_1 \otimes \phi_1) U_1^2 (1 + t \phi_1 \otimes \psi_1)|^2 \geq \rho_0^2 \quad (6.47)
\]
for any $t \in \mathbb{R}$, whenever at least one out of

\begin{align*}
U_j \neq U_i & \quad \text{or } \phi_1 \otimes \psi \neq \phi_i \otimes \psi_i \in S, \quad \text{in the case of (6.46)}, \\
U_j \neq U_i & \quad \text{or } \phi_2 \otimes \psi \neq \phi_i \otimes \psi_i \in S, \quad \text{in the case of (6.47)},
\end{align*}

holds. The amount of cases to be checked is huge. Indeed, there are four different junctions to be checked, that is cases (a–d) each with two subcases. For each of these cases we have to verify two inequalities, namely (6.46)–(6.47), which must hold for six possible different $j$’s, and for forty-eight possible slip-systems. The total amount of cases to be checked is hence $4 \cdot 2 \cdot 2 \cdot (6 \cdot 48 - 1) = 4592$. Since we were not able to identify a unique nice algorithm to verify (6.46)–(6.47), we verified it numerically. Indeed, for any $\lambda > 0$, any $U_j, j = \{1, \ldots, 6\}$ and $\phi_i \otimes \psi_i \in S$ the functions $g_1, g_2$ are fourth order polynomials in $t$ which can be minimised numerically. The smooth dependence on $\lambda$ of $g_1, g_2$ allows to deduce that if we verify the claim for a large enough (but finite) number of different values of $\lambda \in (1, \sqrt{2})$, then it is true for the whole interval. Numerically one observes that the claim is true for any $\lambda \in (1, \sqrt{2})$.

Now, given $\rho_0$ as in the claim, we know that there exists $r = \rho_0 + \max_i |F_i|$ such that if $G \in \mathbb{R}^{3 \times 3}$ satisfies $|G| \geq r$ then $|F_i - G| \geq \rho_0$. Furthermore, the function $H: \{G \in \mathbb{R}^{3 \times 3} : |G| < r\} \to \mathbb{R}^{3 \times 3}$ defined by $H(G) = G^T G$ is Lipschitz on its domain, and hence there exists $c_0 > 0$ such that

$$|F_i - G| \geq c_0 |H(F_i) - H(G)|.$$ 

Therefore, combining this inequality with the claim we obtain that $F_i(s_i)$ enjoys the separation property with $\rho = \rho_0 \min\{1, c_0\}$.

**Local stability and $V_{II}$ junctions.** First, we need to verify the assumption in Theorem 5.1 that $(V_i^2 \phi_i \times \psi) \cdot m \neq 0$. This is done by using (6.44). We plot $(V_i^2 \phi_i \times \psi) \cdot m \neq 0$, against $\lambda$ in Figure 10, and we deduce that it is satisfied for all the cases (a)–(d) and $i = 1, 2$. We just have to construct $\omega$ such that (3)–(4) in Theorem 5.1 are satisfied. But for $(i, \sigma_i)$ as in (a)–(d), fixed $n_1 = n_1^+ \pm$ we can choose $n_2 = \pm n_i^{\sigma_i}$ such that (3)–(4) are satisfied (up to a change of sign
Figure 10: Plotting \(|V_i^2 \phi_i \times \psi_i) \cdot m|\), against \(\lambda\). In black the cases (a) and (c), while in blue the cases (b) and (d). Continuous and dotted lines are respectively for \(i = 1\) and \(i = 2\) for the first out of the two options in (a)–(d), and for \(i = 2\) and \(i = 1\) for the second options in (a)–(d).

of \(\psi\) and/or \(m\). Let us now define \(y\) as in (5.35). The plastic junction is hence stable. By the Hadamard jump condition we can set \(\nabla y = 1\) in \(\omega_c\) and preserve the continuity of the map \(y\).

The proof of the Theorem is thus completed.

\(V_{II}\) junctions between \(1+ a_1^+ \otimes n_1^+\) and \(1+ a_1^- \otimes n_1^-\). In this case there are many slip systems which make plastic junctions possible. However, the only ones which satisfy the necessary conditions of Lemma 4.1, and such that \(\psi_1, \psi_2 \perp \hat{m}\) (where \(\hat{m}\) is parallel to \(n_1 \times n_2\)) as required by hypothesis 4 in Theorem 5.1, are couples of slip systems among

(I) \(\phi = (-1, 1, 1)\) and \(\psi = (2, 1, 1)\);  \hspace{1cm} (III) \(\phi = (1, -1, 1)\) and \(\psi = (0, 1, 1)\);

(II) \(\phi = (1, 1, 1)\) and \(\psi = (-2, 1, 1)\);  \hspace{1cm} (IV) \(\phi = (1, 1, -1)\) and \(\psi = (0, 1, 1)\).

