Leçons Jacques-Louis Lions
Sorbonne Université, 20-22 mai 2019

Transformations de phase, compatibilité et microstructure

John Ball

Heriot-Watt University and

Maxwell Institute for Mathematical Sciences

Notes at http://people.maths.ox.ac.uk/ball/teaching.shtml

Unlike more familiar phase transformations such as

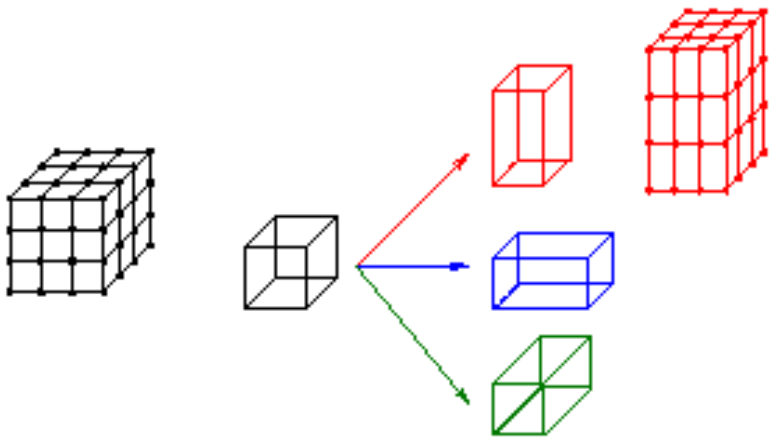
$$\text{ice} \longrightarrow \text{water} \longrightarrow \text{steam}$$

martensitic phase transformations in crystals (metals and alloys) involve a diffusionless *change of shape* of the underlying crystal lattice at some critical temperature.

e.g. cubic to tetragonal

austenite

$\theta > \theta_c$

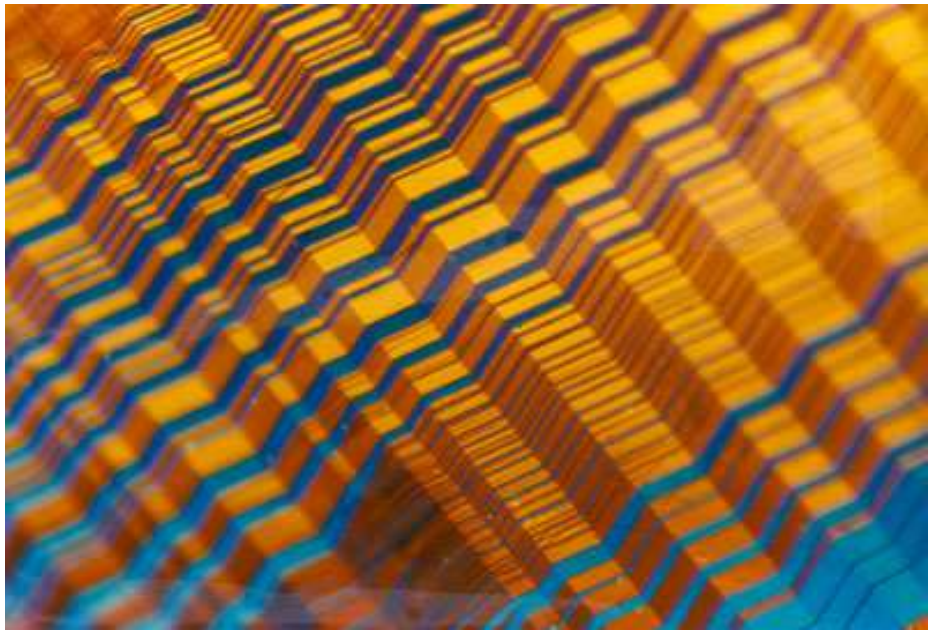


three *variants* of low temperature phase.

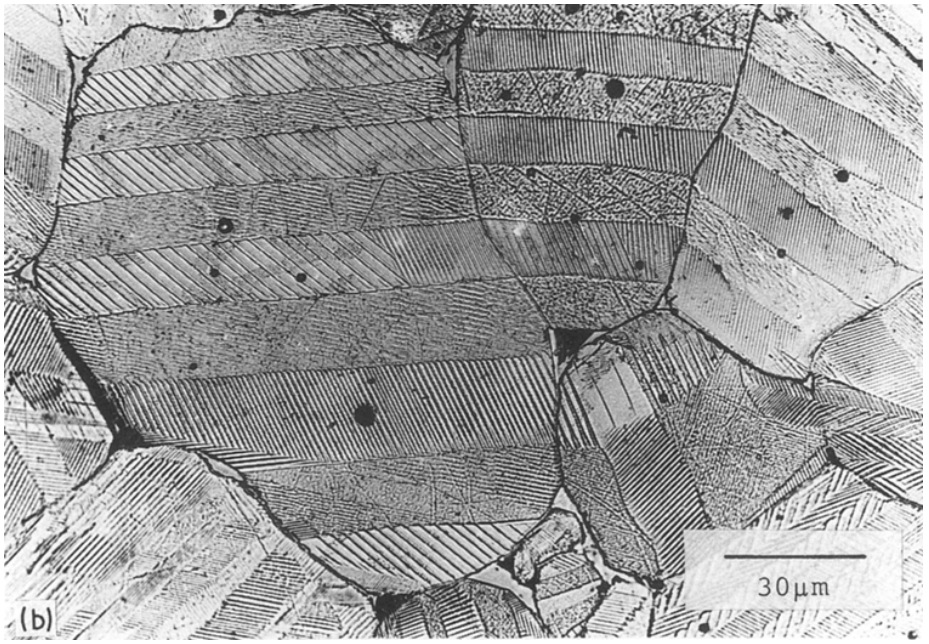
$\theta < \theta_c$

martensite

The requirement that the different variants fit together geometrically (compatibility) leads to characteristic patterns of *microstructure* that are important for determining the macroscopic properties of the material.



CuAlNi single crystal: Chu/James



$BaTiO_3$ polycrystal: G. Arlt 1990

The aim of the course is to try to understand such microstructures, using the following ingredients:

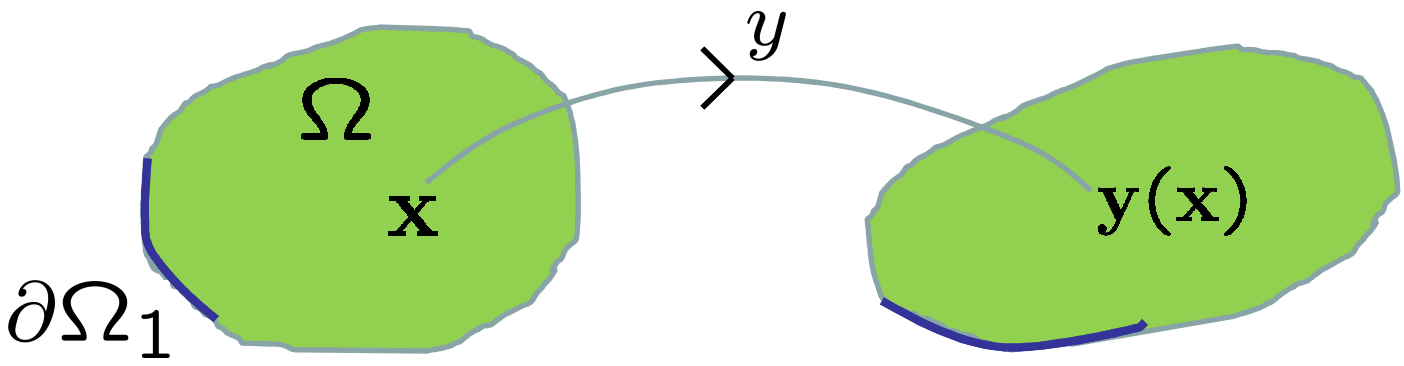
(i) A description of crystal lattices,

(ii) A related nonlinear elasticity model,

(iii) An analysis of possible interfaces and microstructures,

(iv) Techniques of the multi-dimensional calculus of variations (quasiconvexity ...).

Brief review of nonlinear elastostatics



Assume material is homogeneous and occupies a bounded (Lipschitz) domain $\Omega \subset \mathbb{R}^3$ in a reference configuration.

Elastic free energy at constant temperature θ

$$I_\theta(\mathbf{y}) = \int_\Omega \psi(D\mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x}.$$

free-energy density

Properties of free-energy density: $\psi(\mathbf{A}, \theta)$ defined for $\mathbf{A} \in D(\psi), \theta \in I$, where $D(\psi)$ is an open subset of

$$GL^{+}(3, \mathbb{R}) = \{\mathbf{A} \in M^{3\times 3} : \det \mathbf{A} > 0\}.$$

(i) (frame-indifference)

$\psi(\mathbf{QA}, \theta) = \psi(\mathbf{A}, \theta)$ for all $\mathbf{Q} \in SO(3), \mathbf{A} \in D(\psi), \theta \in I$

(ii) (material symmetry)

$\psi(\mathbf{AM}, \theta) = \psi(\mathbf{A}, \theta)$ for all $\mathbf{M} \in \mathcal{S}, \mathbf{A} \in D(\psi), \theta \in I$,
where $\mathcal{S}$ is a subgroup of the set of unimodular matrices
$SL(3) = \{\mathbf{A} \in M^{3\times 3} : \det \mathbf{A} = 1\}$.

For consistency, we need $SO(3)\, D(\psi)\, \mathcal{S} = D(\psi)$.

Energy minimization problem

Minimize

$$I_\theta(\mathbf{y}) = \int_\Omega \psi(D\mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x}$$

among (invertible) $\mathbf{y} : \Omega \to \mathbb{R}^3$ subject to

$$\mathbf{y}|_{\partial\Omega_1} = \bar{\mathbf{y}}.$$

In order that we can be assured that a minimizer exists we typically need that in addition $\psi(\cdot, \theta)$ is quasiconvex and coercive. However we will see that for elastic crystals neither condition is generally satisfied.

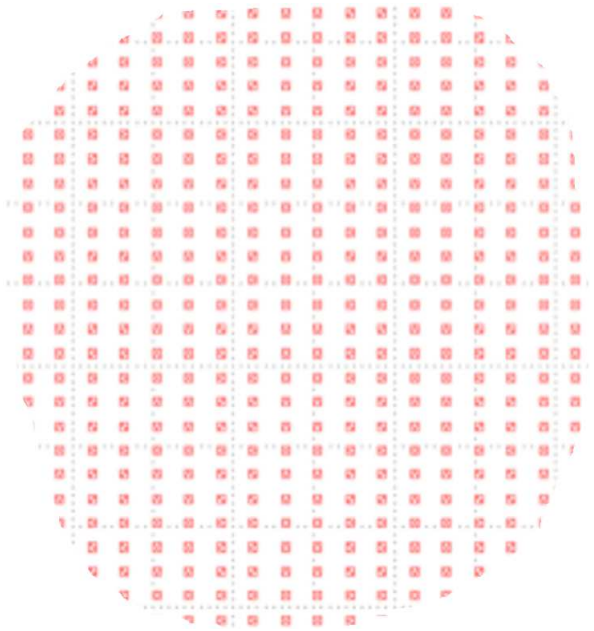
Bravais lattices

A Bravais lattice is an infinite lattice of points in $\mathbb{R}^3$ generated by linear combinations with integer coefficients of three linearly independent basis vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$.

Setting $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3) \in GL(3, \mathbb{R})$ we write the corresponding Bravais lattice as

$$\mathcal{L}(\mathbf{B}) = \{m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 : m_i \in \mathbb{Z}\}.$$

Notice that if $\mathbf{B} = (B_{ij})$ then $B_{ij} = \mathbf{b}_j \cdot \mathbf{e}_i$, where $\mathbf{e}_i$ is the unit vector in the i^{th} coordinate direction.



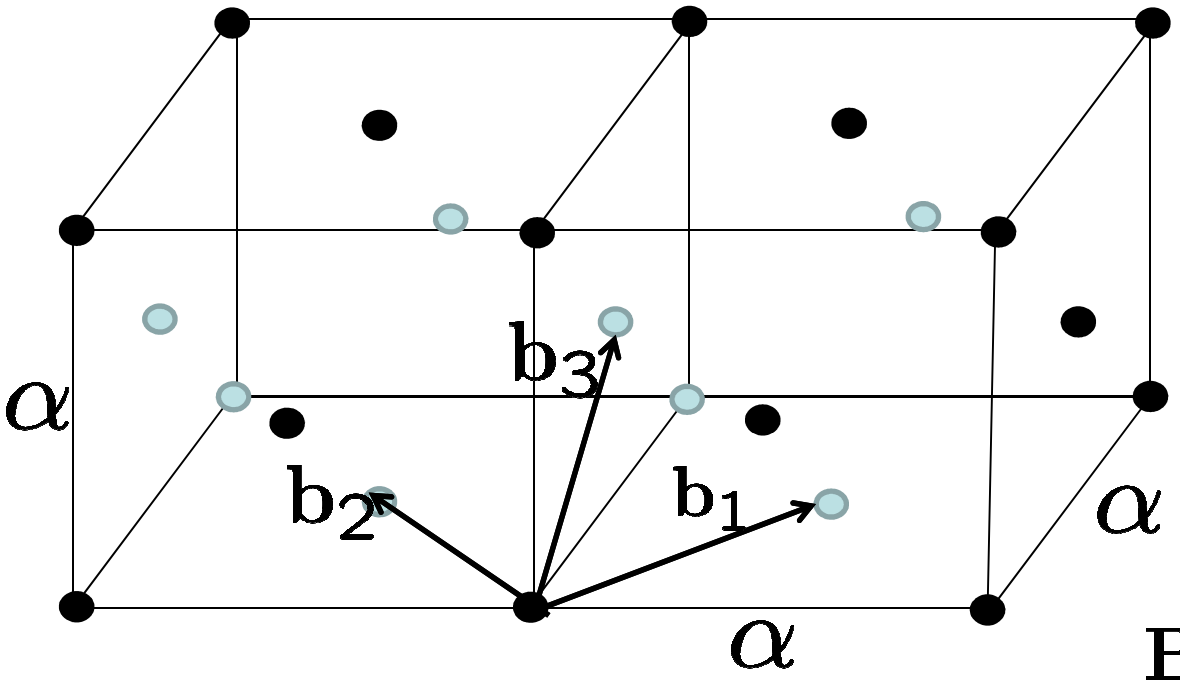
We think of a single crystal as consisting of a part of a Bravais lattice consisting of many points, each point representing an atomic position.

Typical alloys are *solid solutions* of different elements, so that each lattice site has a probability of being occupied by a particular element according to the overall composition.

Some crystals form *multilattices* which are finite unions of translates of a Bravais lattice. We will not consider these.

Examples of Bravais lattices.

1. Face-centred cubic (fcc)



$$\mathbf{B} = \alpha \mathbf{Q} \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} \end{pmatrix},$$

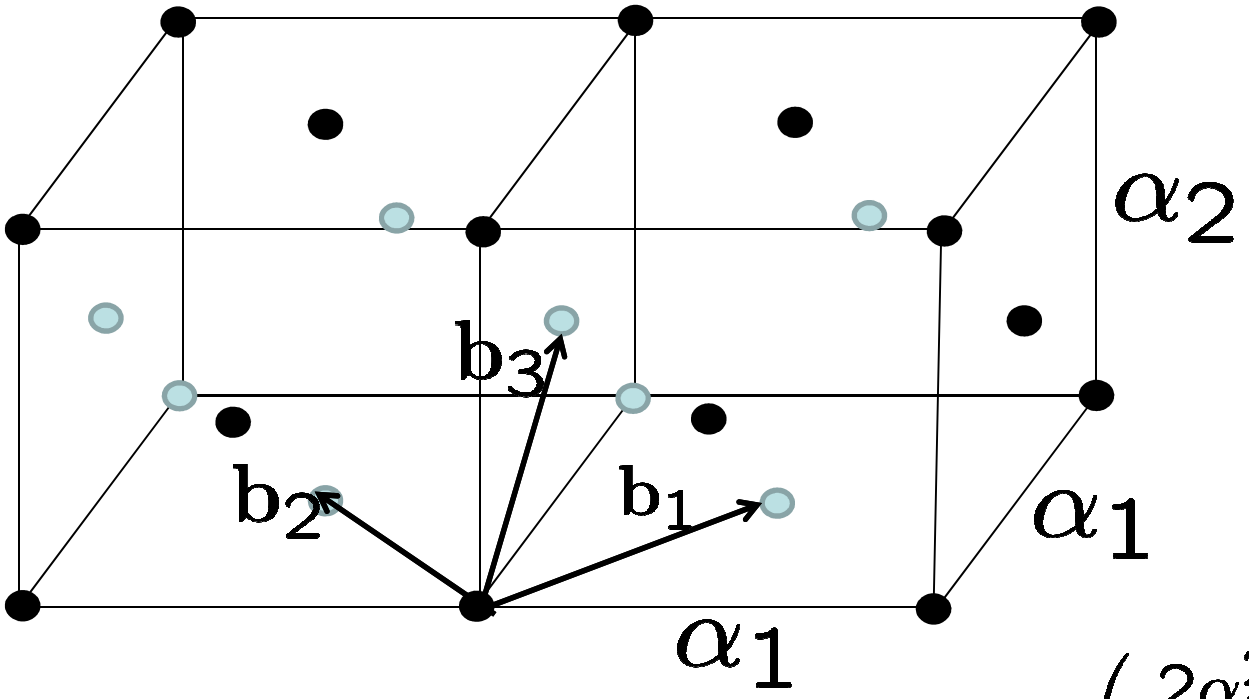
$$\mathbf{Q} \in O(3)$$

Equivalently

$$\mathbf{B}^T\mathbf{B} = \frac{\alpha^2}{4} \begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

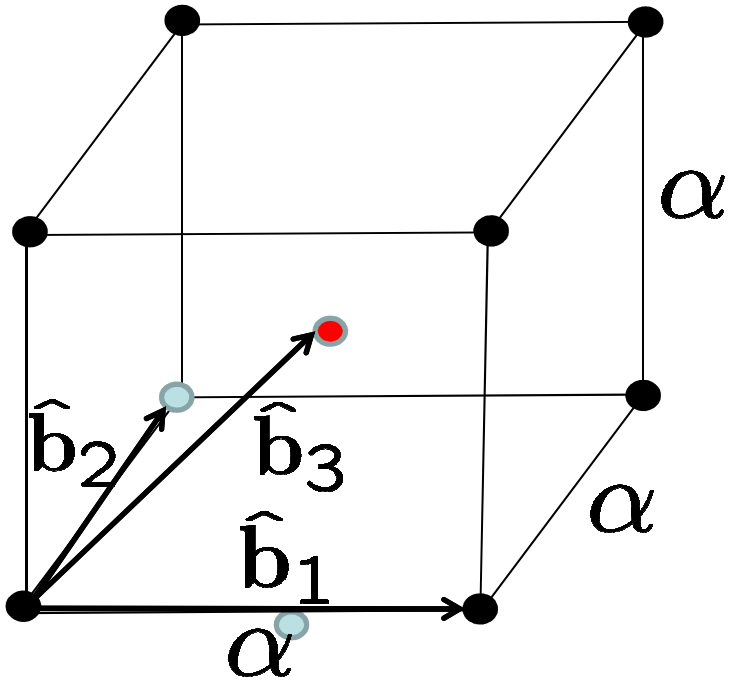
Note that any atom can be taken as the origin.

