Swansea Summer School
in Nonlinear PDEs
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Understanding Material Microstructure

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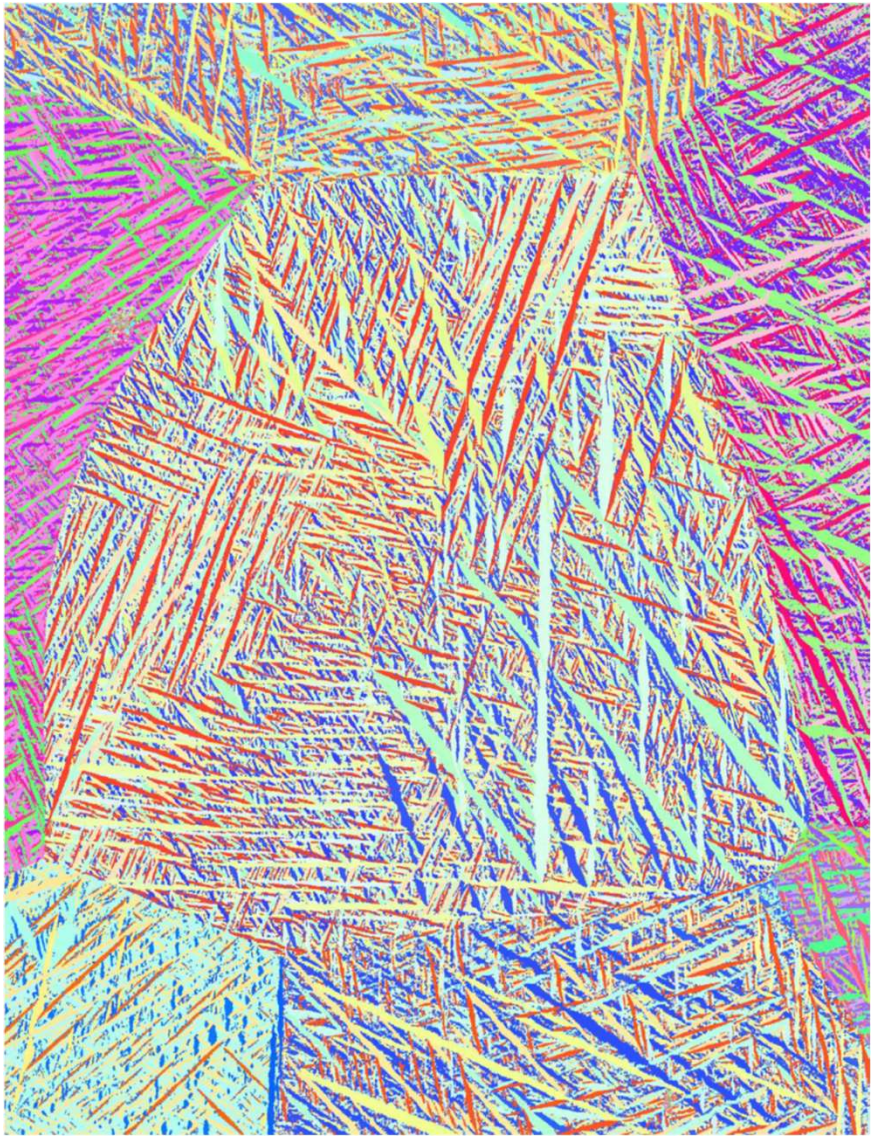
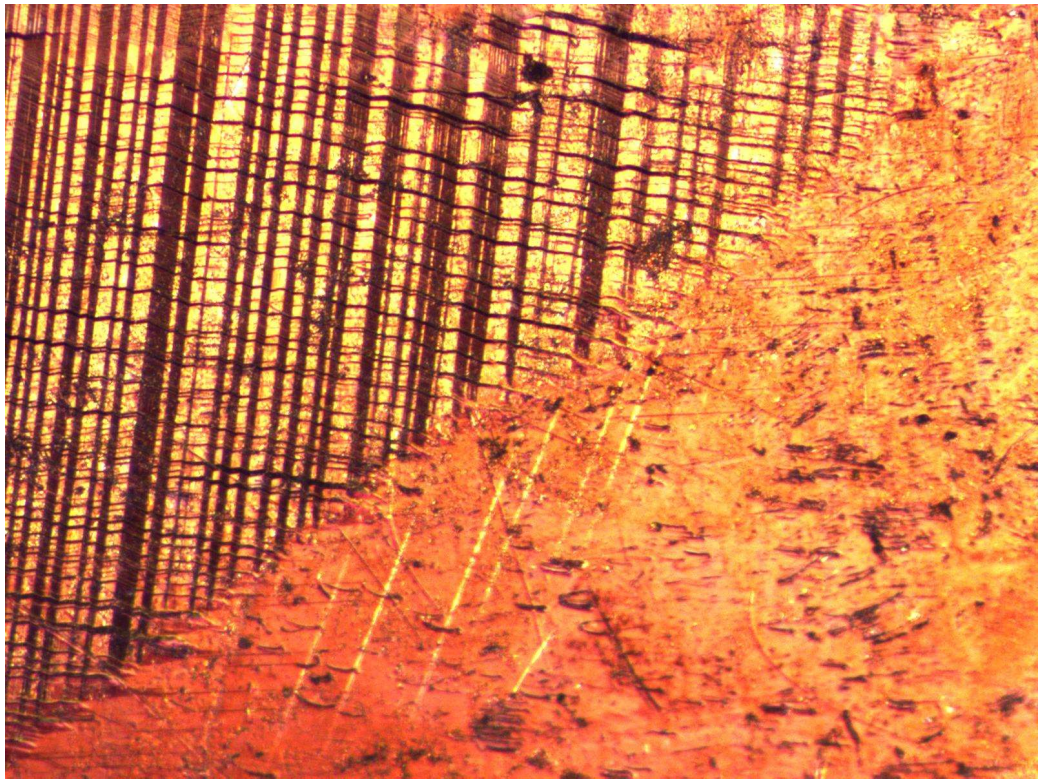
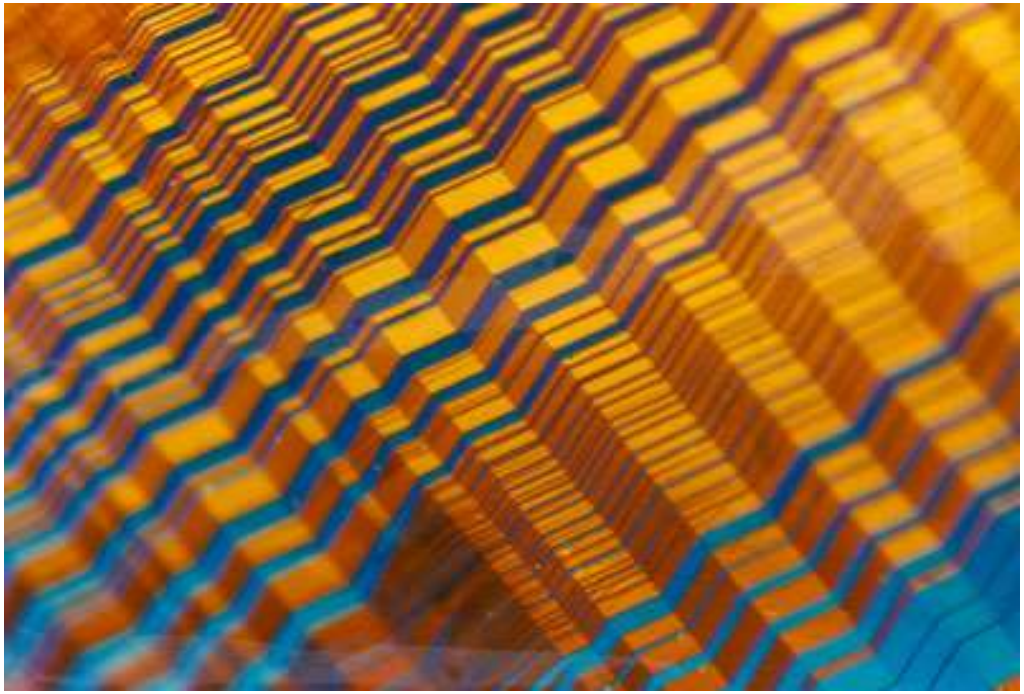
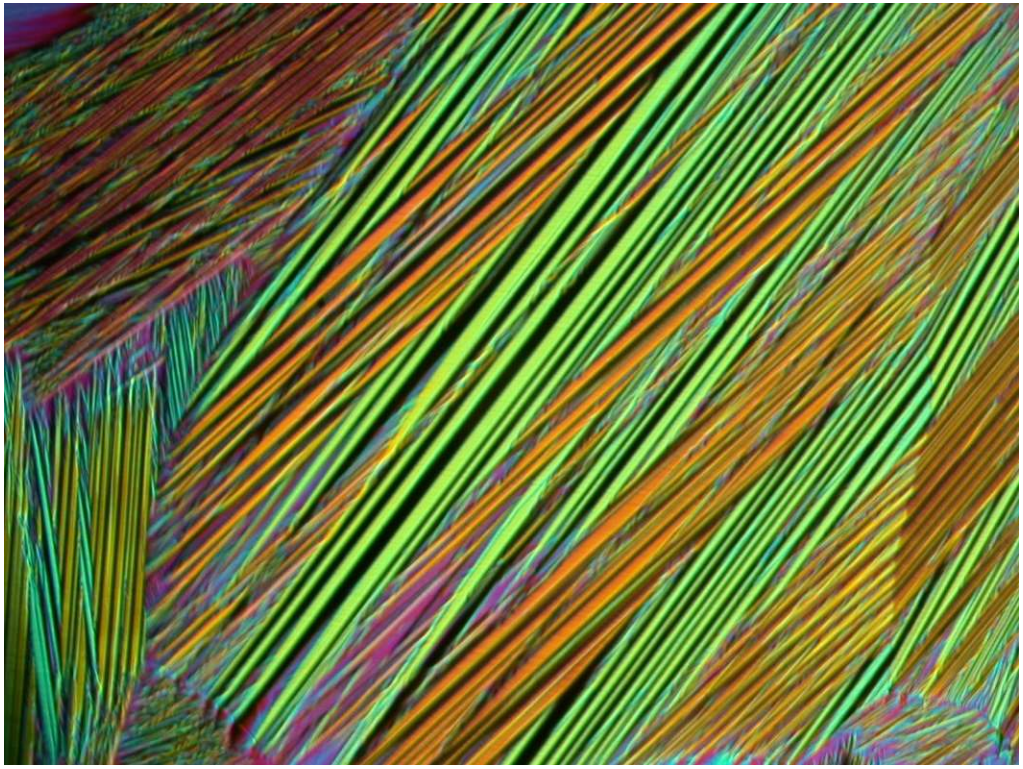