Below we denote by case \((j,k)\) the where \(\phi_1 \otimes \psi_1, \phi_2 \otimes \psi_2\) are respectively given by \(j\) and \(k\) among (I)-(V) above. Let us study the situation in the different cases:

Case (III, III) and case (IV, IV). In these cases Lemma 4.1 guarantees the existence of no plastic junctions.

Cases (I, III), (I, IV), (II, III), (II, IV), (III, I), (III, II), (IV, I), (IV, II). By Proposition 4.1 there exists a unique plastic junction, and \(\dot{t}_i = 0\) for the slip on the plane \((0, 1, 1)\). Therefore, this cases can be studied within the context of cases (I, I) and (II, II) below.

Case (I, II) and case (II, I). In these cases, Proposition 4.1 guarantees the existence of a one parameter family of plastic junctions. However, no local rigidity (in the sense of Definition
4.1) holds. Indeed, let \(\bar{t}_1, \bar{t}_2 \in \mathbb{R}, \ b \in \mathbb{R}^3\) and \(\mathbf{m} \in S^2\) be such that

\[
(1 + a^+_1 \otimes n^+_1)(1 + \bar{t}_1 \phi_1 \otimes \psi_1) - (1 + a^-_1 \otimes n^-_1)(1 + \bar{t}_2 \phi_2 \otimes \psi_2) = b \otimes \mathbf{m}.
\]

Let also \(R \in SO(3)\) be a rotation of angle \(\theta\) and axis \(\hat{m} = \frac{n^+_1 \times n^-_1}{|n^+_1 \times n^-_1|}\). We notice that \(\hat{m} \perp \phi_1, \phi_2, \psi_1, \psi_2, a^+_1, a^-_1\), and hence

\[
0 = (R(1 + a^+_1 \otimes n^+_1)(1 + t_1 \phi_1 \otimes \psi_1) - (1 + a^-_1 \otimes n^-_1)(1 + t_2 \phi_2 \otimes \psi_2)) \hat{m},
\]

for any \(t_1, t_2 \in \mathbb{R}\). Therefore, if for any small \(\theta\) we can show that there exists \(t_1^*, t_2^* \in \mathbb{R}\) such that

\[
0 = (R(1 + a^+_1 \otimes n^+_1)(1 + t_1^* \phi_1 \otimes \psi_1) - (1 + a^-_1 \otimes n^-_1)(1 + t_2^* \phi_2 \otimes \psi_2)) v, \quad v = \frac{m \times \hat{m}}{|m \times \hat{m}|},
\]

we have for any small \(\theta\),

\[
R(1 + a^+_1 \otimes n^+_1)(1 + t_1^* \phi_1 \otimes \psi_1) - (1 + a^-_1 \otimes n^-_1)(1 + t_2^* \phi_2 \otimes \psi_2) = c \otimes \mathbf{m},
\]

for some \(c \in \mathbb{R}^3\), and hence the plastic junction is not rigid. But (6.48) simplifies to

\[
Ra^+_1(n^+_1 \cdot v) - a^-_1(n^-_1 \cdot v) + t_1 R(1 + a^+_1 \otimes n^+_1)\phi_1(\psi_1 \cdot \hat{m})
- t_2(1 + a^-_1 \otimes n^-_1)\phi_2(\psi_2 \cdot \hat{m}) + (\cos(\theta) - 1)v + \sin(\theta)m = 0.
\]

If \(\psi_1 \cdot \hat{m} = 0\) or \(\psi_2 \cdot \hat{m} = 0\), that is if \(\psi_1 \parallel \mathbf{m}\) or if \(\psi_2 \parallel \mathbf{m}\), then by hypothesis 4 in Theorem 5.1 the case reduces to case (I, I) or case (II, II) below. Otherwise, since \((1 + a^+_1 \otimes n^+_1)\phi_1\) and \((1 + a^-_1 \otimes n^-_1)\phi_2\) are linearly independent, there exists an open neighbourhood \(\mathcal{U}\) of 0 such that \(R(1 + a^+_1 \otimes n^+_1)\phi_1\) and \((1 + a^-_1 \otimes n^-_1)\phi_2\) are linearly independent for any \(\theta \in \mathcal{U}\). Keeping in account that all the terms in (6.49) are orthogonal to \(\hat{m}\), (6.49) is solvable for some \(t_1^*, t_2^* \in \mathbb{R}\).

As a consequence the junctions are not locally rigid.