2. Face-centred tetragonal (fct)



$$\mathbf{B}^T\mathbf{B} = \frac{1}{4}\begin{pmatrix} 2\alpha_1^2 & 0 & \alpha_1^2 \\ 0 & 2\alpha_1^2 & \alpha_1^2 \\ \alpha_1^2 & \alpha_1^2 & \alpha_1^2+\alpha_2^2 \end{pmatrix}$$

3. Body-centred cubic (bcc)



Could take the basis vectors as $\hat{\mathbf{b}}_i$ shown, but the conventional and more symmetric choice is

$$\mathbf{B} = \tfrac{\alpha}{2}\mathbf{Q}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \ \mathbf{Q} \in O(3)$$

for which

$$\mathbf{B}^T\mathbf{B} = \tfrac{\alpha^2}{4}\begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

Body-centered tetragonal (bct) treated similarly.

$$GL(3,\mathbb{Z}) = \{\boldsymbol{\mu} = (\mu_{ij}) : \mu_{ij} \in \mathbb{Z}, \det \boldsymbol{\mu} = \pm 1\}.$$

Theorem $\mathcal{L}(\mathbf{B}) = \mathcal{L}(\mathbf{C})$ iff

$$\mathbf{B} = \mathbf{C}\boldsymbol{\mu}, \text{ for some } \boldsymbol{\mu} \in GL(3,\mathbb{Z}).$$

Proof. Let $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$, $\mathbf{C} = (\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3)$.

If $\mathcal{L}(\mathbf{B}) = \mathcal{L}(\mathbf{C})$ then $\mathbf{b}_i = \mu_{ji}\mathbf{c}_j$ for some $\boldsymbol{\mu} = (\mu_{ij}) \in \mathbb{Z}^{3\times 3}$, so that $\mathbf{B} = \mathbf{C}\boldsymbol{\mu}$. Similarly $\mathbf{C} = \mathbf{B}\boldsymbol{\mu}'$ for some $\boldsymbol{\mu}' \in \mathbb{Z}^{3\times 3}$. So $\boldsymbol{\mu}' = \boldsymbol{\mu}^{-1}$ and $\boldsymbol{\mu} \in GL(3,\mathbb{Z})$.

Conversely, if $\mathbf{B} = \mathbf{C}\boldsymbol{\mu}$ then $\mathbf{b}_i = \mu_{ji}\mathbf{c}_j$ and so $\mathcal{L}(\mathbf{B}) \subset \mathcal{L}(\mathbf{C})$. Similarly $\mathcal{L}(\mathbf{C}) \subset \mathcal{L}(\mathbf{B})$. □

Corollary. If $\mathbf{F} \in GL(3,\mathbb{R})$, then $\mathcal{L}(\mathbf{FB}) = \mathcal{L}(\mathbf{B})$ iff

$$\mathbf{F} = \mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \text{ for some } \boldsymbol{\mu} \in GL(3,\mathbb{Z}).$$

Definition. The *point group* $P(\mathbf{B})$ of $\mathcal{L}(\mathbf{B})$ is the set of $\mathbf{Q} \in O(3)$ such that $\mathcal{L}(\mathbf{QB}) = \mathcal{L}(\mathbf{B})$.

By the Corollary,

$$P(\mathbf{B}) = \{\mathbf{Q} \in O(3) : \mathbf{B}^{-1}\mathbf{QB} \in GL(3,\mathbb{Z})\}.$$

If $\mathbf{B}^{-1}\mathbf{QB} = \boldsymbol{\mu} \in GL(3,\mathbb{Z})$ then $\boldsymbol{\mu}^T\boldsymbol{\mu} = \mathbf{B}^T\mathbf{B}^{-T}$, and so $P(\mathbf{B})$ is a *finite* group.

If $\mathbf{R} \in O(3)$ then

$$\begin{aligned} P(\mathbf{RB}) &= \{\mathbf{Q} : \mathbf{R}^T\mathbf{QR} \in \mathcal{L}(\mathbf{B})\} \\ &= \{\mathbf{R}\tilde{\mathbf{Q}}\mathbf{R}^T : \tilde{\mathbf{Q}} \in \mathcal{L}(\mathbf{B})\} \\ &= \mathbf{R}P(\mathbf{B})\mathbf{R}^T, \end{aligned}$$

so that $P(\mathbf{RB})$ is orthogonally conjugate to $P(\mathbf{B})$.

The point groups of the simple cubic ($\mathbf{B} = \alpha\mathbf{Q1}$), fcc and bcc lattices are the same, namely (taking $\mathbf{Q} = \mathbf{1}$) the cubic group P^c consisting of the 48 orthogonal tranformations mapping the unit cube $(0,1)^3$ into itself.

Thus the point group does not discriminate between the different possible cubic lattices, and to do this one needs to consider the *lattice group*

$$L(\mathbf{B}) = \{\boldsymbol{\mu} \in GL(3,\mathbb{Z}) : \mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \in O(3)\}$$

$L(\mathbf{QB}) = L(\mathbf{B})$ for all $\mathbf{Q} \in O(3)$. However $L(\mathbf{B})$ depends on the lattice basis, so that

$$L(\mathbf{B}\boldsymbol{\mu}) = \boldsymbol{\mu}^{-1}L(\mathbf{B})\boldsymbol{\mu} \text{ for all } \boldsymbol{\mu} \in GL(3,\mathbb{Z}).$$

The corresponding conjugacy classes determine 14 distinct Bravais lattices (triclinic, monoclinic, orthorhombic, rhombohedral, tetragonal, hexagonal and cubic).

We now fix a reference lattice $\mathcal{L}(\mathbf{B})$ with $\mathbf{B} \in GL^+(3,\mathbb{R})$, and suppose that there is a free-energy function $\varphi(\mathbf{C},\theta)$ defined for $\mathbf{C}$ in an open neighbourhood D of $\mathbf{B}$ in $GL^+(3,\mathbb{R})$ satisfying

$$\mathbf{Q}D\boldsymbol{\mu} \subset D \text{ for all } \mathbf{Q} \in SO(3), \boldsymbol{\mu} \in GL^+(3,\mathbb{Z})(= SL(3,\mathbb{Z}))$$

and temperatures θ in some interval I, such that for all $\mathbf{C} \in D, \theta \in I$

(i) $\varphi(\mathbf{QC},\theta) = \varphi(\mathbf{C},\theta)$ for all $\mathbf{Q} \in SO(3)$,

(ii) $\varphi(\mathbf{C}\boldsymbol{\mu},\theta) = \varphi(\mathbf{C},\theta)$ for all $\boldsymbol{\mu} \in GL^+(3,\mathbb{Z})$.

That is, the free-energy is rotationally invariant and depends only on the lattice $\mathcal{L}(\mathbf{C})$.

We now use the Cauchy-Born rule (an implicit coarse-graining) to relate the macroscopic free-energy density ψ to φ. Choosing a reference configuration in which the crystal lattice is $\mathbf{B}$, we assume that

$$\psi(\mathbf{A},\theta) = \varphi(\mathbf{AB},\theta), \text{ for } \mathbf{A} \in D(\psi), \theta \in I,$$

where $D(\psi) = D\mathbf{B}^{-1}$.

Thus ψ inherits the invariances for all $\mathbf{A} \in D(\psi), \theta \in I$,
(i) $\psi(\mathbf{QA},\theta) = \psi(\mathbf{A},\theta)$ for all $\mathbf{Q} \in SO(3)$,
(ii) $\psi(\mathbf{AB}\boldsymbol{\mu}\mathbf{B}^{-1},\theta) = \psi(\mathbf{A},\theta)$ for all $\boldsymbol{\mu} \in GL^{+}(3,\mathbb{Z})$.

Hence ψ has symmetry group $\mathcal{S} = \mathbf{B}\,GL^{+}(3,\mathbb{Z})\,\mathbf{B}^{-1}$, which is a subgroup of $SL(3,\mathbb{R})$.

Martensitic phase transformations

We now assume that $\varphi(\cdot, \theta)$ is bounded below for each $\theta \in I$ and attains a minimum. We can suppose that the minimum value is zero. Hence also the minimum value of $\psi(\cdot, \theta)$ is zero.

$$\text{Let } K(\theta) = \{\mathbf{A} \in D(\psi) : \psi(\mathbf{A}, \theta) = 0\}.$$

$$\text{Then } SO(3)K(\theta)\mathcal{S} = K(\theta).$$

We consider a martensitic phase transformation that takes place at the temperature θ_c, with the lattice being cubic (fcc or bcc) for $\theta \geq \theta_c$.

This is described by a change of shape of the lattice with respect to the lattice $\mathbf{B}$ at θ_c given by $\mathbf{U}(\theta) = \mathbf{U}(\theta)^T > 0$.

(Note that by the polar decomposition theorem we can write any $\mathbf{A} \in GL^+(3,\mathbb{R})$ in the form $\mathbf{A} = \mathbf{RU}$ with $\mathbf{R} \in SO(3)$, $\mathbf{U} = \mathbf{U}^T > 0$, so that we can always describe the change of shape by such a $\mathbf{U}$.)

Thus we assume that

$$K(\theta) = \begin{cases} \alpha(\theta) SO(3)\mathcal{S} & \theta > \theta_c \\ SO(3)\mathcal{S} \cup SO(3)\mathbf{U}(\theta_c)\mathcal{S} & \theta = \theta_c \\ SO(3)\mathbf{U}(\theta)\mathcal{S} & \theta < \theta_c \end{cases},$$

where $\alpha(\theta) > 0$ gives the thermal expansion of the cubic lattice, with $\alpha(\theta_c) = 1$.

Reduction of the symmetry group

It is convenient to consider a simplified theory in which we only consider those $\boldsymbol{\mu}$ that generate elements of the point group, thus ignoring large lattice invariant shears that are typically associated with plasticity.

Theorem. (Ericksen-Pitteri neighbourhood) Given a Bravais lattice $\mathbf{B} \in GL^+(3,\mathbb{R})$ there is an open neighbourhood $\mathcal{N}$ of $SO(3)$ in $GL^+(3,\mathbb{R})$ such that
(i) $SO(3)\mathcal{N} = \mathcal{N}$
(ii) if $\boldsymbol{\mu} \in GL^+(3,\mathbb{Z})$ then either $\mathcal{N}\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} = \mathcal{N}$ (in which case $\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \in P(\mathbf{B})$), or $\mathcal{N}\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \cap \mathcal{N} = \emptyset$.

Thus, if we restrict $\psi(\mathbf{A}, \theta)$ to $\mathcal{N}$ then the symmetry group of ψ is reduced to

$$P^+(\mathbf{B}) = P(\mathbf{B}) \cap SO(3) = \mathcal{S} \cap SO(3).$$

Proof. We claim that a suitable neighbourhood is given by

$$\mathcal{N}_\varepsilon = \{\mathbf{A} : |\mathbf{A}^T\mathbf{A} - \mathbf{1}| < \varepsilon\}$$

for $\varepsilon > 0$ sufficiently small.

Note that $SO(3)\mathcal{N}_\varepsilon = \mathcal{N}_\varepsilon SO(3) = \mathcal{N}_\varepsilon$, since if $\mathbf{Q} \in SO(3)$

$$|(\mathbf{AQ})^T\mathbf{AQ} - \mathbf{1}| = |\mathbf{Q}^T(\mathbf{A}^T\mathbf{A} - \mathbf{1})\mathbf{Q}| = |\mathbf{A}^T\mathbf{A} - \mathbf{1}|.$$

Suppose for contradiction that the result is false for $\varepsilon = j^{-1}$, $j = 1, 2 \ldots$. Then for each j there exists $\boldsymbol{\mu}^{(j)}$ with $\mathbf{B}\boldsymbol{\mu}^{(j)}\mathbf{B}^{-1} \notin P(\mathbf{B})$ and $\mathbf{C}^{(j)} = \mathbf{D}^{(j)}\mathbf{B}\boldsymbol{\mu}^{(j)}\mathbf{B}^{-1} \in \mathcal{N}_{1/j}$.

We can assume that $\mathbf{C}^{(j)} \to \mathbf{R}, \mathbf{D}^{(j)} \to \tilde{\mathbf{R}}, \boldsymbol{\mu}^{(j)} \to \boldsymbol{\mu}$, where $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$, and hence $\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \in P(\mathbf{B})$. But $\boldsymbol{\mu}^{(j)} \to \boldsymbol{\mu}$ implies $\boldsymbol{\mu}^{(j)} = \boldsymbol{\mu}$ for j sufficiently large. Contradiction. □

If we apply this result to the phase transformation case then we can restrict the symmetry group to $P^{+}(\mathbf{B})$ provided $\mathbf{U}(\theta)$ is sufficiently close to $\mathbf{1}$ and θ sufficiently close to θ_c.

Thus, restricting ψ to $\mathcal{N}$, and defining as before

$$K(\theta) = \{\mathbf{A} \in \mathcal{N} : \psi(\mathbf{A}, \theta) = 0\},$$

we assume that

$$K(\theta) = \begin{cases} \alpha(\theta) SO(3) & \theta > \theta_c \\ SO(3) \cup \bigcup_{i=1}^{M} SO(3)\mathbf{U}_i(\theta_c) & \theta = \theta_c \\ \bigcup_{i=1}^{M} SO(3)\mathbf{U}_i(\theta) & \theta < \theta_c \end{cases},$$

where $\mathbf{U}_i(\theta)$ are the distinct matrices $\mathbf{Q}^T\mathbf{U}(\theta)\mathbf{Q}$ for $\mathbf{Q} \in P^c \cap SO(3) = P^{24}$.

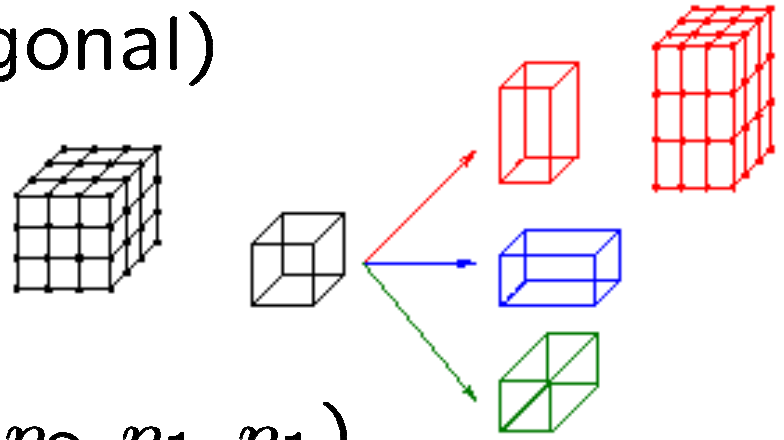
M is the number of *martensitic variants*. If we let

$$G_i = \{\mathbf{Q} \in P^c : \mathbf{Q}^T\mathbf{U}(\theta)\mathbf{Q} = \mathbf{U}_i(\theta)\}$$

then $|G_i|$ is independent of i and so M divides 24.

Example 1. (cubic-to-tetragonal)

(e.g. InTl, NiAl, NiMn, $BaTiO_3$)



$$\mathbf{U}(\theta) = \text{diag}\,(\eta_2, \eta_1, \eta_1),$$

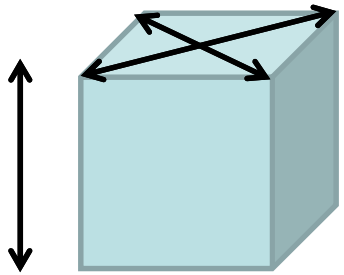
where $\eta_1 = \eta_1(\theta) > 0$, $\eta_2 = \eta_2(\theta) > 0$, $\eta_1 \neq \eta_2$.

Then $M = 3$ and

$$\mathbf{U}_1(\theta) = \text{diag}\,(\eta_2, \eta_1, \eta_1), \mathbf{U}_2(\theta) = \text{diag}\,(\eta_1, \eta_2, \eta_1),$$

$$\mathbf{U}_3(\theta) = \text{diag}\,(\eta_1, \eta_1, \eta_2).$$

Example 2. (cubic-to-orthorhombic)
(e.g. CuAlNi)

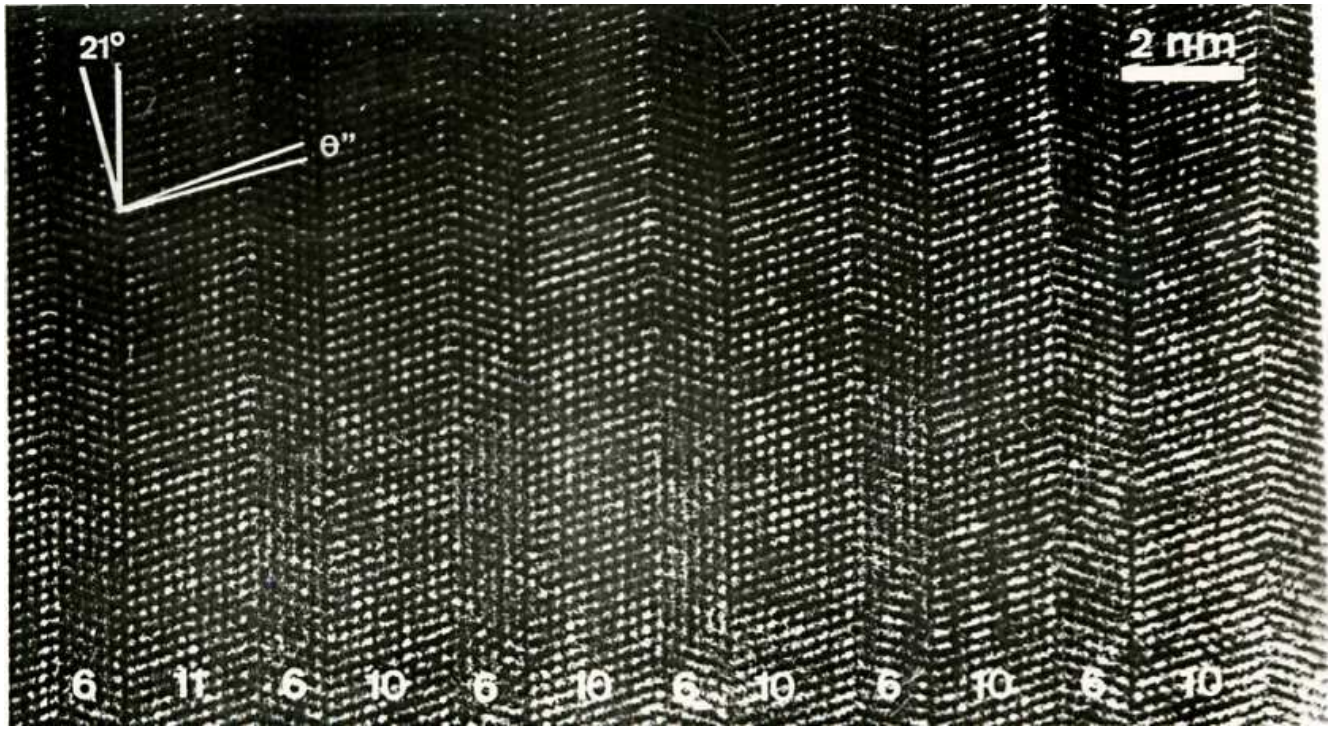


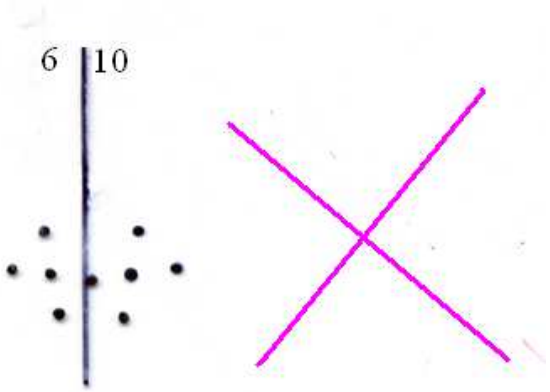
$$\mathbf{U}(\theta) = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \alpha = \alpha(\theta) > 0, \beta = \beta(\theta) > 0, \gamma = \gamma(\theta) > 0$$