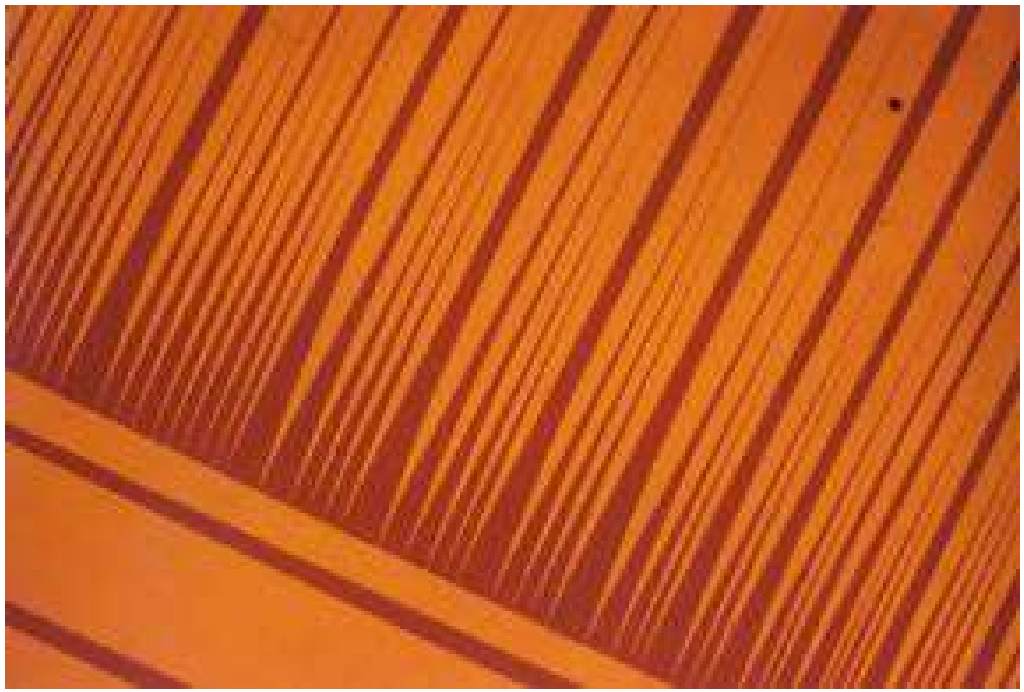


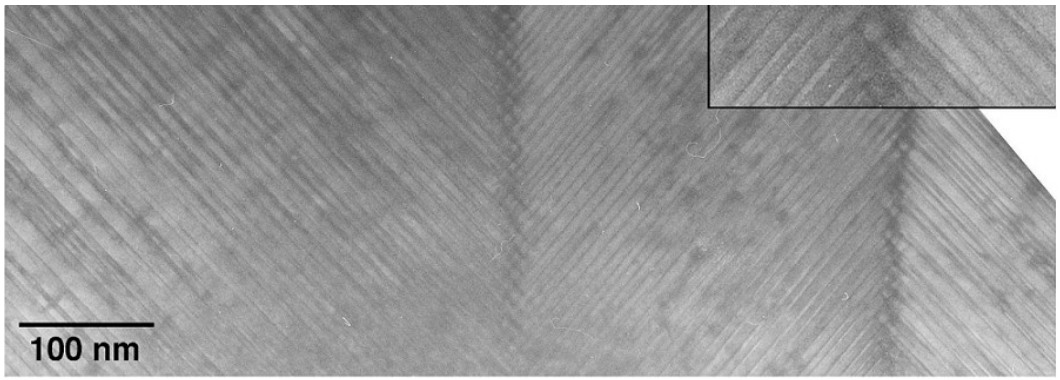


CuAlNi Chu & James



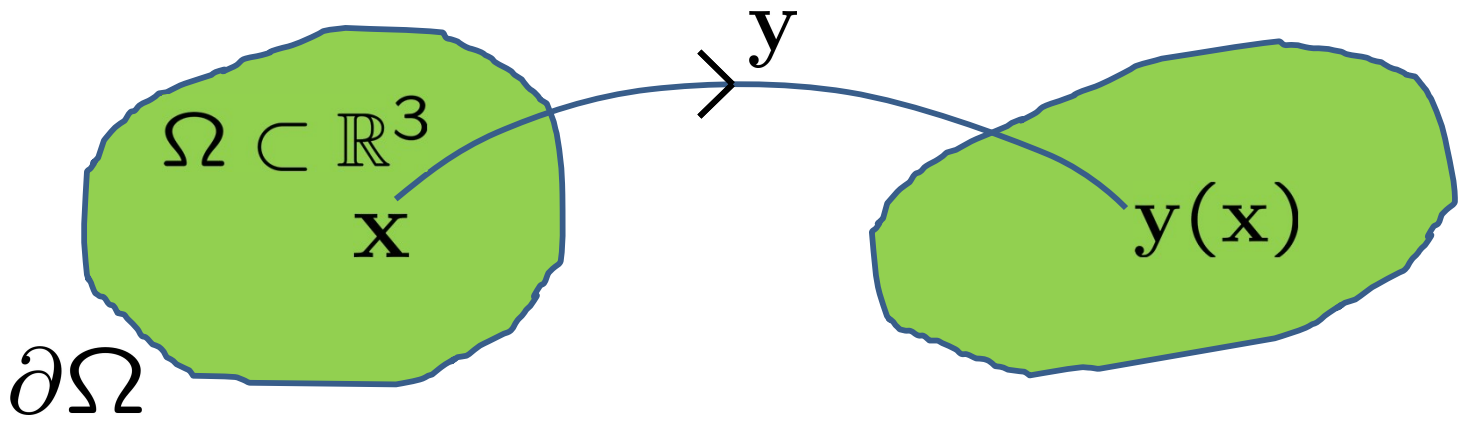
CuZnAl Morin





$Ni_{65}Al_{35}$ Boullay/Schryvers

Nonlinear (thermo)elasticity model



Find a deformation $\mathbf{y} : \Omega \to \mathbb{R}^3$ minimizing

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

subject to suitable boundary conditions, e.g. $\mathbf{y}|_{\partial\Omega} = \bar{\mathbf{y}}$, where θ is the (constant) temperature.