Case (I, I) and case (II, II). In these cases Proposition 4.1 guarantees the existence of a one parameter family of solutions respectively given by

\[
s_1 = s_2 - \frac{\lambda(\lambda^2 - 1)}{\sqrt{2}(2\lambda^4 + 1)}, \quad s_1 = s_2 - \frac{\lambda(\lambda^2 - 1)}{\sqrt{2}(2\lambda^4 + 1)}.
\]

In the cases (I, I) and (II, II), we respectively have

\[
\mathbf{m} \parallel \left(2 - \frac{4(2\lambda^4 + 1)}{4\lambda^4(2s_2 + 1) + \sqrt{2}\lambda^3 - \sqrt{2}\lambda + 4s_2}, 1, 1\right),
\]

\[
\mathbf{m} \parallel \left(\frac{4(2\lambda^4 + 1)}{4\lambda^4(2s_2 + 1) - \sqrt{2}\lambda^3 + \sqrt{2}\lambda + 4s_2} - 2, 1, 1\right).
\]

By arguing as in the case (I, II) and the case (II, I) we can deduce that, as long as \((2, 1, 1) \parallel \mathbf{m}\) and \((-2, 1, 1) \parallel \mathbf{m}\) then the plastic junctions constructed in the case (I, I) and in the case
(II, II) are not locally rigid. But we notice that, given \( \lambda \in (1, \sqrt{2}) \) and \( \mathbf{m} \) as in (6.50) this never occurs, concluding that no local rigidity holds for these junctions.

**Case (III, IV) and case (IV, III).** In these cases there exists plastic junctions if and only if \( s_2 = -s_1 = \frac{\lambda(\lambda^2-1)}{2\sqrt{2}} \), and \( \mathbf{m} = (1, 0, 0) \). Let now \( R \in SO(3) \) be a rotation of angle \( \theta \in (-\pi, \pi] \) and axis \( \mathbf{m} = \frac{n_1^+ \times n_2^-}{|n_1^+ \times n_2^-|} \). In this case we can solve explicitly

\[
\cof(RR_1 V_1 (1 + t_1 \phi_1 \otimes \psi_1) - (R_1 V_1 + b_1 \otimes m_1 + b_2 \otimes m_2)(1 + t_2 \phi_2 \otimes \psi_2)) = 0,
\]

in terms of \( (t_1, t_2) \), and deduce that the unique solution is given by

\[
\bar{t}_2 = -\bar{t}_1 = \frac{\lambda^2(\lambda^2 - 1) \cos(\theta/2) - 2\lambda \sin(\theta/2)}{\sqrt{2}(\lambda^2 - 1) \sin(\theta/2) + 2\lambda \cos(\theta/2)}.
\]

In this case, however,

\[
RR_1 V_1 (1 + t_1 \phi_1 \otimes \psi_1) - (R_1 V_1 + b_1 \otimes m_1 + b_2 \otimes m_2)(1 + t_2 \phi_2 \otimes \psi_2) = b \otimes m,
\]

for some \( b \in \mathbb{R}^3 \) depending on \( \theta \). Therefore, also in this case no local rigidity holds.

### 6.2 Comparison with experimental results

We can now compare the results obtained in Theorem 6.1 to the experimental observations in [22] for Ti74Nb23Al3. We recall that for Ti74Nb23Al3, \( V_{II} \) junctions with \( 1 + \mathbf{a}_i^+ \otimes \mathbf{n}_1^+ \) are observed only for \( (i, \sigma_i) \) equal to \((4, -)\) and \((6, -)\). This is coherent with the result in Theorem 6.1 Indeed, although Theorem 6.1 predicts the existence of \( V_{II} \) junctions also for the cases \((i, \sigma_i)\) equal to \((3, +)\) and \((5, +)\), Figure 7 shows that the energy required for a single slip in these cases is consistently bigger than the energy required in the case \((i, \sigma_i)\) equal to \((4, -)\) and \((6, -)\). If we approximate the transformation matrices for the phase transition in Ti74Nb23Al3 with the matrices in (6.40) with \( d = \frac{1}{3} \), \( \lambda \in (1.033, 1.035) \) we get that, in some regions of the domain, the shear amount required to form \( V_{II} \) junctions in the cases \((i, \sigma_i)\) equal to \((3, +)\) and \((5, +)\), is about ten times bigger than in the case \((i, \sigma_i)\) equal to \((4, -)\) and \((6, -)\). Therefore, one can explain the lack of \( V_{II} \) junctions between \( 1 + \mathbf{a}_i^+ \otimes \mathbf{n}_1^+ \) and \( 1 + \mathbf{a}_i^+ \otimes \mathbf{n}_1^+ \), with \((i, \sigma_i)\) equal to \((3, +)\) and \((5, +)\) with the fact that they are energetically expensive. We report the above discussed results in Table 1. Another factor influencing the presence of \( V_{II} \) junctions may be the norm of the dislocation density tensor \( \nabla \times \mathbf{F}^p \) (see e.g., [27]). For \( V_{II} \) junctions as in Definition 5.2 we have that \( \nabla \times \mathbf{F}^p \) is a Radon measure and \( \nabla \times \mathbf{F}^p = (\tilde{t}_1 \phi_1 \otimes \psi_1 - \tilde{t}_2 \phi_2 \otimes \psi_2) \times \mathbf{m} \mathcal{H}^2 \subset \{ \mathbf{x} \cdot \mathbf{m} = 0 \} \). Here \( \mathcal{H}^2 \subset \{ \mathbf{x} \cdot \mathbf{m} = 0 \} \) is the two-dimensional Hausdorff measure restricted to the plane \( \{ \mathbf{x} \cdot \mathbf{m} = 0 \} \), and the cross product is taken row-wise. We report in Figure 11 the values of \( |(\tilde{t}_1 \phi_1 \otimes \psi_1 - \tilde{t}_2 \phi_2 \otimes \psi_2) \times \mathbf{m}| \) for the constructed \( V_{II} \) junctions. Again, the results confirm that the cases \((i, \sigma_i)\) equal to \((4, -)\) and \((6, -)\) are more preferable than the cases \((i, \sigma_i)\) equal to \((3, +)\) and \((5, +)\).
Figure 11: Plotting $|\nabla \times F^p|$ against $\lambda$. In black the cases $(i, \sigma_i)$ equal to (3, +) and (5, +), while in blue the cases $(i, \sigma_i)$ equal to (4, −) and (6, −). On the right a zoom of the plot.