$M = 6$

$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \mathbf{U}_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \mathbf{U}_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},$$

$$\mathbf{U}_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix}, \quad \mathbf{U}_5 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}, \quad \mathbf{U}_6 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}.$$

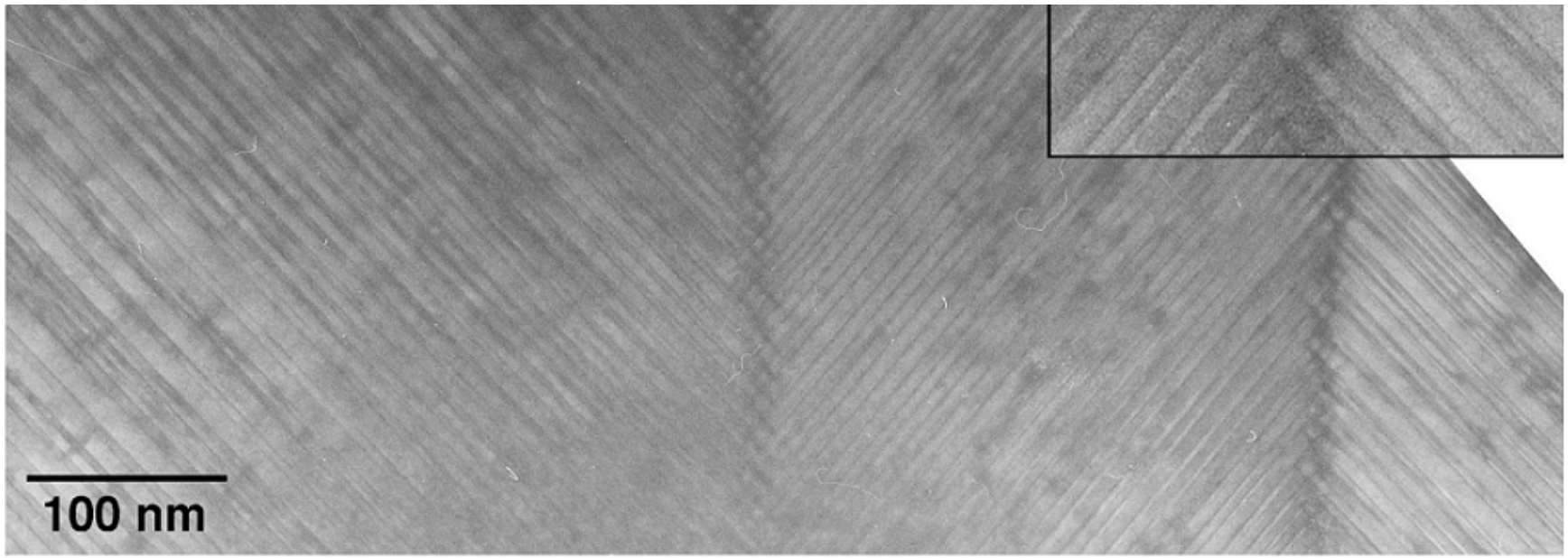




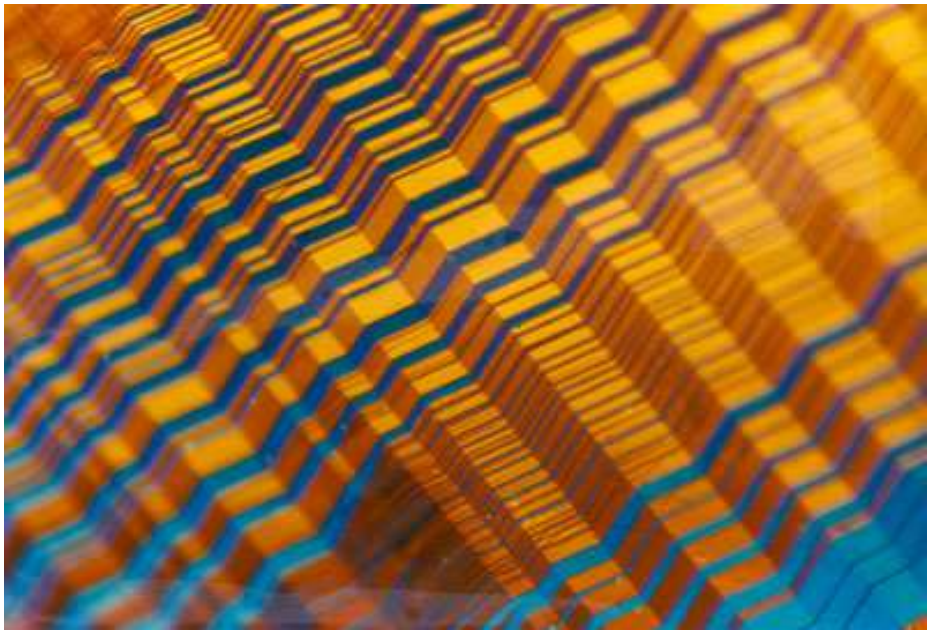
Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

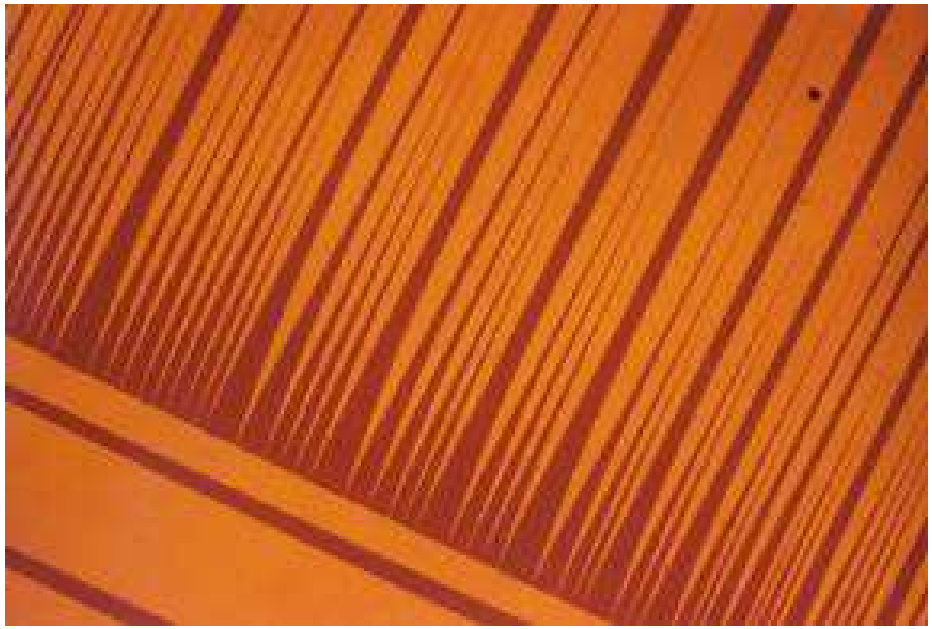
Baele, van Tenderloo, Amelinckx

Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



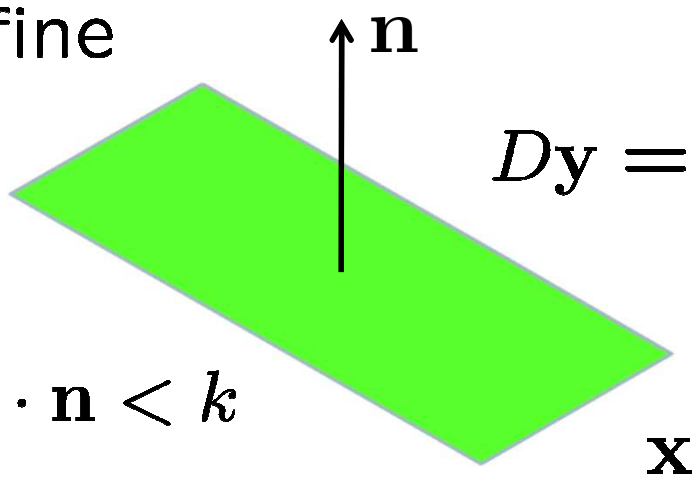
Martensitic microstructures in CuAlNi (Chu/James)





The Hadamard jump condition

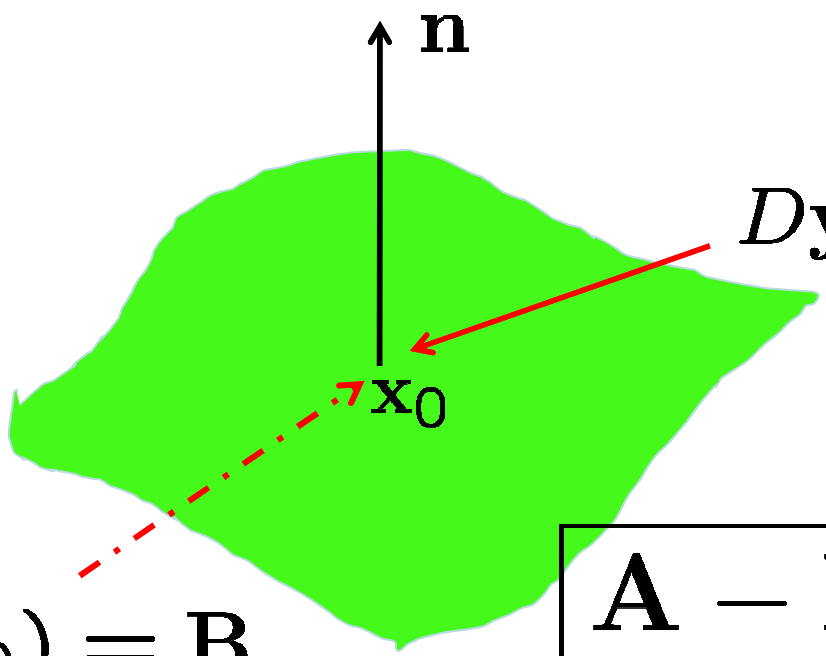
$\mathbf{y}$ piecewise affine



Let $\mathbf{C} = \mathbf{A} - \mathbf{B}$. Then $\mathbf{Cx} = \mathbf{0}$ if $\mathbf{x}\cdot\mathbf{n} = 0$. Thus $\mathbf{C}(\mathbf{z} - (\mathbf{z}\cdot\mathbf{n})\mathbf{n}) = \mathbf{0}$ for all $\mathbf{z}$, and so $\mathbf{Cz} = (\mathbf{Cn}\otimes\mathbf{n})\mathbf{z}$.

Hence $\boxed{\mathbf{A} - \mathbf{B} = \mathbf{a}\otimes\mathbf{n}}$ Hadamard jump condition

More generally this holds for $\mathbf{y}$ piecewise C^1, with $D\mathbf{y}$ jumping across a C^1 surface.



$$D\mathbf{y}^+(\mathbf{x}_0) = \mathbf{A}$$

$$D\mathbf{y}^-(\mathbf{x}_0) = \mathbf{B}$$

$$\boxed{\mathbf{A} - \mathbf{B} = \mathbf{a} \otimes \mathbf{n}}$$

(See later for generalizations when $\mathbf{y}$ not piecewise C^1.)

Theorem

Let $\mathbf{U} = \mathbf{U}^T > 0$, $\mathbf{V} = \mathbf{V}^T > 0$. Then $\mathrm{SO}(3)\,\mathbf{U}$, $\mathrm{SO}(3)\,\mathbf{V}$ are rank-one connected iff

$$\mathbf{U}^2 - \mathbf{V}^2 = c(\mathbf{n} \otimes \tilde{\mathbf{n}} + \tilde{\mathbf{n}} \otimes \mathbf{n}) \qquad (*)$$

for unit vectors $\mathbf{n}$, $\tilde{\mathbf{n}}$ and some $c \neq 0$.

If $\tilde{\mathbf{n}} \neq \pm\mathbf{n}$ there are exactly two rank-one connections between $\mathbf{V}$ and $\mathrm{SO}(3)\,\mathbf{U}$ given by

$$\mathbf{R}\mathbf{U} = \mathbf{V} + \mathbf{a} \otimes \mathbf{n}, \quad \tilde{\mathbf{R}}\mathbf{U} = \mathbf{V} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}},$$

for suitable $\mathbf{R}, \tilde{\mathbf{R}} \in \mathrm{SO}(3)$, $\mathbf{a}, \tilde{\mathbf{a}} \in \mathbb{R}^3$.

(JB/Carstensen version of standard result cf. Ericksen, Gurtin, JB/James ...)

Proof. Note first that

$$\begin{aligned}\det(\mathbf{V}+\mathbf{a}\otimes\mathbf{n}) &= \det\mathbf{V}\cdot\det(1+\mathbf{V}^{-1}\mathbf{a}\otimes\mathbf{n})\\ &= \det\mathbf{V}\cdot(1+\mathbf{V}^{-1}\mathbf{a}\cdot\mathbf{n}).\end{aligned}$$

Hence if $1+\mathbf{V}^{-1}\mathbf{a}\cdot\mathbf{n}>0$, then by the polar decomposition theorem $\mathbf{RU}=\mathbf{V}+\mathbf{a}\otimes\mathbf{n}$ for some $\mathbf{R}\in\mathrm{SO}(3)$ if and only if

$$\begin{aligned}\mathbf{U}^2 &= (\mathbf{V}+\mathbf{n}\otimes\mathbf{a})(\mathbf{V}+\mathbf{a}\otimes\mathbf{n})\\ &= \mathbf{V}^2+\mathbf{V}\mathbf{a}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{V}\mathbf{a}+|\mathbf{a}|^2\mathbf{n}\otimes\mathbf{n}\\ &= \mathbf{V}^2+\left(\mathbf{V}\mathbf{a}+\frac{1}{2}|\mathbf{a}|^2\mathbf{n}\right)\otimes\mathbf{n}+\mathbf{n}\otimes\left(\mathbf{V}\mathbf{a}+\frac{1}{2}|\mathbf{a}|^2\mathbf{n}\right).\end{aligned}$$

If $\mathbf{a} \neq \mathbf{0}$ then $\mathbf{V}\mathbf{a} + \frac{1}{2}|\mathbf{a}|^2\mathbf{n} \neq \mathbf{0}$, since otherwise

$$\mathbf{V}\mathbf{a} \cdot \mathbf{V}^{-1}\mathbf{a} + \frac{1}{2}|\mathbf{a}|^2\mathbf{V}^{-1}\mathbf{a} \cdot \mathbf{n} = 0,$$

i.e. $2 + \mathbf{V}^{-1}\mathbf{a} \cdot \mathbf{n} = 0$. This proves the necessity of (*).

Conversely, suppose $(*)$ holds. We need to find $\mathbf{a} \neq \mathbf{0}$ such that $\mathbf{V}\mathbf{a} + \frac{1}{2}|\mathbf{a}|^2\mathbf{n} = c\tilde{\mathbf{n}}$ and $1 + \mathbf{V}^{-1}\mathbf{a} \cdot \mathbf{n} > 0$. So we need to find t such that

$$\mathbf{a} = c\mathbf{r} + t\mathbf{s}$$

where $|c\mathbf{r} + t\mathbf{s}|^2 + 2t = 0$ and $1 + (c\mathbf{r} + t\mathbf{s}) \cdot \mathbf{s} > 0$, where we have written $\mathbf{r} = \mathbf{V}^{-1}\tilde{\mathbf{n}}$, $\mathbf{s} = \mathbf{V}^{-1}\mathbf{n}$.

The quadratic for t has the form

$$t^2|\mathbf{s}|^2 + 2t(1 + c\mathbf{r}\cdot\mathbf{s}) + c^2|\mathbf{r}|^2 = 0 \text{ with roots}$$

$$t = \frac{-(1 + c\mathbf{r}\cdot\mathbf{s}) \pm \sqrt{(1 + c\mathbf{r}\cdot\mathbf{s})^2 - c^2|\mathbf{r}|^2|\mathbf{s}|^2}}{|\mathbf{s}|^2}.$$

Since $\det \mathbf{U}^2 = \det \mathbf{V}^2 \det(1 + c(\mathbf{r}\otimes\mathbf{s} + \mathbf{s}\otimes\mathbf{r}))$,

$$\det(1 + c(\mathbf{r}\otimes\mathbf{s} + \mathbf{s}\otimes\mathbf{r})) = (1 + c\mathbf{r}\cdot\mathbf{s})^2 - c^2|\mathbf{r}|^2|\mathbf{s}|^2$$

is positive and the roots are real. In order to satisfy $1 + c\mathbf{r}\cdot\mathbf{s} + t|\mathbf{s}|^2 > 0$ we must take the $+$ sign, giving a unique $\mathbf{a}$, and thus unique $\mathbf{R}$ such that $\mathbf{RU} = \mathbf{V} + \mathbf{a}\otimes\mathbf{n}$.

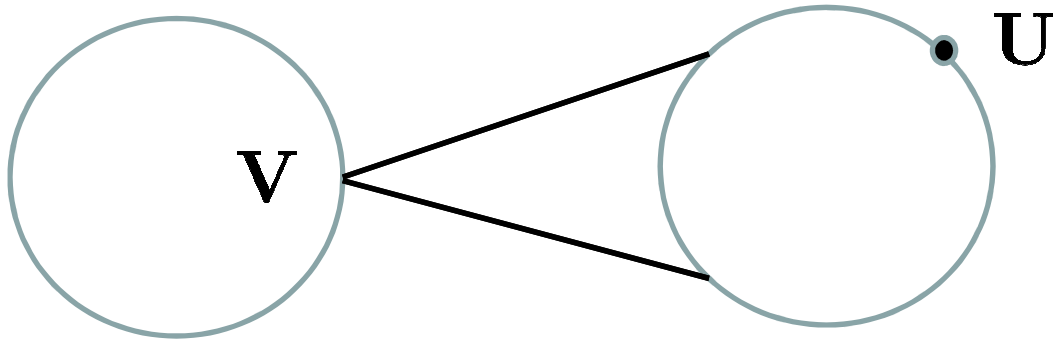
Similarly we get a unique $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{R}}$ such that $\tilde{\mathbf{R}}\mathbf{U} = \mathbf{V} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$.

To complete the proof it suffices to check the following

Lemma

If $c(\mathbf{n} \otimes \tilde{\mathbf{n}} + \tilde{\mathbf{n}} \otimes \mathbf{n}) = c'(\tilde{\mathbf{p}} \otimes \mathbf{p} + \mathbf{p} \otimes \tilde{\mathbf{p}})$ for unit vectors $\mathbf{p}, \tilde{\mathbf{p}}$ and some constant c', then either $\mathbf{p} \otimes \tilde{\mathbf{p}} = \pm \mathbf{n} \otimes \tilde{\mathbf{n}}$ or $\mathbf{p} \otimes \tilde{\mathbf{p}} = \pm \tilde{\mathbf{n}} \otimes \mathbf{n}$.

□



Corollaries:

1. There are no rank-one connections between matrices $\mathbf{A}, \mathbf{B}$ belonging to the *same* energy well.

Proof. In this case $\mathbf{U} = \mathbf{V}$, contradicting $c \neq 0$. □

2. There is a rank-one connection between pairs of matrices $\mathbf{A} \in SO(3)$ and $\mathbf{B} \in SO(3)\mathbf{U}$ *if and only if* $\mathbf{U}$ *has middle eigenvalue 1.*

(Thus it is in generically impossible to have an interface between constant gradients in the austenite and martensite energy wells.)

Proof. If there is a rank-one connection then 1 is an eigenvalue since $\det(\mathbf{U}^2 - 1) = 0$.