Here $D\mathbf{y}(\mathbf{x}) = \left(\frac{\partial y_i}{\partial x_\alpha}\right) = y_{i,\alpha}$ is the *deformation gradient*, and $\psi(\mathbf{F}, \theta)$ is the *free-energy density* of the material, defined for $\mathbf{F} \in GL^+(3, \mathbb{R}) := \{3 \times 3 \text{ real matrices } \mathbf{F} \text{ with } \det \mathbf{F} > 0\}$.

To avoid interpenetration of matter $\mathbf{y}$ should be *invertible*. Also we require that $\mathbf{y}$ is *orientation-preserving*, so that $\det D\mathbf{y}(\mathbf{x}) > 0$. In order to help ensure this it is typically supposed that $\psi(\mathbf{F}, \theta) \to \infty$ as $\det \mathbf{F} \to 0+$.

By *Cauchy's polar decomposition theorem* any $\mathbf{F} \in GL^+(3, \mathbb{R})$ can be decomposed uniquely as $\mathbf{F} = \mathbf{RU}$ with $\mathbf{R} \in SO(3)$ and $\mathbf{U} = \mathbf{U}^T > 0$.

We assume that ψ is *frame-indifferent*, that is

$$\psi(\mathbf{QF}, \theta) = \psi(\mathbf{F}, \theta) \text{ for all } \mathbf{Q} \in SO(3),$$

so that, choosing $\mathbf{Q} = \mathbf{R}^T$, $\psi(\mathbf{F}, \theta) = \psi(\mathbf{U}, \theta)$.

In particular, the set of matrices minimizing $\psi(\cdot, \theta)$ is invariant to left multiplication by rotations.

Applying polar decomposition to $D\mathbf{y}(\mathbf{x})$ we have that

$$D\mathbf{y}(\mathbf{x}) = \mathbf{R}(\mathbf{x})\mathbf{U}(\mathbf{x}),$$

where $\mathbf{R}(\mathbf{x}) \in SO(3)$ and $\mathbf{U}(\mathbf{x}) = \mathbf{U}^T(\mathbf{x}) > 0$.

Theorem

Let $\mathbf{y} \in W^{1,2}(\Omega, \mathbb{R}^3)$. Then $\mathbf{U}(\mathbf{x})$ constant implies $D\mathbf{y}(\mathbf{x})$ constant.

Proof (cf Shield 1971). By considering $\tilde{\mathbf{y}}(\mathbf{x}) = \mathbf{y}(\mathbf{U}^{-1}\mathbf{x})$ we may assume that $\mathbf{U}(\mathbf{x}) = \mathbf{1}$.

Then $\operatorname{cof} D\mathbf{y}(\mathbf{x}) = \operatorname{cof} \mathbf{R}(\mathbf{x}) = \mathbf{R}(\mathbf{x}) = D\mathbf{y}(\mathbf{x})$ and since $\operatorname{div} \operatorname{cof} D\mathbf{y}(\mathbf{x}) = \mathbf{0}$ we have that $\Delta \mathbf{y}(\mathbf{x}) = \mathbf{0}$. In particular $\mathbf{y}$ is smooth.

But $|D\mathbf{y}(\mathbf{x})|^2 = y_{i,\alpha} y_{i,\alpha} = 3$ and so

$$(y_{i,\alpha} y_{i,\alpha})_{,\beta\beta} = \cancel{2 y_{i,\alpha\beta\beta} y_{i,\alpha}} + 2 y_{i,\alpha\beta} y_{i,\alpha\beta} = 0. \quad \square$$

Compatibility

Suppose $\mathbf{F}(\mathbf{x})$ is a smooth field of 3×3 matrices in Ω.

When is $\mathbf{F}(\mathbf{x})$ a gradient? i.e. when does there exist $\mathbf{y} : \Omega \to \mathbb{R}^3$ with $\mathbf{F}(\mathbf{x}) = D\mathbf{y}(\mathbf{x})$, that is