7 Concluding remarks

In Section 5 we provided a mathematical characterisation of $V_{II}$ junctions in martensitic transformations. Our $V_{II}$ are weak local minimisers of a physically relevant energy introduced in Section 2. In Section 6 we have showed that our model is successful in capturing the $V_{II}$ junctions observed in Ti$_{74}$Nb$_{23}$Al$_3$. There are nonetheless a few directions in which the present work can be extended or improved.

Despite $V_{II}$ junctions look very similar to the inexact junctions observed in Ni$_{65}$Al$_{35}$ [9,13], the theory developed in this paper cannot be applied to that case. This is mainly for three reasons: first, as reported in [8] elastic distortions are experimentally observed and seem to play an important role for the formation of incompatible junctions in Ni$_{65}$Al$_{35}$. Second, when considering average deformation gradients like laminates (and hence a relaxed elastic energy), one should also consider average plastic shears (and thus a relaxed plastic energy). In that case, also the compatibility results of Section 4 should be re-proven. Third, it seems that a rigidity argument based on the separation of wells as the one in the proof of Theorem 5.1 does not work for a relaxed elastic energy.

The aim of this work is to study $V_{II}$ junctions, but would be interesting to understand also $V_I$ junctions within this framework. This would allow to better understand nucleation of martensite in Ti$_{74}$Nb$_{23}$Al$_3$. Indeed, as reported in [22], nucleation in Ti$_{74}$Nb$_{23}$Al$_3$ occurs mostly through the formation of new $V_I$ junctions. However we were not able to find a mathematical characterisation of $V_I$ junctions which is both simple and well-defined, as in this case one should consider plastic deformations both in austenite and in the martensite plates. This will hopefully be discussed in future work.

In our opinion, keeping in account small elastic effects would improve the physical accuracy of the model discussed in Section 2 but would make the proof of local stability much harder. The context of linear elasto-plasticity and the linear elasticity model for martensitic transformations (see e.g., [12]) may provide a better framework to approach this problem analytically.
Table 1: Incompatible junctions observed in Ti$_{74}$Nb$_{23}$Al$_3$: comparison between experimental data and results obtained in Theorem 6.1. In the second column we give the incompatibility between $1 + a_i^+ \otimes n_i^+$ and $1 + a_i^- \otimes n_i^-$ measured as in [9] (see Introduction). The approximate values obtained for the angles of incompatibility $\theta$ are expressed in degrees. In the third column we report the type of incompatible junction observed in experiments. In the last column we report the values of $|\bar{t}_1|$, $|\bar{t}_2|$, the amount of simple shear for the $V_{II}$ junctions given by Theorem 6.1. For this values we have given a range, corresponding to the value of $\lambda = 1.033$ and $\lambda = 1.035$ respectively. This range approximates the deformation gradient for Ti$_{74}$Nb$_{23}$Al$_3$ best. The obtained results confirm that $V_{II}$ junctions are energetically convenient when $(i, \sigma_i)$ is equal to $(4, -)$ or $(6, -)$. The data in the second and third column are taken from [22, Table 4].

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