Choosing $\mathbf{e}$ with $\tilde{\mathbf{n}}\cdot\mathbf{e} > 0, \mathbf{n}\cdot\mathbf{e} > 0$ and $\tilde{\mathbf{n}}\cdot\mathbf{e} > 0$, $\mathbf{n}\cdot\mathbf{e} < 0$, we see that 1 is the middle eigenvalue. Conversely, if

$$\mathbf{U} = \lambda_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3$$

with eigenvectors $\mathbf{e}_i$ and eigenvalues $\lambda_1 \leq 1 \leq \lambda_3$ then

$$\begin{aligned}\mathbf{U}^2 - 1 = \frac{\lambda_3^2 - \lambda_1^2}{2}\Big(&(\alpha\mathbf{e}_1 + \beta\mathbf{e}_3) \otimes (-\alpha\mathbf{e}_1 + \beta\mathbf{e}_3) \\ &+ (-\alpha\mathbf{e}_1 + \beta\mathbf{e}_3) \otimes (\alpha\mathbf{e}_1 + \beta\mathbf{e}_3)\Big),\end{aligned}$$

where $\alpha = \sqrt{\frac{1-\lambda_1^2}{\lambda_3^2-\lambda_1^2}}, \beta = \sqrt{\frac{\lambda_3^2-1}{\lambda_3^2-\lambda_1^2}}$. □

3. If $\mathbf{U}_i, \mathbf{U}_j$ are distinct martensitic variants then $SO(3)\mathbf{U}_i$ and $SO(3)\mathbf{U}_j$ are rank-one connected if and only if $\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$, and the possible interface normals are orthogonal. Variants separated by such interfaces are called *twins*.

Proof. Clearly $\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$ is necessary, since the matrix on the RHS of (*) is of rank at most 2.

Conversely suppose that $\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$.
Then $\mathbf{U}_i^2 - \mathbf{U}_j^2$ has the spectral decomposition

$$\mathbf{U}_i^2 - \mathbf{U}_j^2 = \lambda \mathbf{e} \otimes \mathbf{e} + \mu \hat{\mathbf{e}} \otimes \hat{\mathbf{e}}.$$

Since $\mathbf{U}_j = \mathbf{R}\mathbf{U}_i\mathbf{R}^T$ for some $\mathbf{R} \in P^{24}$ it follows that $\mathrm{tr}\,(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$. Hence $\mu = -\lambda$ and

$$\begin{aligned}\mathbf{U}_i^2 - \mathbf{U}_j^2 &= \lambda(\mathbf{e}\otimes\mathbf{e} - \hat{\mathbf{e}}\otimes\hat{\mathbf{e}}) \\ &= \lambda\left(\frac{\mathbf{e}+\hat{\mathbf{e}}}{\sqrt{2}}\otimes\frac{\mathbf{e}-\hat{\mathbf{e}}}{\sqrt{2}} + \frac{\mathbf{e}-\hat{\mathbf{e}}}{\sqrt{2}}\otimes\frac{\mathbf{e}+\hat{\mathbf{e}}}{\sqrt{2}}\right),\end{aligned}$$

as required. □

Remark: Another equivalent condition due to Forclaz is that $\det(\mathbf{U}_i - \mathbf{U}_j) = 0$. This is because of the surprising identity (not valid in higher dimensions)

$$\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = (\lambda_1+\lambda_2)(\lambda_2+\lambda_3)(\lambda_3+\lambda_1)\det(\mathbf{U}_i - \mathbf{U}_j).$$

Mallard's law

Let $\mathbf{U} = \mathbf{U}^T > 0$, $\mathbf{V} = \mathbf{V}^T > 0$ be such that

$$\mathbf{V} = (-\mathbf{1} + 2\mathbf{e} \otimes \mathbf{e})\mathbf{U}(-\mathbf{1} + 2\mathbf{e} \otimes \mathbf{e}), \qquad (\dagger)$$

where $|\mathbf{e}| = 1$. Then $SO(3)\mathbf{U}$ and $SO(3)\mathbf{V}$ are rank-one connected with rank-one connections given by

$$\mathbf{QV} = \mathbf{U} + \mathbf{a} \otimes \mathbf{n},$$

$$\mathbf{a} \otimes \mathbf{n} = \begin{cases} 2\left(\frac{\mathbf{U}^{-1}\mathbf{e}}{|\mathbf{U}^{-1}\mathbf{e}|^2} - \mathbf{Ue}\right) \otimes \mathbf{e} & \text{(Type I)}, \\ 2\mathbf{Ue} \otimes \left(\mathbf{e} - \frac{\mathbf{U}^2\mathbf{e}}{|\mathbf{Ue}|^2}\right) & \text{(Type II)}. \end{cases}$$

(In fact Chen et al (2013) show that if $\mathbf{V} = \mathbf{RUR}^T$ for some $\mathbf{R} \in SO(3)$ then $SO(3)\mathbf{U}$ and $SO(3)\mathbf{V}$ are rank-one connected iff (†) holds for some $\mathbf{e}$.)

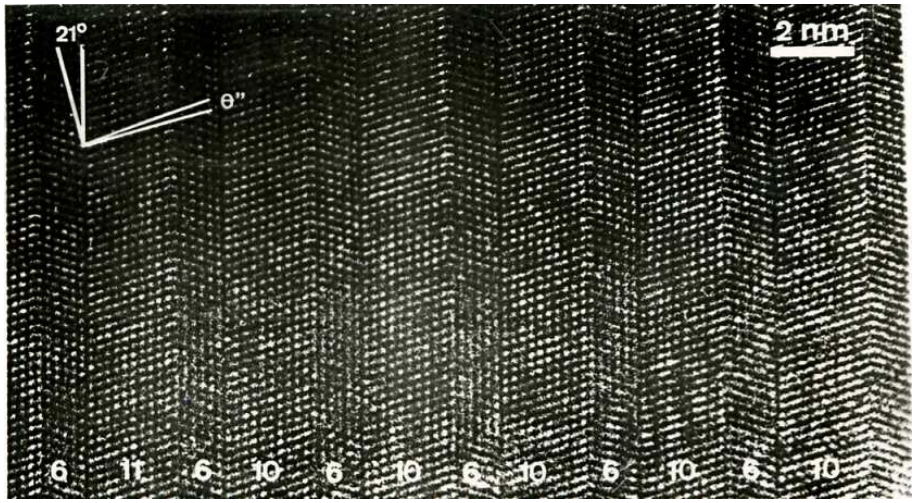
For example, for cubic-to-tetragonal we can take

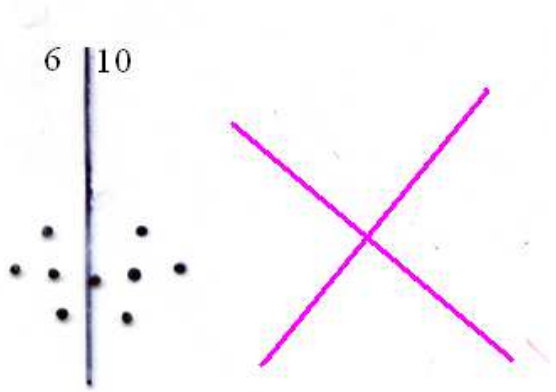
$$\mathbf{U}_1 = \text{diag}\,(\eta_2, \eta_1, \eta_1), \quad \mathbf{U}_2 = \text{diag}\,(\eta_1, \eta_2, \eta_1),$$

and then

$$\mathbf{U}_1^2 - \mathbf{U}_2^2 = \frac{1}{2}(\eta_2^2 - \eta_1^2)\Big((\mathbf{e}_2 - \mathbf{e}_1)\otimes(\mathbf{e}_2 + \mathbf{e}_1) + (\mathbf{e}_2 + \mathbf{e}_1)\otimes(\mathbf{e}_2 - \mathbf{e}_1)\Big),$$

so that twinning is on [110] planes.





Convexity conditions

Let $\psi : M^{3\times 3} \to \mathbb{R}$ be continuous. We say that

ψ is *rank-one convex* if $t \mapsto \psi(\mathbf{A} + t\mathbf{a}\otimes\mathbf{n})$ is convex for all $\mathbf{A} \in M^{3\times 3}$, and $\mathbf{a}, \mathbf{n} \in \mathbb{R}^3$,

Null Lagrangians

ψ is *polyconvex* if $\psi(\mathbf{A}) = g(\mathbf{A}, \operatorname{cof}\mathbf{A}, \det\mathbf{A})$ for all $\mathbf{A} \in M^{3\times 3}$ for some convex g,

ψ is *quasiconvex* if

$$\int_\Omega \psi(D\mathbf{z}(\mathbf{x}))\, d\mathbf{x} \geq \int_\Omega \psi(\mathbf{A})\, d\mathbf{x}$$

whenever $\mathbf{z} \in \mathbf{A}\mathbf{x} + W_0^{1,\infty}(\Omega;\mathbb{R}^3)$

definition independent of Ω

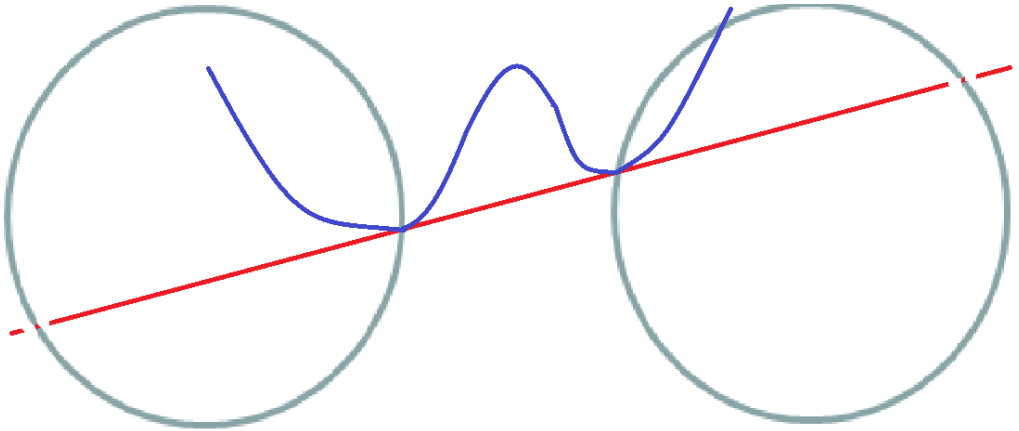
or $C_0^\infty(\Omega;\mathbb{R}^3)$

ψ polyconvex $\Rightarrow$ ψ quasiconvex $\Rightarrow$ ψ rank-one convex

$\not\Leftarrow$ Roughly N&S $\not\Leftarrow$

for existence

of minimizers

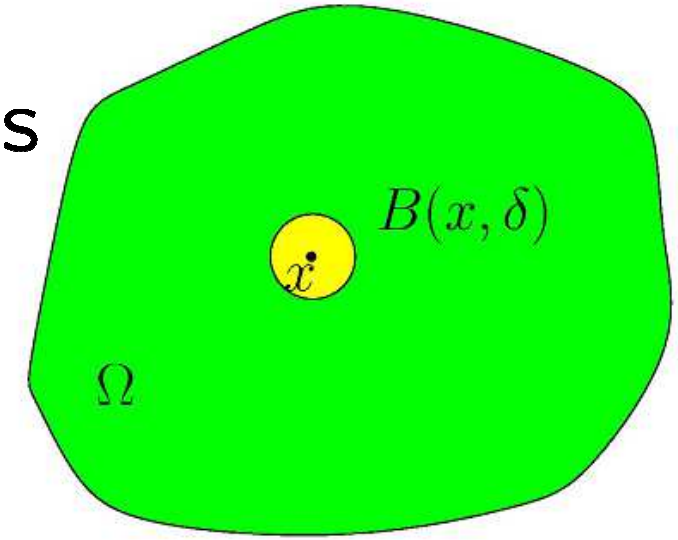


The free-energy function $\psi(\cdot,\theta)$ is not quasiconvex because the existence of rank-one connections between energy wells implies that $\psi(\cdot,\theta)$ is not rank-one convex.

So we expect the minimum of the energy in general not to be attained, with the gradients $D\mathbf{y}^{(j)}$ of minimizing sequences generating *infinitely fine* microstructures.

Gradient Young measures

Given a sequence of gradients $D\mathbf{y}^{(j)}$, fix $j, \mathbf{x}, \delta$.



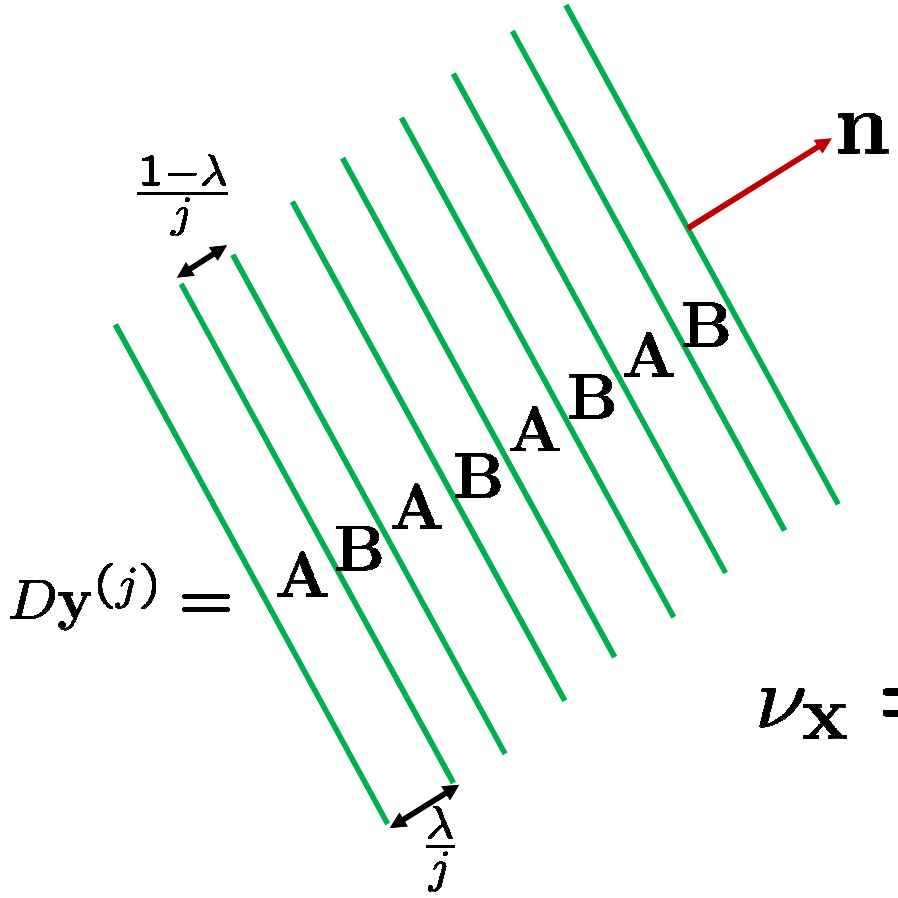
Let $E \subset M^{3\times 3}$.

$$\nu_{\mathbf{x},j,\delta}(E) = \frac{\text{vol } \{\mathbf{z} \in B(\mathbf{x},\delta) : D\mathbf{y}^{(j)}(\mathbf{z}) \in E\}}{\text{vol } B(\mathbf{x},\delta)}$$

$$\nu_{\mathbf{x}}(E) = \lim_{\delta \to 0} \lim_{j \to \infty} \nu_{\mathbf{x},j,\delta}(E)$$

Gradient Young measure

Gradient Young measure of a simple laminate



$$\mathbf{A} - \mathbf{B} = \mathbf{a} \otimes \mathbf{n}$$

$$0 < \lambda < 1$$

$$\nu_{\mathbf{x}} = \lambda \delta_{\mathbf{A}} + (1 - \lambda)\delta_{\mathbf{B}}$$

$$Dy^{(j)} \rightharpoonup \lambda \mathbf{A} + (1 - \lambda)\mathbf{B} = \bar{\nu}_{\mathbf{x}} = \int_{M^{3\times 3}} \mathbf{C}\, d\nu_x(\mathbf{C})$$

Theorem (Kinderlehrer/Pedregal)

A family of probability measures $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ *is the Young measure of a sequence of gradients* $D\mathbf{y}^{(j)}$ *bounded in* L^∞ *if and only if*

(i) $\bar{\nu}_{\mathbf{x}}$ *is a gradient (*$D\mathbf{y}$*, the weak limit of* $D\mathbf{y}^{(j)}$*)*

(ii) $\langle \nu_{\mathbf{x}}, f\rangle := \int_{M^{3\times 3}} f(\mathbf{C})\, d\nu_{\mathbf{x}}(\mathbf{C}) \geq f(\bar{\nu}_{\mathbf{x}})$

for all quasiconvex f*.*

Convexifications with respect to a cone

Let G be a convex cone of continuous functions $f : M^{3\times 3} \to \mathbb{R}$. Examples are the cones of convex, polyconvex, quasiconvex and rank-one convex functions.

For a continuous $\psi : M^{3\times 3} \to \mathbb{R}$ define the $G-$convexification ψ^G of ψ by

$$\psi^G = \sup\{f \in G : f \leq \psi\}.$$

Then $\psi^c \leq \psi^{pc} \leq \psi^{qc} \leq \psi^{rc}$.

$\psi^{\mathrm{qc}}(\mathbf{A}, \theta)$ is the macroscopic free-energy function corresponding to ψ.

Similarly, for $K \subset M^{3\times 3}$ compact define (Šverák)

$$K^G = \{\mathbf{A} : f(\mathbf{A}) \leq \max_K f \text{ for all } f \in G\}.$$

Then $K^{rc} \subset K^{qc} \subset K^{pc} \subset K^c$.

Theorem (JB/Carstensen (to appear) following Krucik 2000)

$$K^G = \{\mathbf{A} \in M^{3\times 3} : \exists \mu \in \mathcal{P}(K) \text{ with } f(\mathbf{A}) \leq \langle \mu, f\rangle \ \forall f \in G\}$$

In particular

$$K^{qc} = \{\bar{\nu} : \nu \text{ homogeneous gradient YM}, \operatorname{supp}\nu \subset K\}.$$

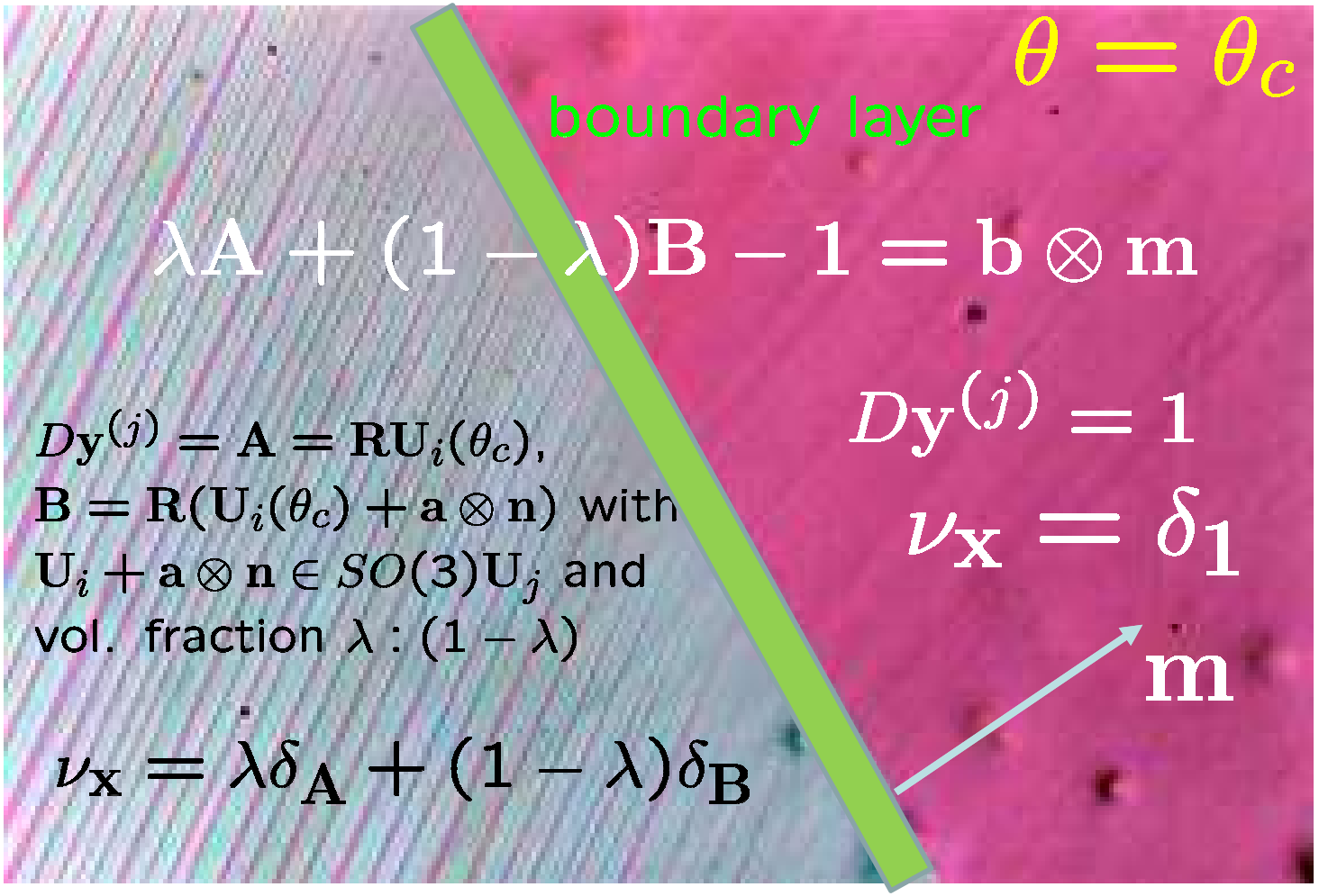
$K(\theta)^{\mathrm{qc}}$ is the set of macroscopic deformation gradients corresponding to zero-energy microstructures.