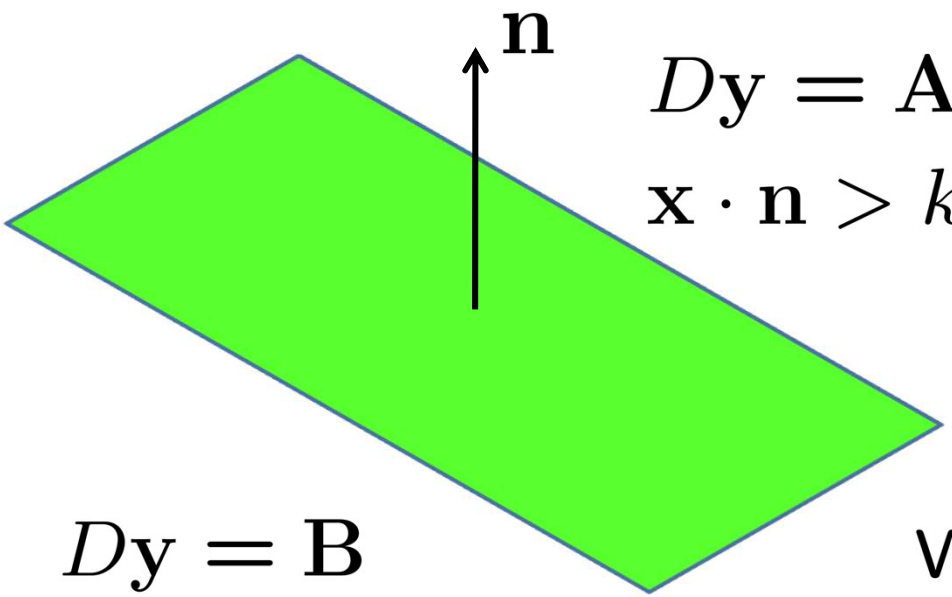
$$F_{i\alpha}(\mathbf{x}) = y_{i,\alpha}(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega.$$

A necessary condition, which is sufficient if Ω is simply-connected, is that

$$F_{i\alpha,\beta}(\mathbf{x}) = F_{i\beta,\alpha}(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega.$$

Another necessary and sufficient condition is the vanishing of the Riemann curvature tensor, which is a nonlinear function of the metric $\mathbf{g}(\mathbf{x}) = \mathbf{F}^T(\mathbf{x})\mathbf{F}(\mathbf{x}) = \mathbf{U}(\mathbf{x})^2$ and its first and second derivatives, expressing the fact that Euclidean space is flat.

An important special case of compatibility is the *Hadamard jump condition* for a continuous piecewise affine map.



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

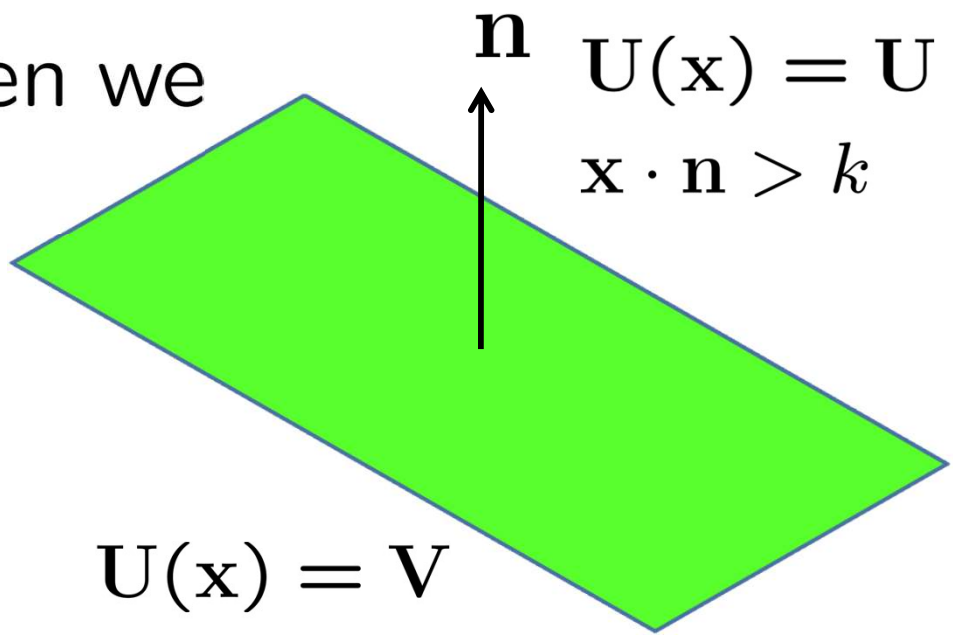
where $(\mathbf{a} \otimes \mathbf{n})_{i\alpha} := a_i n_\alpha$

(a matrix of rank one if $\mathbf{A} \neq \mathbf{B}$)

Proof. 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 $\mathbf{Cz} = (\mathbf{Cn} \otimes \mathbf{n})\mathbf{z}$. $\square$

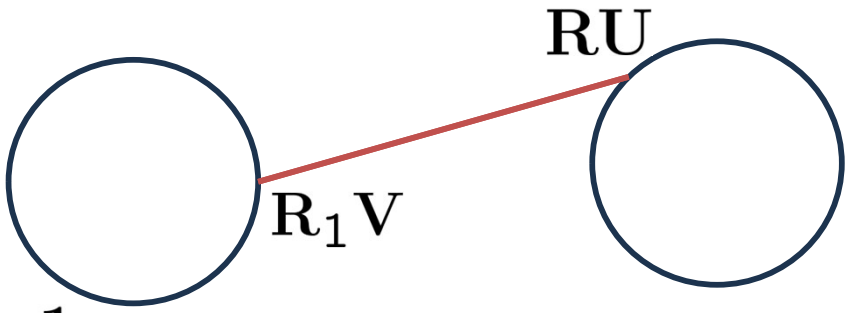
Open Problem. Give necessary and sufficient conditions for a nonsmooth (e.g. in L^∞) map $\mathbf{x} \mapsto \mathbf{U}(\mathbf{x})$, $\mathbf{U}(\mathbf{x}) = \mathbf{U}(\mathbf{x})^T > 0$, to be such that $D\mathbf{y}(\mathbf{x})^T D\mathbf{y}(\mathbf{x}) = \mathbf{U}(\mathbf{x})^2$ for some $\mathbf{y}$.