Phase nucleation

How does austenite transform to martensite as θ passes through θ_c?

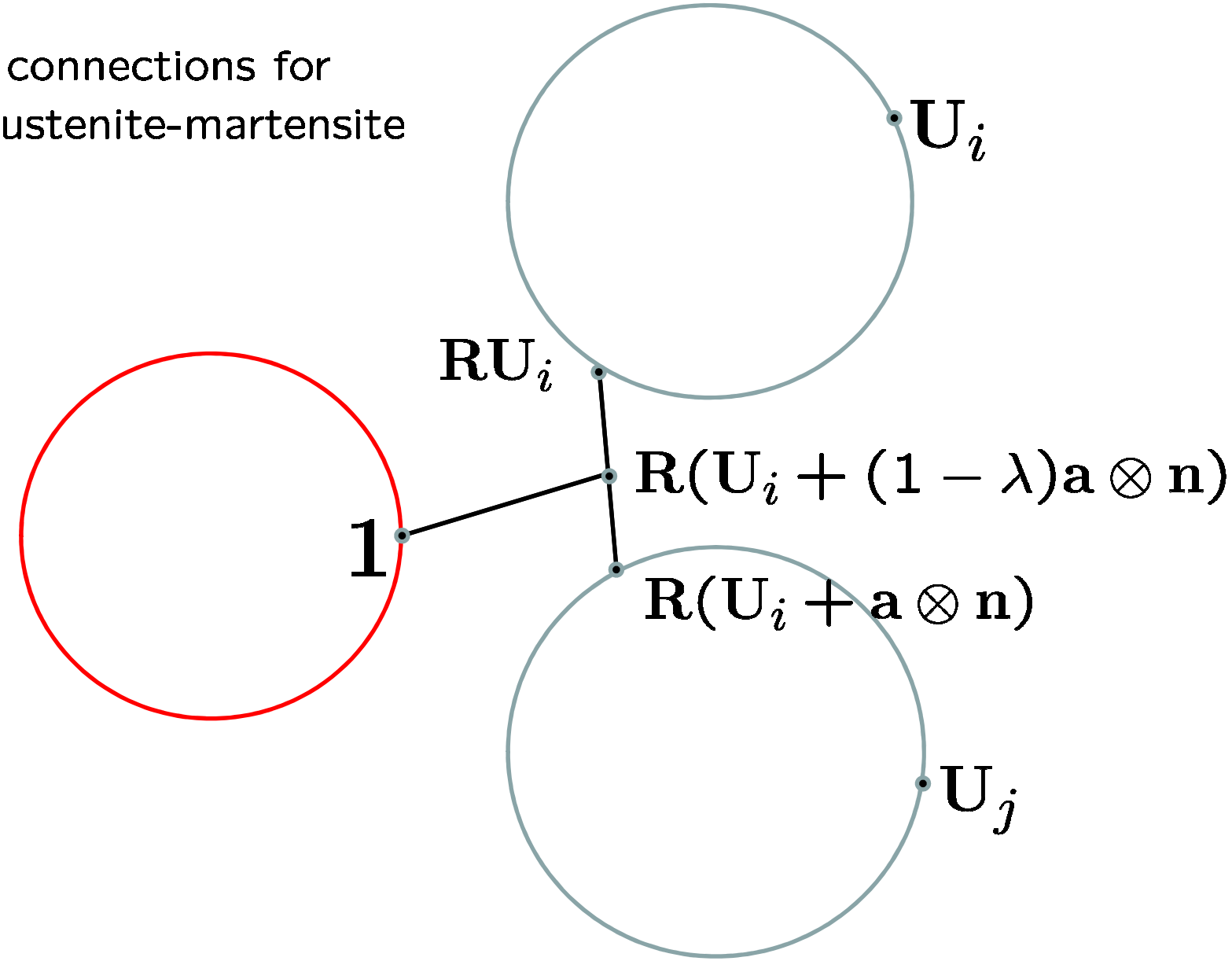
It cannot do this by means of an exact interface between austenite and martensite, because this requires the middle eigenvalue of $\mathbf{U}_i(\theta)$ to be one, which in general is not the case (but see later).

So what does it do?



(Classical) austenite-martensite interface in CuAlNi (courtesy C-H Chu and R. D. James)

Rank-one connections for classical austenite-martensite interface



We have to solve

$$\mathbf{R}(\mathbf{U}_i + (1-\lambda)\mathbf{a} \otimes \mathbf{n}) - \mathbf{1} = \mathbf{b} \otimes \mathbf{m}$$

for $\mathbf{R} \in SO(3), \lambda \in [0,1]$ and $\mathbf{b}, \mathbf{m} \in \mathbb{R}^3$.

The solutions (JB/James 1987) give the formulae of the *crystallographic theory of martensite* (Wechsler, Lieberman & Read 1953)

Let $\delta^* = \mathbf{a} \cdot \mathbf{U}_i(\mathbf{U}_i^2 - \mathbf{1})^{-1}\mathbf{n}$.

Case 1. If $\mathbf{U}_i$ does not have an eigenvalue 1 then there is a solution iff $\delta^* \leq -2$ and

$$\operatorname{tr} \mathbf{U}_i^2 - \det \mathbf{U}_i^2 - 2 + \frac{1}{2\delta^*}|\mathbf{a}|^2 \geq 0,$$

and if $\delta^* < -2$ there are exactly four solutions

$$(\mathbf{R}_1, \lambda^*, \mathbf{b}_1^+ \otimes \mathbf{m}_1^+), \quad (\mathbf{R}_2, \lambda^*, \mathbf{b}_1^- \otimes \mathbf{m}_1^-),$$
$$(\mathbf{R}_3, 1-\lambda^*, \mathbf{b}_2^+ \otimes \mathbf{m}_2^+), \quad (\mathbf{R}_4, 1-\lambda^*, \mathbf{b}_2^- \otimes \mathbf{m}_2^-),$$

where $\lambda^* = \frac{1}{2}\left(1 - \sqrt{1 + \frac{2}{\delta^*}}\right)$.

Case 2. There are solutions for *every* $\lambda \in [0,1]$ iff the following *cofactor conditions*

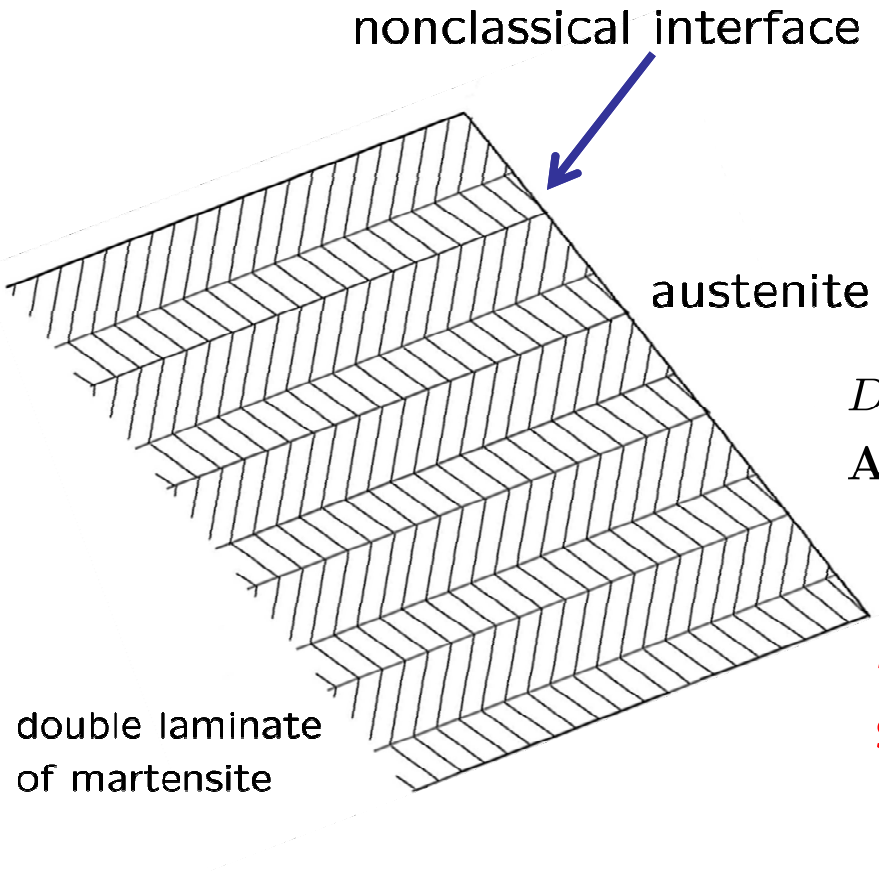
$\mathbf{U}_i$ has middle eigenvalue 1

$\mathbf{a} \cdot \operatorname{cof}(\mathbf{U}_i^2 - \mathbf{1})\mathbf{n} = 0,$

$\operatorname{tr} \mathbf{U}_i^2 - \det \mathbf{U}_i^2 - \frac{|\mathbf{a}|^2}{4} - 2 \geq 0$

hold.

But why (cf JB/Carstensen 1997) should the martensitic microstructure be a simple laminate, rather than something more complicated, such as a double laminate?



$$D\mathbf{y}(\mathbf{x}) = 1$$

$\mathbf{m}$

$\nu_{\mathbf{x}} = \delta_1$

$$D\mathbf{y}(\mathbf{x}) = \mathbf{A} = \bar{\nu}$$

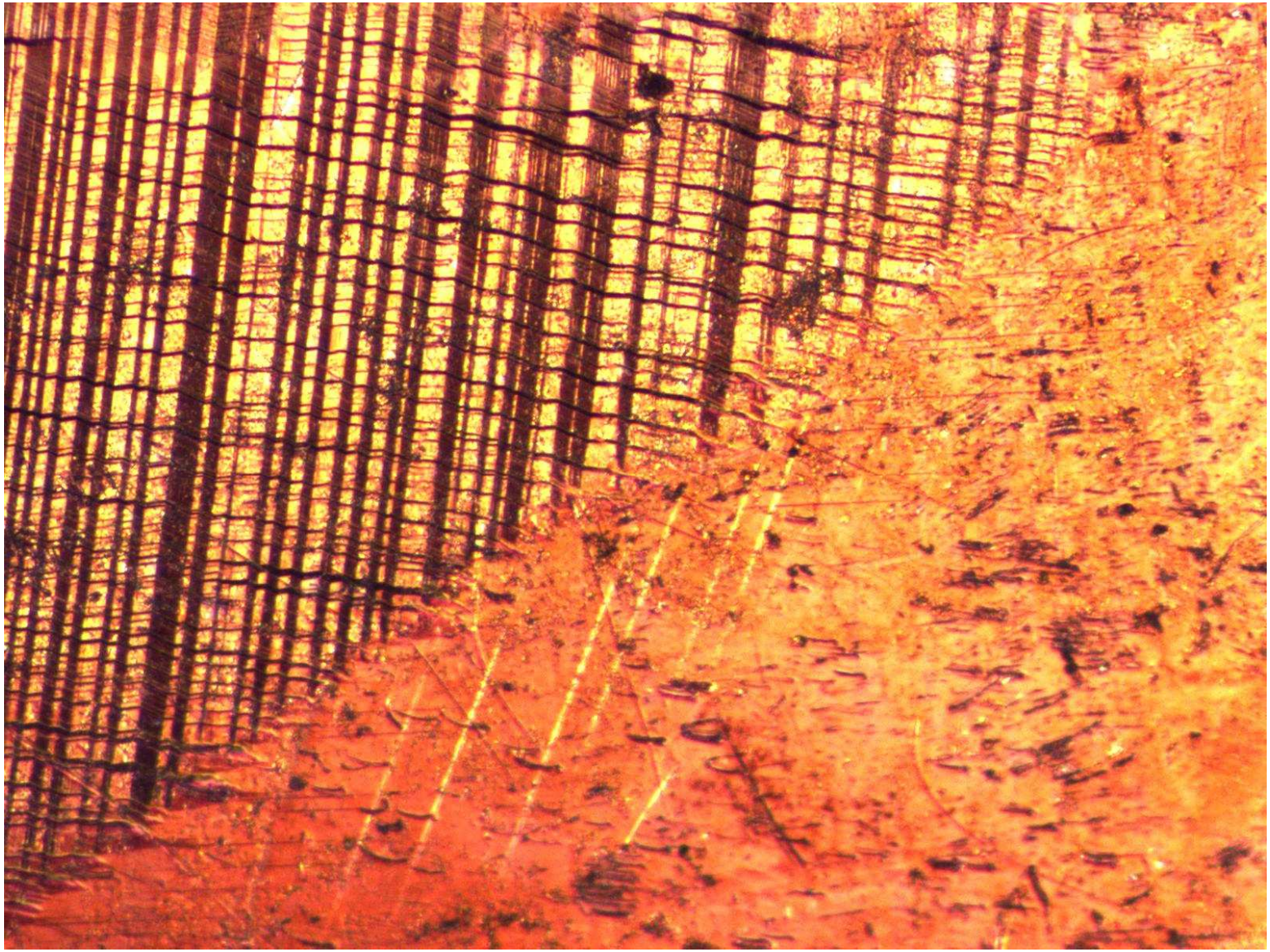
$$\mathbf{A} \in \left(\cup_{i=1}^{M} \mathrm{SO}(3)\mathbf{U}_i(\theta_c)\right)^{\mathrm{qc}}$$

(unknown unless $M = 2$)

$\nu_{\mathbf{x}} = \nu$

$\operatorname{supp} \nu \subset \cup_{i=1}^{M} \mathrm{SO}(3)\mathbf{U}_i(\theta_c)$

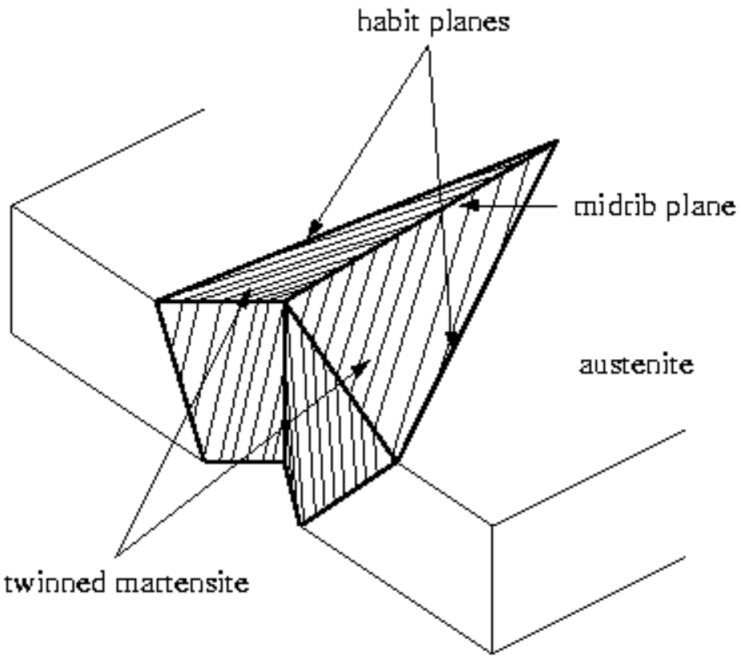
$$\mathbf{A} = 1 + \mathbf{b} \otimes \mathbf{m}$$

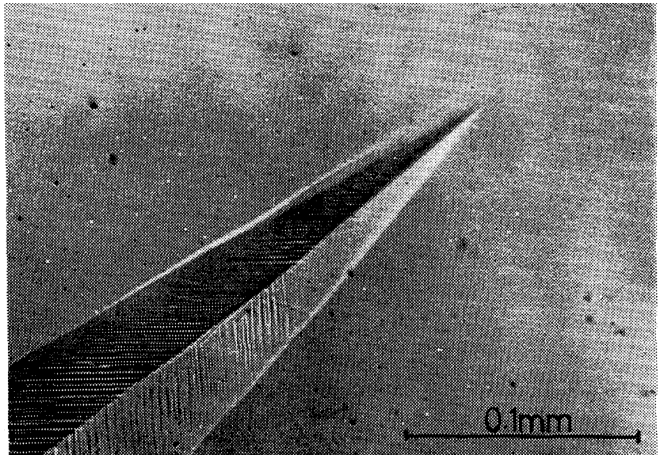


Nonclassical austenite-martensite interface in CuAlNi (H. Seiner)

Special compositions and the discovery of low hysteresis alloys.

1. The wedge microstructure (Bhattacharya 1991)





Wedge microstructure in CuAlNi
Otsuka & Shimizu (1969)

Microstructure supported on energy wells impossible for cubic-to-tetragonal, possible for cubic to orthorhombic iff the eigenvalues α, β, γ of the transformation strain $\mathbf{U}_i(\theta_c)$ satisfy a special relation $f(\alpha, \beta, \gamma) = 0$, which holds to high accuracy for the actual compositions close to Cu-14.2wt.%AI-4.3wt.%Ni used in shape-memory alloys.

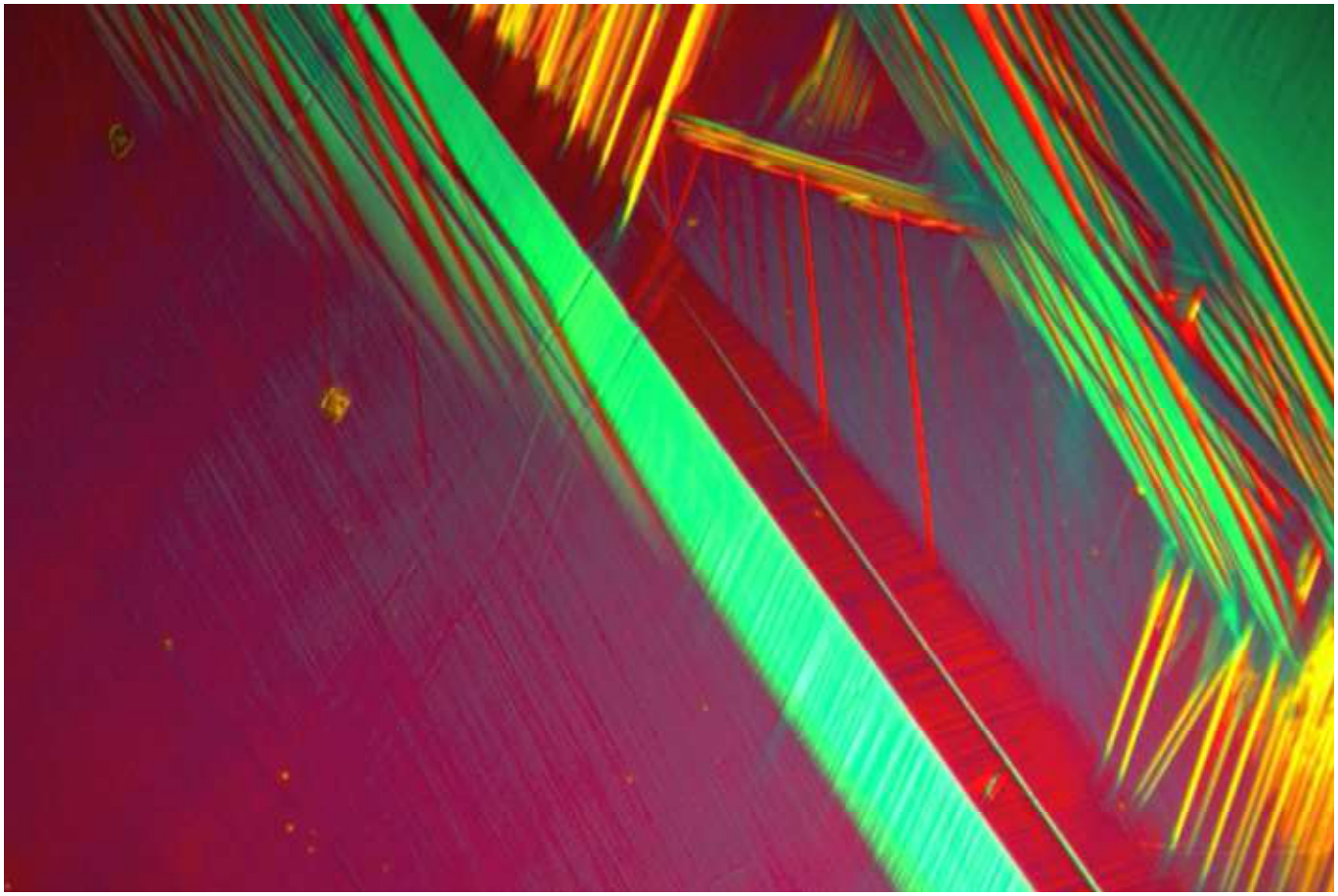
2. Ultra-low hysteresis alloys

James *et.al.* (2013) tuned the composition of a ZnAuCu alloy so that the cofactor conditions were very nearly satisfied, with dramatic results.

(i) the thermal hysteresis was reduced from typical values of $50° - 70°$C to about $2°$C.

(ii) Material undamaged after thousands of thermal cycles (millions for a material discovered later by Quandt, Wuttig et al 2014).

(iii) During thermal cycling remarkable martensitic microstructures are observed that are completely different in each cycle.



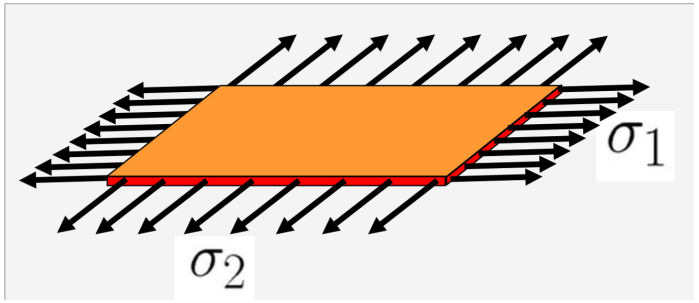
$Zn_{45}Au_{30}Cu_2$ ultra-low hysteresis alloy Song, Chen, Dabade, Shield, James, 2013

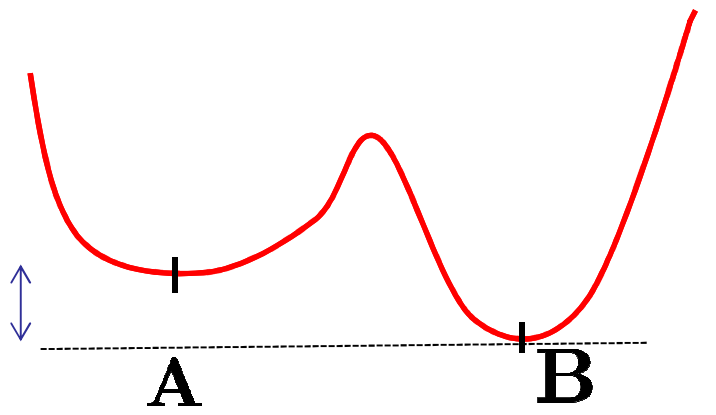
'Moving mask' approximation analyzed by Della Porta (2018), who has also identified further conditions on the $\mathbf{U}_i$ allowing new microstructures, closely satisfied in this alloy.

Incompatibility-induced metastability

Example 1

Special case of JB/James 2014 designed to explain hysteresis in the bi-axial experiments of Chu & James on CuAlNi single crystals, in which a transformation occurs under load between two martensitic variants.





Consider the integral

$$I(\mathbf{y}) = \int_\Omega W(D\mathbf{y})\, d\mathbf{x},$$

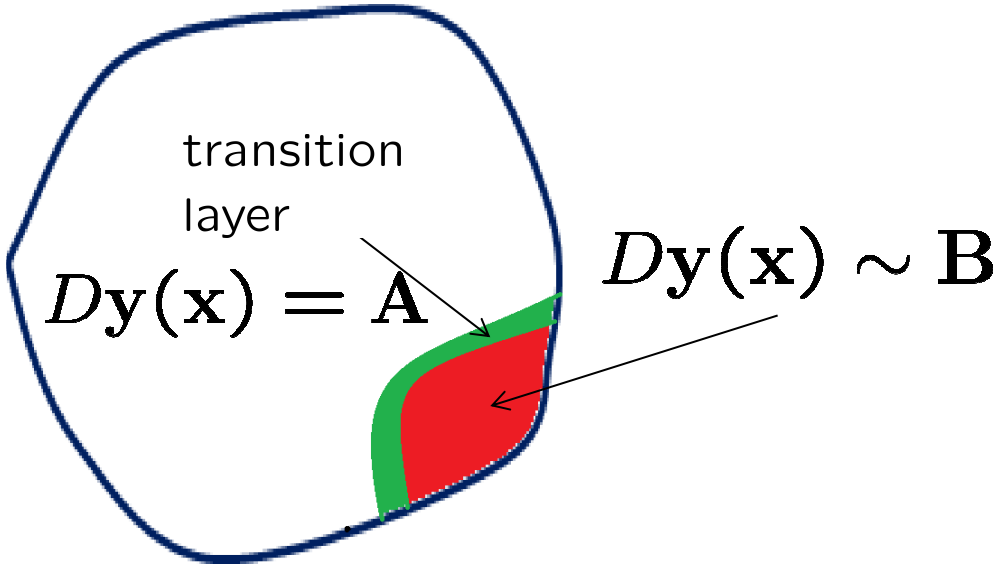
where $W : GL^+(3,\mathbb{R}) \to \mathbb{R}$ and W has two local minimizers at $\mathbf{A}, \mathbf{B}$ with $\text{rank}\,(\mathbf{A} - \mathbf{B}) > 1$ and $W(\mathbf{A}) - W(\mathbf{B}) > 0$ sufficiently small.

$$W(\mathbf{A}) = \psi(\mathbf{A}, \theta) - \mathbf{T} \cdot \mathbf{A}$$

Claim. Under suitable growth hypotheses on W, $\bar{\mathbf{y}}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{c}$ is a local minimizer of I in $L^1(\Omega; \mathbb{R}^3)$, i.e. there exists $\varepsilon > 0$ such that $I(\mathbf{y}) \geq I(\bar{\mathbf{y}})$ if $\int_\Omega |\mathbf{y} - \bar{\mathbf{y}}|\, d\mathbf{x} < \varepsilon$.

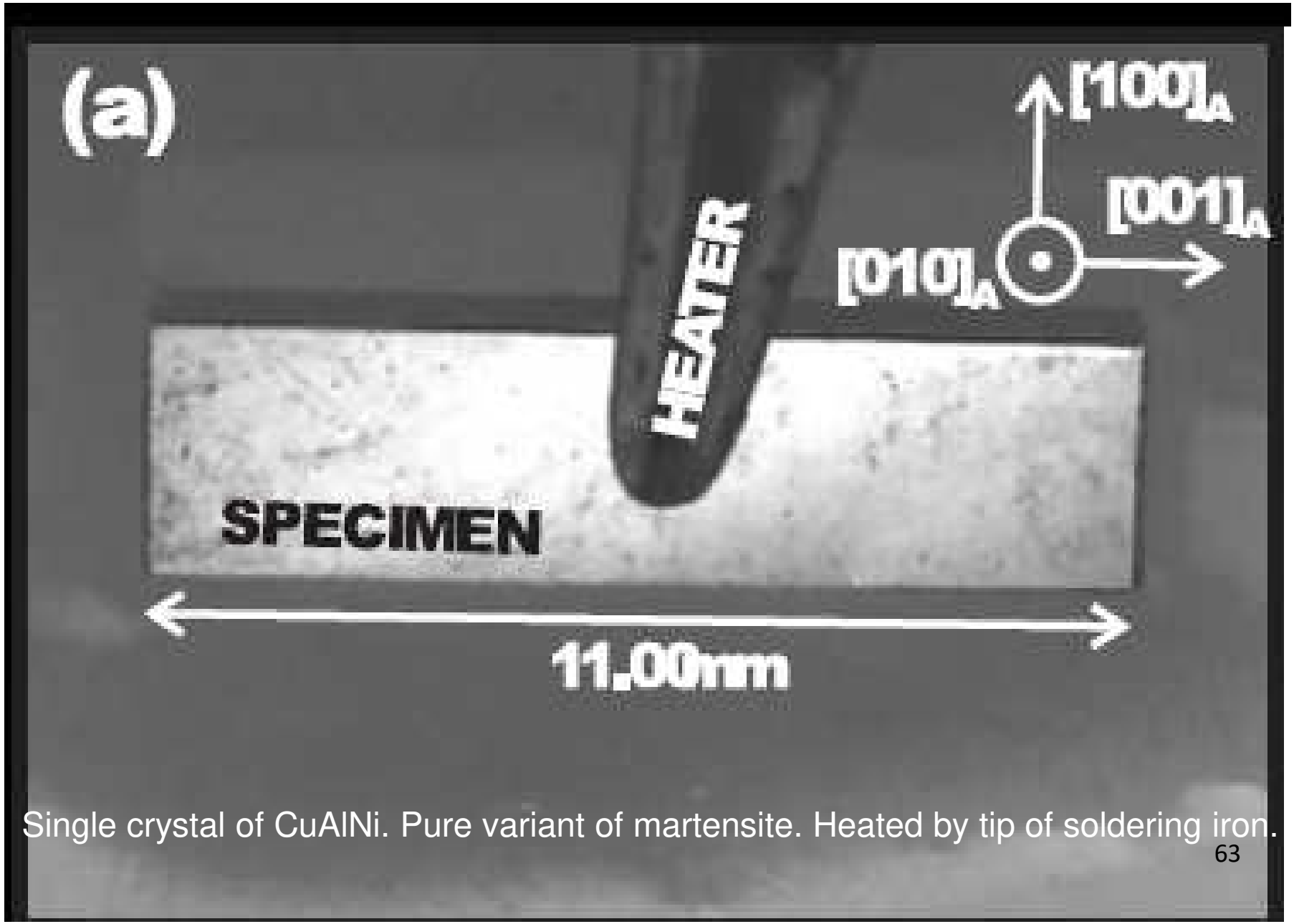
Idea: since $\mathbf{A}$ and $\mathbf{B}$ are incompatible, if we nucleate a region in which $D\mathbf{y}(\mathbf{x}) \sim \mathbf{B}$ there must be a transition layer in which the increase of energy is greater than the decrease of energy in the nucleus.

Related work:
Kohn & Sternberg 1989,
Grabovsky & Mengesha 2009

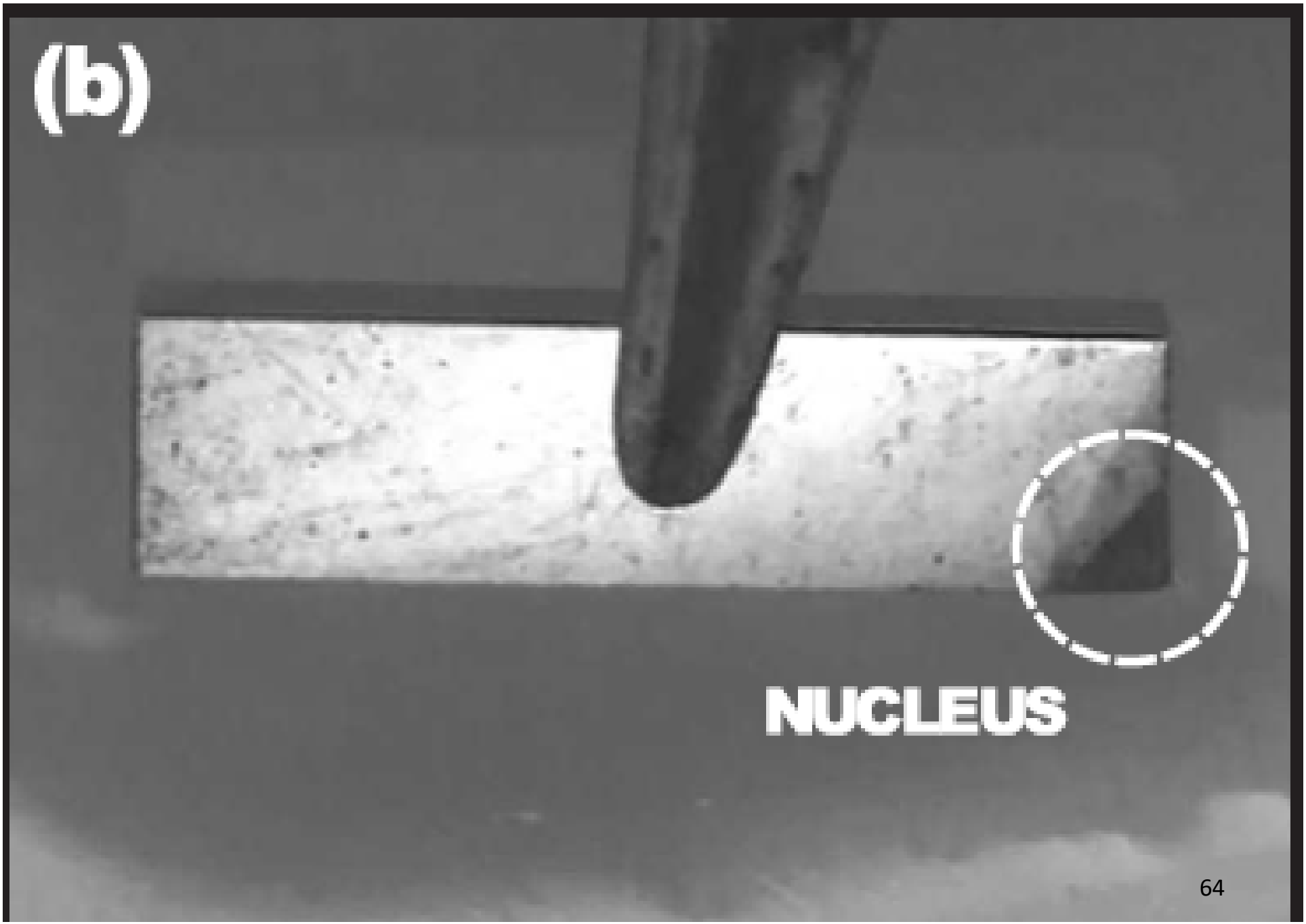


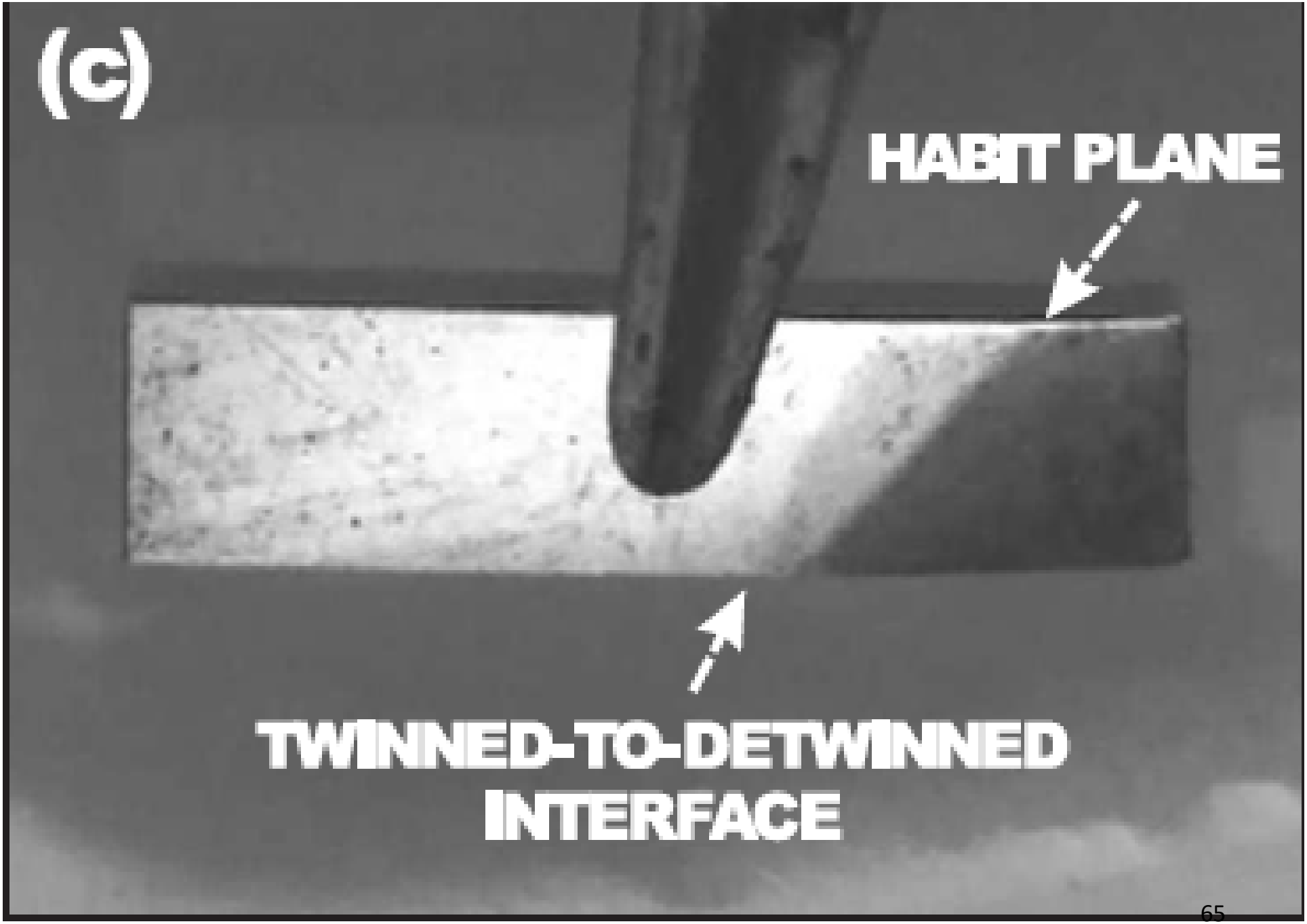
Example 2. Nucleation of austenite in martensite

(JB/K. Koumatos/H. Seiner 2013,2014)



Single crystal of CuAlNi. Pure variant of martensite. Heated by tip of soldering iron.