Here is a simple case when we can give an answer.



When is this possible for $\mathbf{U} \neq \mathbf{V}$? Equivalently, when is there a rank-one connection between $SO(3)\mathbf{U}$ and $SO(3)\mathbf{V}$?

$$\mathbf{RU} - \mathbf{R}_1\mathbf{V} = \mathbf{a} \otimes \mathbf{n}$$



Note that we can suppose $\mathbf{R}_1 = \mathbf{1}$.

Theorem

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

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

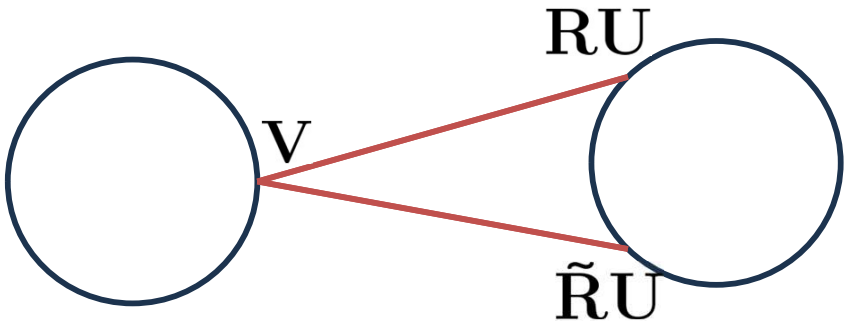
for unit vectors $\mathbf{n}$, $\tilde{\mathbf{n}}$ and some $c \neq 0$.

If $\tilde{\mathbf{n}} \neq \pm\mathbf{n}$ there are exactly two rank-one connections between $\mathbf{V}$ and $SO(3)\,\mathbf{U}$ 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 $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$, $\mathbf{a}, \tilde{\mathbf{a}} \in \mathbb{R}^3$.

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



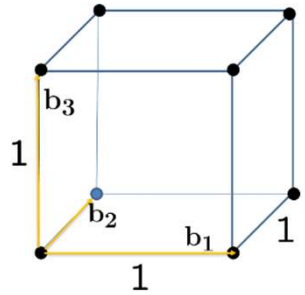
A Bravais lattice is an infinite lattice of points in $\mathbb{R}^3$ generated by linear combinations with integer coefficients of three linearly independent basis vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$.

Setting $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$, so that $B_{ij} = \mathbf{b}_j \cdot \mathbf{e}_i$, we write the corresponding Bravais lattice as

$$\mathcal{L}(\mathbf{B}) = \{m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 : m_i \in \mathbb{Z}\} = \{\mathbf{Bm} : \mathbf{m} \in \mathbb{Z}^3\}$$

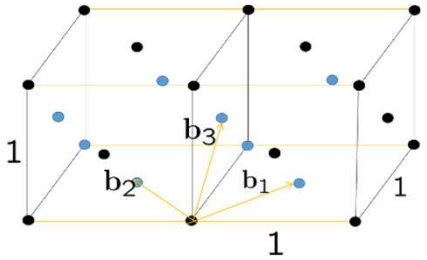
Cubic lattices

Simple cubic



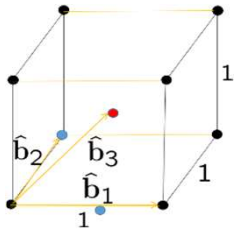
$$\mathbf{B}_{\mathrm{c}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbf{1},$$

Face-centred cubic (fcc)

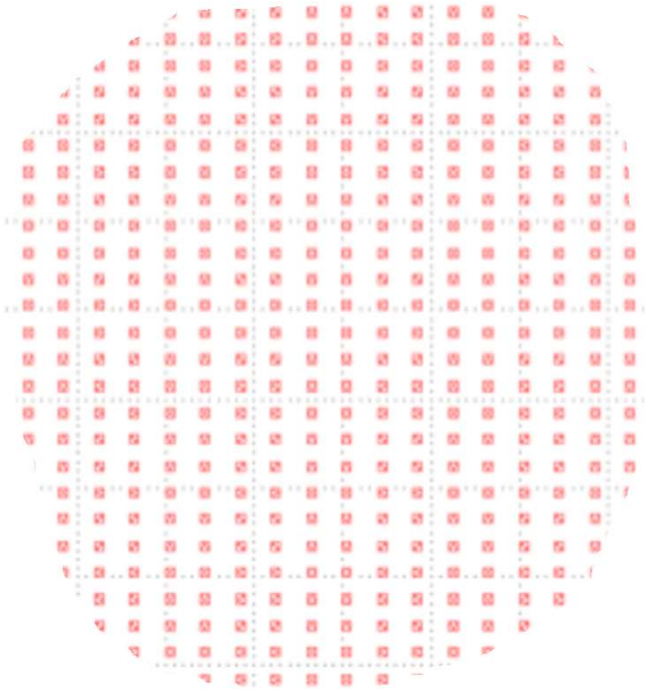


$$\mathbf{B}_{\mathrm{fcc}} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix},$$

Body-centred cubic (bcc)



$$\mathbf{B}_{\mathrm{bcc}} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$



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.

Pure metal examples include Fe, Cr, W, Nb (bcc) and Al, Cu, Au, Ag (fcc).

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.

Theorem (on equivalent lattices)

= integer 3×3 matrices with determinant ± 1

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

(See e.g. Ericksen (1977), Pitteri & Zanzotto (2003).)