(b)
NUCLEUS


(c)
HABIT PLANE
TWINNED-TO-DETWINNED
INTERFACE

Twinning and slip in Bravais lattices

Consider a Bravais lattice $\mathbf{B}$. What are the rank-one connections between $SO(3)$ and $SO(3)\mathbf{M}$, where $\mathbf{M} = \mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \notin P(\mathbf{B})$?

We try $\boldsymbol{\mu} = -\mathbf{1} + \mathbf{p} \otimes \mathbf{q}$ with $\mathbf{p}, \mathbf{q} \in \mathbb{Z}^3$ and $\mathbf{p} \cdot \mathbf{q} = 2$, when

$$\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} = -\mathbf{1} + \mathbf{B}\mathbf{p} \otimes \mathbf{B}^{-T}\mathbf{q},$$

$$\begin{aligned}
\mathbf{M}^T\mathbf{M} - \mathbf{1} &= (-\mathbf{1} + \mathbf{B}^{-T}\mathbf{q} \otimes \mathbf{B}\mathbf{p})(-\mathbf{1} + \mathbf{B}\mathbf{p} \otimes \mathbf{B}^{-T}\mathbf{q}) - \mathbf{1} \\
&= -\mathbf{B}^{-T}\mathbf{q} \otimes \mathbf{B}\mathbf{p} - \mathbf{B}\mathbf{p} \otimes \mathbf{B}^{-T}\mathbf{q} + |\mathbf{B}\mathbf{p}|^2 \mathbf{B}^{-T}\mathbf{q} \otimes \mathbf{B}^{-T}\mathbf{q} \\
&= (-\mathbf{B}\mathbf{p} + \frac{1}{2}|\mathbf{B}\mathbf{p}|^2 \mathbf{B}^{-T}\mathbf{q}) \otimes \mathbf{B}^{-T}\mathbf{q} \\
&\qquad + \mathbf{B}^{-T}\mathbf{q} \otimes (-\mathbf{B}\mathbf{p} + \frac{1}{2}|\mathbf{B}\mathbf{p}|^2 \mathbf{B}^{-T}\mathbf{q}).
\end{aligned}$$

Hence $SO(3)$ and $SO(3)\mathbf{M}$ are rank-one connected, with normals parallel to $\mathbf{B}^{-T}\mathbf{q}$ and $-\mathbf{Bp}+\frac{1}{2}|\mathbf{Bp}|^2\mathbf{B}^{-T}\mathbf{q}$.

Note also that if $\mathbf{1}+\mathbf{a}\otimes\mathbf{n}=\mathbf{QM}$ then

$$\begin{aligned}\operatorname{tr}\mathbf{M}^T\mathbf{M}-3 &= \operatorname{tr}(\mathbf{1}+\mathbf{n}\otimes\mathbf{a})(\mathbf{1}+\mathbf{a}\otimes\mathbf{n})-3\\ &= |\mathbf{Bp}|^2|\mathbf{B}^{-T}\mathbf{q}|^2-4,\end{aligned}$$

so that $|\mathbf{a}|^2=|\mathbf{Bp}|^2|\mathbf{B}^{-T}\mathbf{q}|^2-4$.

For a bcc lattice we can take

$$\mathbf{B} = \tfrac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \mathbf{B}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

Then the first case with $\mathbf{p} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, $\mathbf{q} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$ gives

the normals $\begin{pmatrix} \pm 1 \\ \pm 1 \\ 2 \end{pmatrix}$ and $|\mathbf{a}|^2 = \frac{1}{2}$.

These are the most commonly observed normals for bcc metals and alloys, and work of Bevis & Crocker (1968,1969), Jaswon & Dove (1956,1957,1960) probably shows that they minimize $|\mathbf{a}|$.

For fcc we can take

$$\mathbf{B} = \tfrac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}, \mathbf{B}^{-1} = \begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & -1 \\ 0 & 0 & 2 \end{pmatrix}.$$

Then with $\mathbf{p} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$, $\mathbf{q} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$ we get the commonly observed normals $\begin{pmatrix} \pm 1 \\ \pm 1 \\ 1 \end{pmatrix}$ and $|\mathbf{a}|^2 = \frac{1}{2}$.

Another possibility is to take $\boldsymbol{\mu} = \mathbf{1} + \hat{\mathbf{p}} \otimes \hat{\mathbf{q}}$ with $\hat{\mathbf{p}} \cdot \hat{\mathbf{q}} = 0$, when we have $\mathbf{M} = \mathbf{1} + \mathbf{B}\hat{\mathbf{p}} \otimes \mathbf{B}^{-T}\hat{\mathbf{q}}$ and

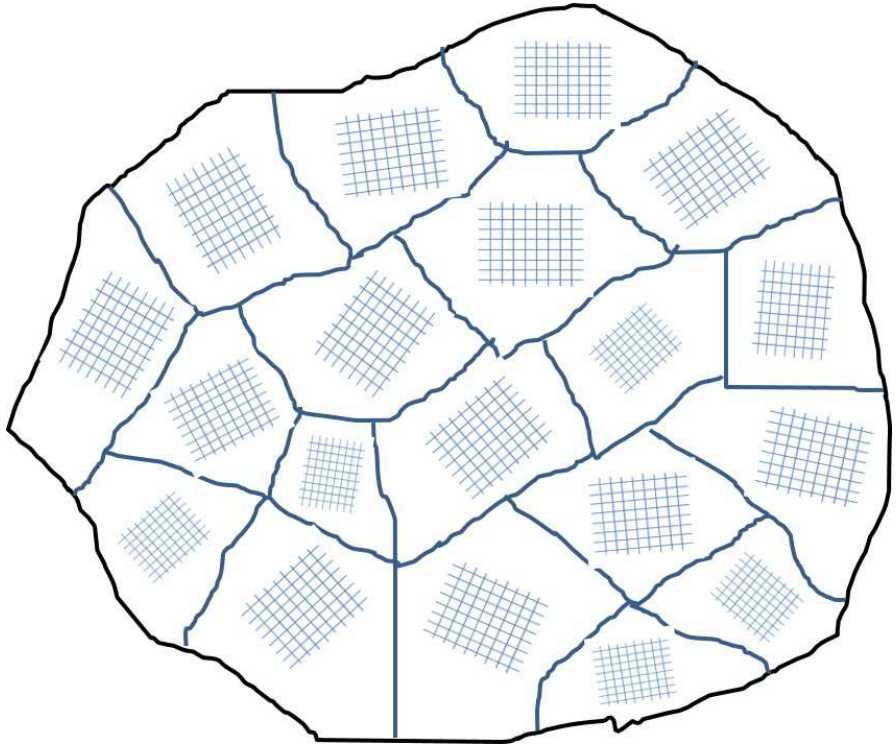
$$\begin{aligned}\mathbf{M}^T\mathbf{M} - 1 &= \mathbf{B}^{-T}\hat{\mathbf{q}} \otimes \mathbf{B}\hat{\mathbf{p}} + \mathbf{B}\hat{\mathbf{p}} \otimes \mathbf{B}^{-T}\hat{\mathbf{q}} + |\mathbf{B}\hat{\mathbf{p}}|^2 \mathbf{B}^{-T}\hat{\mathbf{q}} \otimes \mathbf{B}^{-T}\hat{\mathbf{q}} \\ &= (\mathbf{B}\hat{\mathbf{p}} + \frac{1}{2}|\mathbf{B}\hat{\mathbf{p}}|^2 \mathbf{B}^{-T}\hat{\mathbf{q}}) \otimes \mathbf{B}^{-T}\hat{\mathbf{q}} \\ &\quad + \mathbf{B}^{-T}\hat{\mathbf{q}} \otimes (\mathbf{B}\hat{\mathbf{p}} + \frac{1}{2}|\mathbf{B}\hat{\mathbf{p}}|^2 \mathbf{B}^{-T}\hat{\mathbf{q}}),\end{aligned}$$

so that again $SO(3)$ and $SO(3)\mathbf{M}$ are rank-one connected with normals $\mathbf{B}^{-T}\hat{\mathbf{q}}$ and $\mathbf{B}\hat{\mathbf{p}} + \frac{1}{2}|\mathbf{B}\hat{\mathbf{p}}|^2 \mathbf{B}^{-T}\hat{\mathbf{q}}$ and $|\mathbf{a}|^2 = |\mathbf{B}\hat{\mathbf{p}}|^2 |\mathbf{B}^{-T}\hat{\mathbf{q}}|^2$.

For bcc with $\hat{\mathbf{p}}v = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$, $\hat{\mathbf{q}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, we get the normals $\begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix}$ (twinning), $\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$ (slip) with $|\mathbf{a}|^2 = 2$.

Polycrystals

Different orientations of the crystal lattice in each grain.



No diffusion, within the grains, or of the grain boundaries.

Description of grain geometry

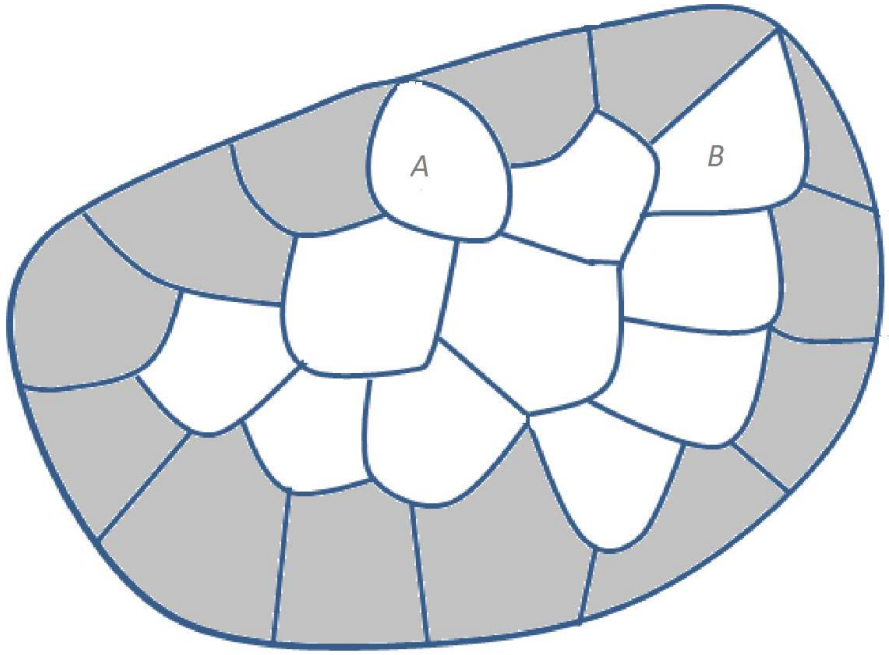
Consider a polycrystal that occupies in a reference configuration a bounded domain (open, connected set) $\Omega \subset \mathbb{R}^3$ composed of a finite number of disjoint grains Ω_j, $j = 1, \ldots, N$, where each Ω_j is a bounded domain with Lipschitz boundary $\partial\Omega_j$, so that

$$\Omega = \text{int} \bigcup_{i=1}^{N} \overline{\Omega}_j.$$

Topology and graphs

Some topological information is encoded in the graph whose vertices are the grains (labelled $1, \ldots, N$) and with edges (i, j) corresponding to grains Ω_i, Ω_j with $\mathcal{H}^2(\partial\Omega_i \cap \partial\Omega_j) > 0$ (in 2D this is used in the proof of the four colour theorem).

For each grain i let $M(i)$ be the number of $j \neq i$ for which (i, j) is an edge.



A and B are interior grains but touch $\partial\Omega$.

Interior grains are ones for which $\partial\Omega_j \subset \bigcup_{k\neq j} \partial\Omega_k$, and the others are *boundary* grains.

The set of *triple points* is

$$T = \bigcup_{1\leq i_1<i_2<i_3\leq N} \partial\Omega_{i_1} \cap \partial\Omega_{i_2} \cap \partial\Omega_{i_3}.$$

Theorem Suppose each grain Ω_j is convex. Then every interior grain Ω_i is a convex polyhedron (i.e. an intersection of a finite number of open half-spaces) with at most $M(i)$ faces.

Theorem If each $\overline{\Omega}_j$ is a topological manifold with boundary then T is nowhere dense in $\bigcup_{j=1}^{N} \partial\Omega_j$.

Zero-energy microstructures for a polycrystal

For a polycrystal the total free energy is given by

$$I(\mathbf{y}) = \int_\Omega W(D\mathbf{y}(\mathbf{x}), \mathbf{x})\, d\mathbf{x},$$

where $W(\mathbf{A}, \mathbf{x}) = \psi(\mathbf{A}\mathbf{R}_i^T)$ for $\mathbf{x} \in \Omega_i$ and $\mathbf{R}_i \in SO(3)$.

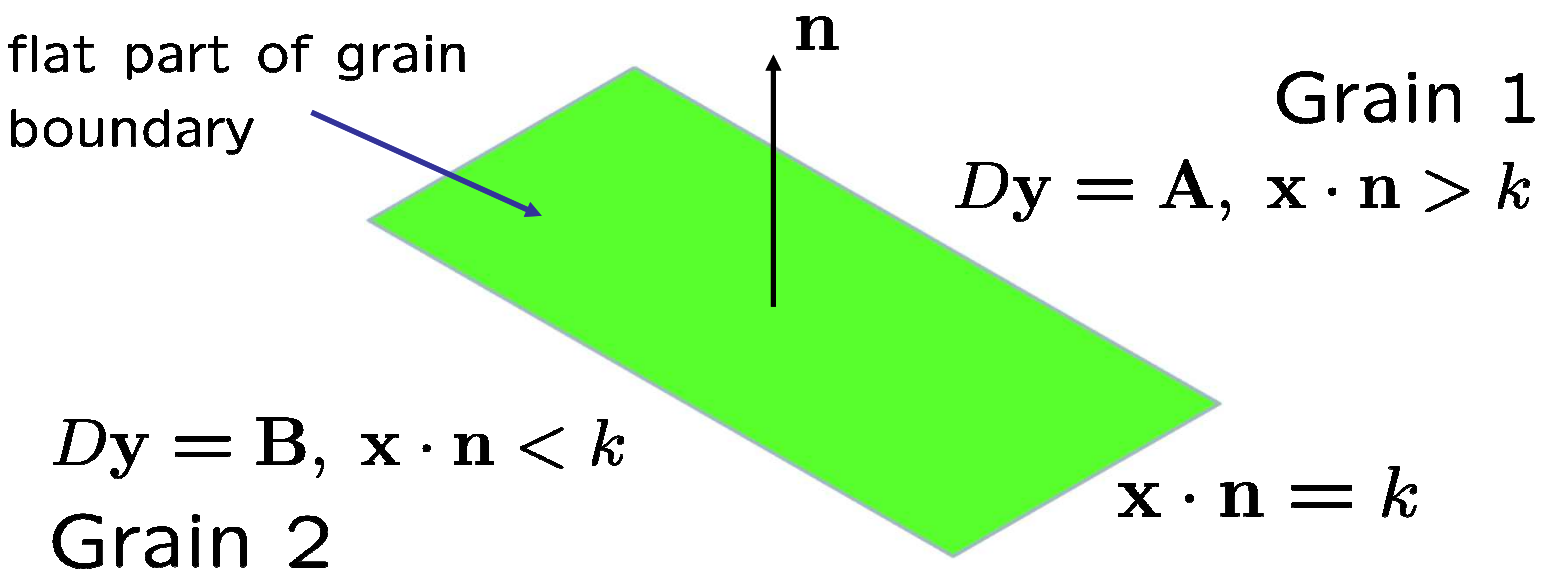
We fix $\theta < \theta_c$ and write $K = K(\theta)$, $\mathbf{U} = \mathbf{U}(\theta)$ etc.

Then a zero-energy microstructure corresponds to a gradient YM $(\nu_\mathbf{x})_{\mathbf{x}\in\Omega}$ with $\operatorname{supp} \nu_\mathbf{x} \subset K\mathbf{R}_i$ for a.e. $\mathbf{x} \in \Omega_i$, or equivalently to a macroscopic deformation gradient with

$$D\mathbf{y}(\mathbf{x}) \in (K\mathbf{R}_i)^{\mathrm{qc}} = K^{\mathrm{qc}}\mathbf{R}_i$$

for a.e. $\mathbf{x} \in \Omega_i$.

Constant deformation gradient in adjacent grains



We can assume that grain 1 has unrotated crystal axes. Hence for this to be a zero-energy deformation $\mathbf{A} = \mathbf{Q_1 U_i}$, $\mathbf{B} = \mathbf{Q_2 U_j \tilde{R}}$, where $\mathbf{Q_1}, \mathbf{Q_2} \in SO(3)$ and $\tilde{\mathbf{R}} \in SO(3)$ is the rotation of grain 2.

Note that $\mathbf{U}_j = \bar{\mathbf{R}}^T \mathbf{U}_i \bar{\mathbf{R}}$ for some $\bar{\mathbf{R}} \in P^{24}$.

Thus for a rank-one connection we must have

$$\det(\mathbf{U_i^2} - (\bar{\mathbf{R}}\tilde{\mathbf{R}})^{\mathbf{T}} \mathbf{U_i^2} \bar{\mathbf{R}}\tilde{\mathbf{R}}) = 0.$$

The function

$$\mathbf{R} \mapsto \det(\mathbf{U_i^2} - \mathbf{R}^{\mathbf{T}} \mathbf{U_i^2} \mathbf{R})$$

is real analytic on $SO(3)$ and for $\mathbf{U}_i$ not a multiple of 1 is not identically zero. Hence (c.f. Mityagin 2015) its zero set is of measure zero. Thus for generic grain rotations such a zero-energy deformation is impossible.

Zero-energy microstructures possible for any grain geometry and rotations

These correspond to gradient YMs $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ such that $\operatorname{supp}\nu_{\mathbf{x}} \subset \bigcap_{\mathbf{R}\in SO(3)} K\mathbf{R}$ a.e., or equivalently to macroscopic deformation gradients satisfying

$$D\mathbf{y}(\mathbf{x}) \in \mathcal{E} := \bigcap_{\mathbf{R}\in SO(3)} K^{\mathrm{qc}}\mathbf{R} \text{ for a.e. } \mathbf{x}\in\Omega.$$

The set $\mathcal{E}$ was essentially defined in Bhattacharya & Kohn (1996,1997) in connection with the 'Taylor bound'.

Note that $\mathcal{E}$ is *isotropic*, i.e.

$$\mathbf{Q}\mathcal{E}\mathbf{R} = \mathcal{E} \text{ for all } \mathbf{Q},\mathbf{R}\in SO(3).$$

The case of two wells

We take

$$K = SO(3)\mathbf{U}_1 \cup SO(3)\mathbf{U}_2,$$

$$\mathbf{U}_1 = \text{diag}\,(\eta_1, \eta_2, \eta_3), \quad \mathbf{U}_2 = \text{diag}\,(\eta_2, \eta_1, \eta_3),$$

and $\eta_2 > \eta_1 > 0$, $\eta_3 > 0$ (e.g. tetragonal to orthorhombic, or special orthorhombic to monoclinic transformations).

The advantage of this case is that it is the only one for which K^{qc} is known.