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 $\mathcal{L}(\mathbf{C}) \subset \mathcal{L}(\mathbf{B})$. □

= real invertible 3×3 matrices

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

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

Ericksen energy well picture

Suppose that the free energy per unit volume of a crystalline material with atoms at the points of the Bravais lattice $\mathcal{L}(\mathbf{C})$, where $\mathbf{C} \in GL^+(3,\mathbb{R})$, at temperature θ, is given by $\varphi(\mathbf{C},\theta) \geq 0$. By adding a function of θ to φ we can and will suppose that $\min_{\mathbf{C}} \varphi(\mathbf{C},\theta) = 0$ for all θ.

Natural requirements are
(i) (frame-indifference) $\varphi(\mathbf{QC},\theta) = \varphi(\mathbf{C},\theta)$ for all $\mathbf{Q} \in SO(3)$,
(ii) (lattice invariance) $\varphi(\mathbf{C}\boldsymbol{\mu},\theta) = \varphi(\mathbf{C},\theta)$ for all $\boldsymbol{\mu} \in GL^+(3,\mathbb{Z})$.

We now use the *Cauchy-Born rule* to relate the mesoscopic free-energy density ψ to φ, thus defining an elastic free energy

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

for a deformation $\mathbf{y} : \Omega \to \mathbb{R}^3$.

Choosing a reference configuration in which the crystal lattice is $\mathcal{L}(\mathbf{B})$, where $\mathbf{B} \in GL^+(3,\mathbb{R})$, assume that

$$\psi(\mathbf{F},\theta) = \varphi(\mathbf{FB},\theta), \text{ for } \mathbf{F} \in GL^+(3,\mathbb{R}).$$

Thus $\psi \geq 0$ inherits from φ the invariances:
(i) (frame-indifference) $\psi(\mathbf{QF},\theta) = \psi(\mathbf{F},\theta)$ for all $\mathbf{Q} \in SO(3)$,
(ii) (symmetry) $\psi(\mathbf{FB}\boldsymbol{\mu}\mathbf{B}^{-1},\theta) = \psi(\mathbf{F},\theta)$ 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 the unimodular group $SL(3,\mathbb{R}) := \{\mathbf{A} \in GL^+(3,\mathbb{R}) : \det \mathbf{A} = 1\}$.

In particular, setting

$$K(\theta) = \{\mathbf{F} \in GL^+(3,\mathbb{R}) : \psi(\mathbf{F},\theta) = 0\}$$

we have that $SO(3)K(\theta)\mathcal{S} = K(\theta)$.

First let us suppose that

$$K(\theta) = SO(3)\mathcal{S},$$

so that, up to rotations and lattice-invariant transformations, $\mathbf{F} = \mathbf{1}$ (corresponding to the Bravais lattice $\mathbf{B}$) is the unique minimizer of $\psi(\cdot, \theta)$.

Thus

$$K(\theta) = \bigcup_{\boldsymbol{\mu} \in GL^+(3,\mathbb{Z})} SO(3)\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1}$$

is a union of energy wells, infinitely many of which are distinct.

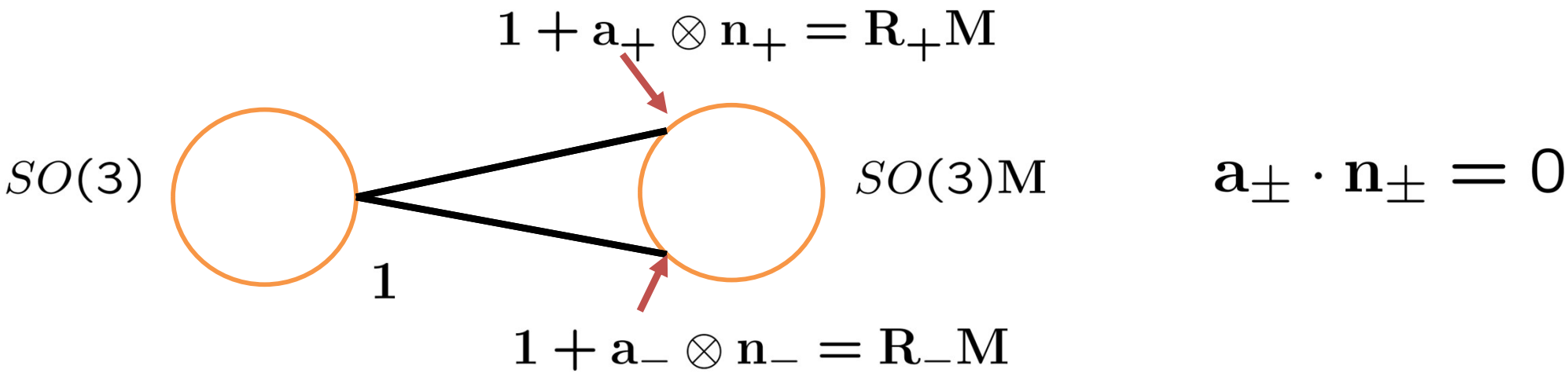
Are these energy wells rank-one connected?