Theorem (B/James 92) K^{qc} consists of the matrices $\mathbf{A} \in GL^+(3,\mathbb{R})$ such that

$$\mathbf{A}^T\mathbf{A} = \begin{pmatrix} a & c & 0 \\ c & b & 0 \\ 0 & 0 & \eta_3^2 \end{pmatrix},$$

where $a > 0, b > 0, a+b+|2c| \leq \eta_1^2+\eta_2^2,\ ab-c^2 = \eta_1^2\eta_2^2$.

In addition (B/James 91), if $D\mathbf{y}(\mathbf{x}) \in K^{\text{qc}}$ a.e. then $\mathbf{y}$ is a plane strain, i.e.

$$\mathbf{y}(\mathbf{x}) = \mathbf{Q}(y_1(\mathbf{x}), y_2(\mathbf{x}), \eta_3 x_3 + a),$$

where $y_{1,3} = y_{2,3} = 0$, $\mathbf{Q} \in SO(3)$ and $a \in \mathbb{R}$.

Theorem

$$\mathcal{E} = \begin{cases} \emptyset & \text{if } \eta_3 \neq \sqrt{\eta_1 \eta_2} \\ SO(3)\eta_3 & \text{if } \eta_3 = \sqrt{\eta_1 \eta_2} \end{cases}$$

Proof. Suppose $\mathbf{D} = \operatorname{diag}(d_1, d_2, d_3) \in \mathcal{E}$. Then for any $\mathbf{R} \in SO(3)$ we have $\mathbf{DR} \in \mathcal{E}$, and so there exist a, b, c with $a > 0$, $b > 0$, $ab - c^2 = \eta_1^2 \eta_2^2$, $a + b + |2c| \leq \eta_1^2 + \eta_2^2$ and

$$\begin{pmatrix} a & c & 0 \\ c & b & 0 \\ 0 & 0 & \eta_3^2 \end{pmatrix} = \mathbf{R} \begin{pmatrix} d_1^2 & 0 & 0 \\ 0 & d_2^2 & 0 \\ 0 & 0 & d_3^2 \end{pmatrix} \mathbf{R}^T.$$

Hence $d_1 = d_2 = d_3 = \eta_3$ and both sides equal $\eta_3^2 \mathbf{1}$, so that we must have $a = b = \eta_3^2, c = 0$. Thus $\eta_3 = \sqrt{\eta_1 \eta_2}$, when indeed $2\eta_3^2 + 0 \leq \eta_1^2 + \eta_2^2$.

(For particular grain geometries and rotations there could be additional zero-energy microstructures.)

Now consider the set

$$\mathcal{E}_{2\mathrm{D}} = \bigcap_{\mathbf{R}\in SO(3),\, \mathbf{R}\mathbf{e}_3 = \pm\mathbf{e}_3} K^{\mathrm{qc}}\mathbf{R}.$$

Theorem

$\mathbf{A} \in \mathcal{E}_{2\mathrm{D}}$ iff $\mathbf{A} = \mathbf{R}\mathbf{D}\tilde{\mathbf{R}}$, where $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$, $\tilde{\mathbf{R}}\mathbf{e}_3 = \pm\mathbf{e}_3$,

$$\mathbf{D} = \begin{pmatrix} v_1 & 0 & 0 \\ 0 & v_2 & 0 \\ 0 & 0 & \eta_3 \end{pmatrix},$$

and $v_1 > 0, v_2 > 0$, $v_1 v_2 = \eta_1 \eta_2$, $|v_i| \leq \sqrt{\frac{\eta_1^2 + \eta_2^2}{2}}$.

(See Kohn & Niethammer (2000) and the book of Dolzmann (2003).)

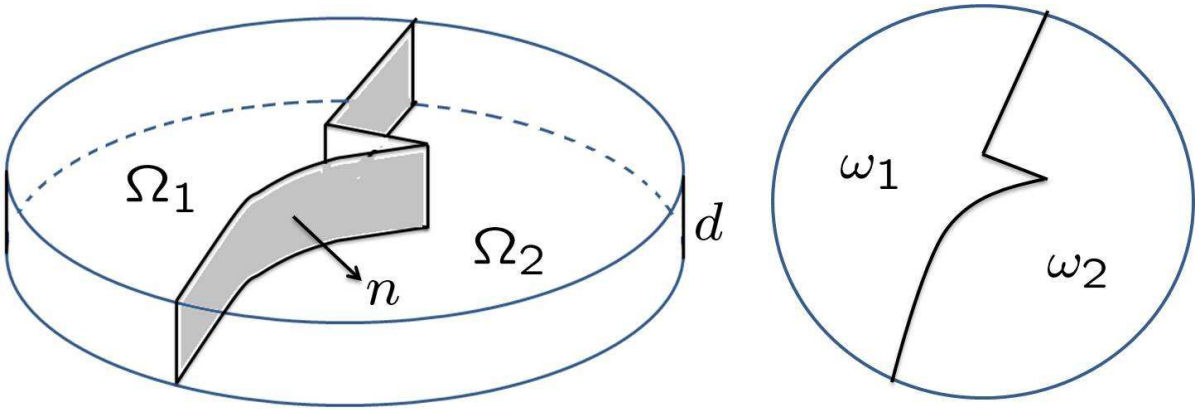
There are nontrivial deformations $\mathbf{y}$ with $D\mathbf{y}(\mathbf{x}) \in \mathcal{E}_{2D}$ a.e. $\mathbf{x} \in \Omega$, such as

$$\mathbf{y}(\mathbf{x}) = (\sqrt{\eta_1\eta_2}\, x_1, \sqrt{\eta_1\eta_2}\, x_2, \eta_3 x_3) + \varepsilon g(\mathbf{x}\cdot\mathbf{e}^{\perp})\mathbf{e},$$

where $|\mathbf{e}| = |\mathbf{e}^{\perp}| = 1, \mathbf{e}^{\perp}\cdot\mathbf{e} = \mathbf{e}\cdot\mathbf{e}_3 = 0$, $|g'| \leq M < \infty$ and $|\varepsilon|$ sufficiently small.

Such deformations nontrivially deform the grain boundaries (it would be interesting to have experimental results on grain boundary deformation resulting from martensitic transformations).

Zero-energy microstructures for a bicrystal



Energy wells $K = \mathrm{SO}(3)\mathbf{U}_1 \cup \mathrm{SO}(3)\mathbf{U}_2$

$\mathbf{U}_1 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_3), \mathbf{U}_2 = \mathrm{diag}\,(\eta_1, \eta_2, \eta_3),$

$\eta_2 > \eta_1 > 0, \eta_3 > 0$

Grain 1

$\Omega_1 = \omega_1 \times (0, d)$

$\mathrm{supp}\,\nu_x \subset K$ a.e. $x \in \Omega_1$

Grain 2

$\Omega_2 = \omega_2 \times (0, d)$

$\mathrm{supp}\,\nu_{\mathbf{x}} \subset K\mathbf{R}(\alpha)$ a.e. $\mathbf{x} \in \Omega_2$

$\mathbf{R}(\alpha)\mathbf{e}_3 = \mathbf{e}_3$

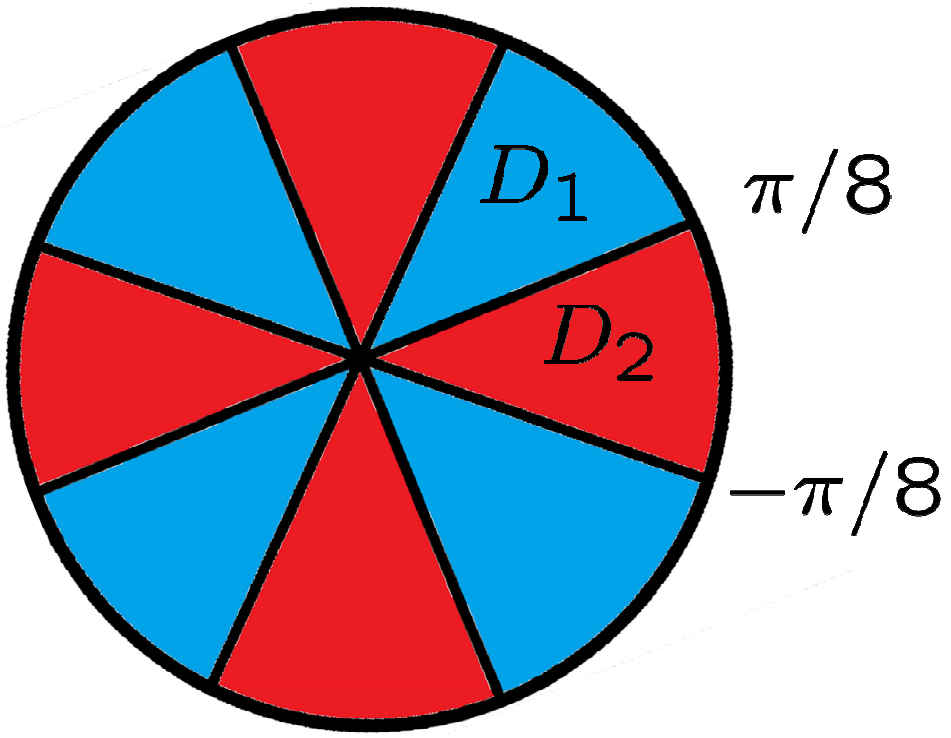
Question: Is it true that every zero-energy microstructure is nontrivial (i.e. not a pure phase $\nu_{\mathbf{x}} = \delta_{\mathbf{A}}$) in each of the grains?

(If the interface between the grains were not vertical, so that it had the form $x_3 = g(x_1, x_2)$ for some open set of (x_1, x_2), we cannot have a pure phase in one of the grains because a short calculation shows that it violates the microstructure being a plane strain in the other grain.)

Result 1. If the interface is *planar* then whatever its normal $\mathbf{n}$ there always exists a zero-energy microstructure which has a pure phase (i.e. $\nu_{\mathbf{x}} = \delta_{\mathbf{A}}$) in one of the grains.

Therefore the interface needs to be curved in order to show that the microstructure has to be nontrivial. Write the normal to the interface as $\mathbf{n} = (\cos\theta, \sin\theta, 0)$.

Result 2. Suppose that $\alpha = \pi/4$. Then it is impossible to have a zero-energy microstructure with a pure phase in one of the grains if the boundary between the grains contains a normal with $\theta \in D_1$ and another normal with $\theta' \in D_2$.

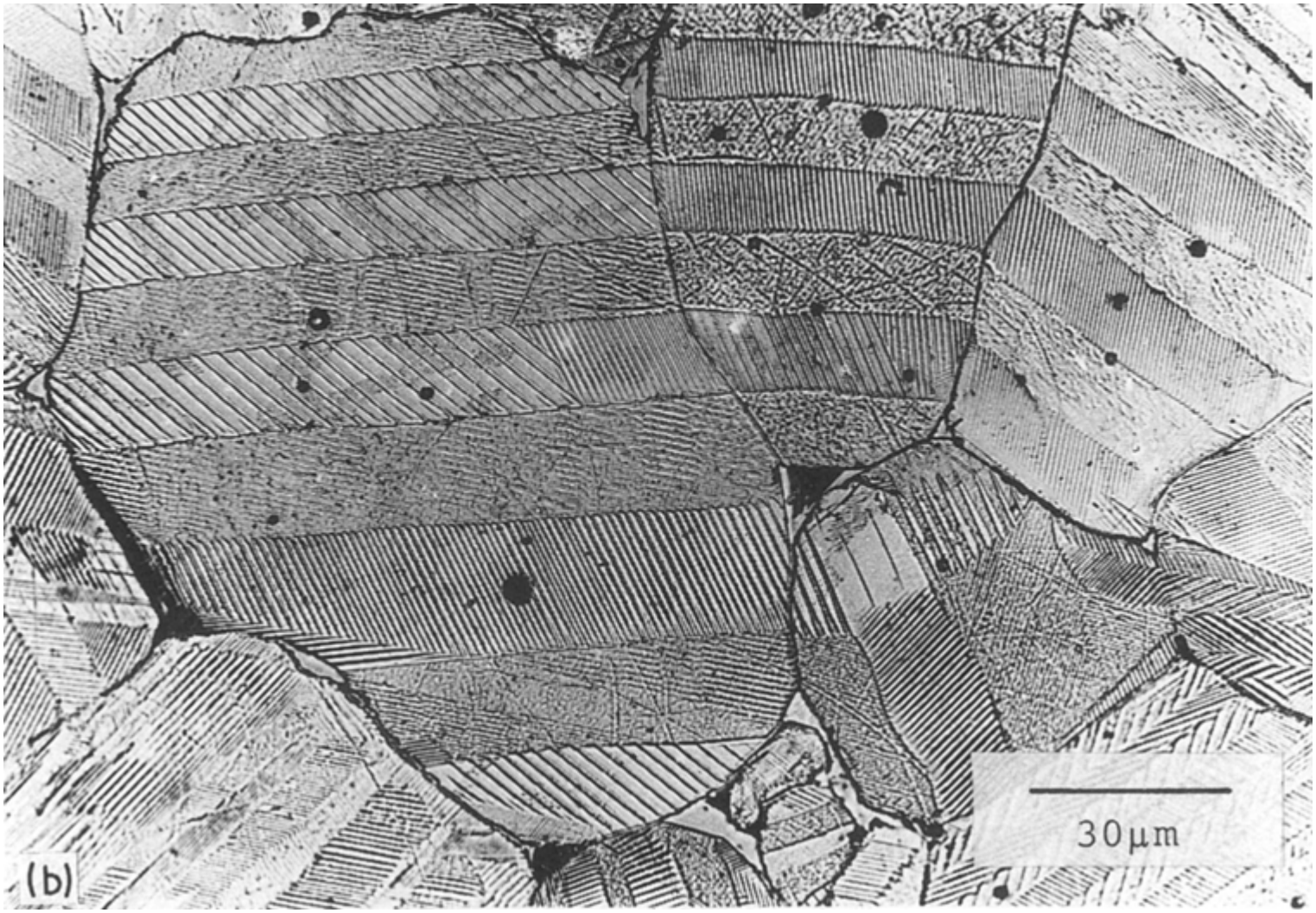


Proofs use:

1. A reduction to 2D using the plane strain result for the two-well problem.
2. The characterization of the quasiconvex hull of two wells.
3. Use of a *generalized Hadamard jump condition* in 2D to show that there has to be a rank-one connection $\mathbf{b} \otimes \mathbf{N}$ between the polyconvex hulls for each grain.
4. Long and detailed calculations.

For the details see, JB & C. Carstensen, *Interaction of martensitic microstructures in adjacent grains*, ICOMAT 2017 Proceedings.

Polycrystal microstructures for more than two wells



$BaTiO_3$ ceramic: G. Arlt, J. Materials Science, 25 (1990) 2655-2666.

Consider a cubic-to-tetragonal transformation with

$$K = \bigcup_{i=1}^{3} SO(3)\mathbf{U}_i,$$

$$\mathbf{U}_1 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_1),\ \mathbf{U}_2 = \mathrm{diag}\,(\eta_1, \eta_2, \eta_1),$$
$$\mathbf{U}_3 = \mathrm{diag}\,(\eta_1, \eta_1, \eta_2).$$

Theorem

$\mathcal{E}$ contains a relatively open neighbourhood of $(\eta_1^2\eta_2)^{\frac{1}{3}}SO(3)$ in $\mathcal{D} := \{\mathbf{A} \in GL^+(3,\mathbb{R}) : \det \mathbf{A} = \eta_1^2\eta_2\}$.

Proof. $\mathcal{E}$ is isotropic and by Dolzmann & Kirchheim (2013) K^{qc} contains a relatively open neighbourhood of $(\eta_1^2\eta_2)^{\frac{1}{3}}\mathbf{1}$ in $\mathcal{D}$.

In fact, if the austenite is cubic and the transformation strain $\mathbf{U}$ is not a dilatation then K^{qc} always contains a nontrivial set of tetragonal wells (c.f. Bhattacharya (1992), B/Koumatos (2014)) and so $\mathcal{E}$ contains a relatively open neighbourhood of $(\det \mathbf{U})^{\frac{1}{3}} SO(3)$ in $\mathcal{D} := \{\mathbf{A} \in GL^+(3,\mathbb{R}) : \det \mathbf{A} = \det \mathbf{U}\}$. Hence, for example, we have a nontrivial $\mathcal{E}$ for cubic to orthorhombic transformations.

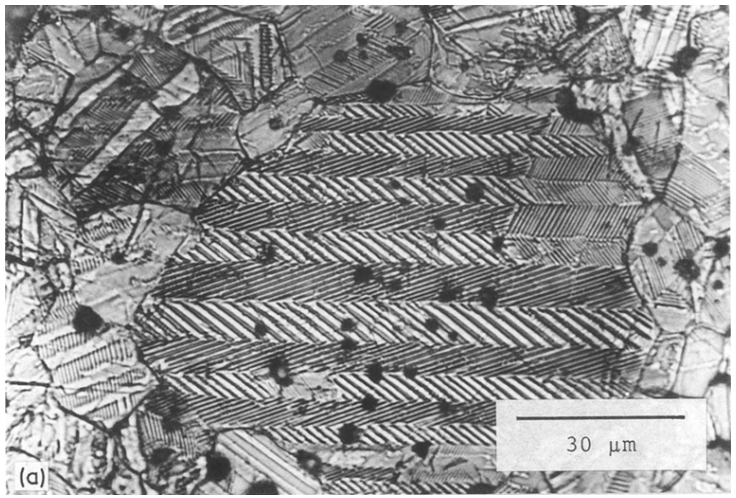
A related remark is:

Theorem There is no homogeneous gradient Young measure

$$\nu = \sum_{i=1}^{4} \lambda_i \delta_{\mathbf{A}_i}, \quad \lambda_i \geq 0, \sum_{i=1}^{4} \lambda_i = 1,$$

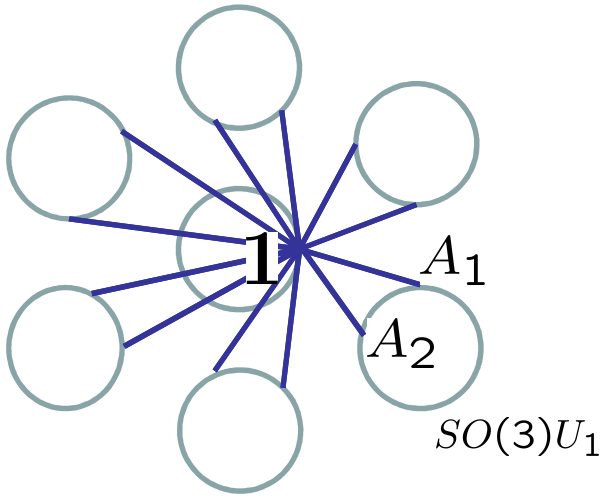
with $\mathbf{A}_i \in K$ and $\bar{\nu} = (\eta_1^2 \eta_2)^{1/3} \mathbf{1}$.

Arlt (1990).
Microstructure with approximately four gradients in $BaTiO_3$.



Is the apparent conflict with experiment due to ignoring interfacial energy, or because the deformation is not a dilatation on the boundary?

Another issue (c.f. recent work of F. Della Porta) is whether all microstructures with $\operatorname{supp}\nu_{\mathbf{x}} \subset K^{\mathrm{qc}}\mathbf{R}_i$ for a.e. $\mathbf{x} \in \Omega_i$ are obtainable by a suitable path starting from the austenite.



$\operatorname{rank}(\mathbf{A_i} - \mathbf{1}) = 1,$
$i = 1, \ldots, 12$

$\operatorname{rank}(\mathbf{A_i} - \mathbf{A_j}) > 1,$
$i \neq j$

What is $\{\mathbf{A}_1, \ldots, \mathbf{A}_{12}\}^{\mathrm{qc}}$?

$Ti_{76}Nb_{22}Al_2$ (T. Inamura) cubic to orthorhombic, $\lambda_2 = 1$