Without loss of generality we can consider rank-one connections between $SO(3)$ and $SO(3)\mathbf{M}$, where $\mathbf{M} = \mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1}$ and $\mathbf{M}^T\mathbf{M} \neq \mathbf{1}$. Thus we require that

$$\mathbf{M}^T\mathbf{M} - \mathbf{1} = c(\mathbf{n} \otimes \tilde{\mathbf{n}} + \tilde{\mathbf{n}} \otimes \mathbf{n})$$

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

Since $\det \mathbf{M}^T\mathbf{M} = 1$ a necessary and sufficient condition for this is that $\mathbf{M}^T\mathbf{M}$ has an eigenvalue 1 (which is the middle eigenvalue). Then there are exactly two rank-one connections:



Two possible kinds of rank-one connections $\mathbf{F} = \mathbf{1} + \mathbf{a} \otimes \mathbf{n} = \mathbf{RM}$ are:

(i) *slip*, for which $\mathbf{R} = \mathbf{1}$

(ii) *twins*, for which the lattices $\mathcal{L}(\mathbf{B})$ and $\mathbf{F}\mathcal{L}(\mathbf{B})$ on either side of the interface are nontrivially reflected with respect to each other, so that $\mathbf{F}$ is not a slip and satisfies for some unit vector $\mathbf{m}$

$$\mathbf{F}\mathcal{L}(\mathbf{B}) = (\mathbf{1} - 2\mathbf{m} \otimes \mathbf{m})\mathcal{L}(\mathbf{B}) = (-\mathbf{1} + 2\mathbf{m} \otimes \mathbf{m})\mathcal{L}(\mathbf{B}).$$

Type 1 twins are those for which $\mathbf{m} = \mathbf{n}$, so that

$$\mathbf{1} + \mathbf{a} \otimes \mathbf{n} = (-\mathbf{1} + 2\mathbf{n} \otimes \mathbf{n})\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1},$$

and *Type* 2 twins are those for which $\mathbf{m} = \frac{\mathbf{a}}{|\mathbf{a}|}$.

There are twins that are neither Type 1 or Type 2, and rank-one connections that are neither slips not twins.

One can rigorously calculate (an integer minimization problem) the slips and Type 1/Type 2 twins that minimize $|\mathbf{a}|^2$, a popular criterion loosely related to energetics.

For example, for fcc the minimum value for slips is given by $|\mathbf{a}|^2 = \frac{3}{2}$, while for Type 1/Type 2 twins it is $|\mathbf{a}|^2 = \frac{1}{2}$ (and these twins minimize $|\mathbf{a}|^2$ among *all* rank-one connections). In both cases the normals are parallel to $\mathbf{e}_i + \mathbf{e}_j \pm \mathbf{e}_k$ with i, j, k distinct.

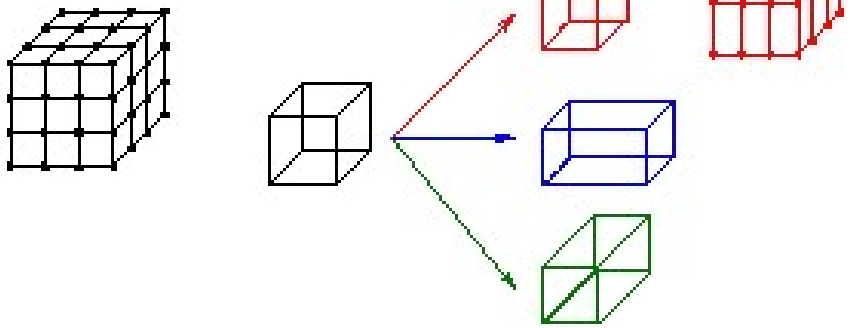
These results correspond to experiment and calculations in the materials science literature due to Chalmers & Martius (1952), Jaswon & Dove (1956,1957,1960), Bilby & Crocker (1965), Bevis & Crocker (1968,1969) and summarized in Christian & Mahajan (1995).

Martensitic phase transformations

These involve a change of shape of the crystal lattice of some alloy at a critical temperature.

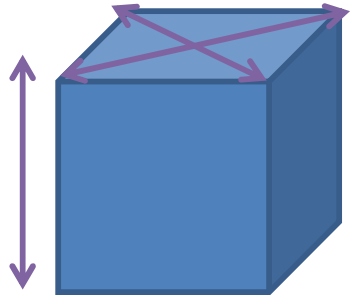
e.g. cubic to tetragonal

$\theta > \theta_c$
cubic
austenite



$\theta < \theta_c$
three tetragonal variants
of martensite

cubic to
orthorhombic



$\theta < \theta_c$
six orthorhombic variants
of martensite

Taking the reference configuration to be the cubic Bravais lattice at temperature θ_c, the change of shape of the lattice with respect to $\mathbf{B}$ is given by $\mathbf{U}(\theta) = \mathbf{U}(\theta)^T > 0$.

For example, in the case of a cubic to tetragonal transformation we can take

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

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

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 $\alpha(\theta_c) = 1$.

To restrict the model to a finite number of energy wells, and to eliminate e.g. large lattice invariant shears associated with plasticity, we replace $\mathcal{S} = \mathbf{B}\, GL^+(3,\mathbb{Z})\, \mathbf{B}^{-1}$ by

$$\mathcal{S} = \mathbf{B}\, P^{24}\, \mathbf{B}^{-1},$$

where $P^{24} = GL^+(3,\mathbb{Z}) \cap SO(3)$ (the proper rotations in the *point group*), i.e. the 24 rotations mapping a cube to itself.

Thus

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

where the $\mathbf{U}_i(\theta)$ are the distinct matrices $\mathbf{Q}\mathbf{U}(\theta)\mathbf{Q}^T$ for $\mathbf{Q} \in P^{24}$, the N *variants* of martensite.

For cubic-to-tetragonal (e.g. InTl, NiAl, NiMn, $BaTiO_3$) $N = 3$ and

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

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

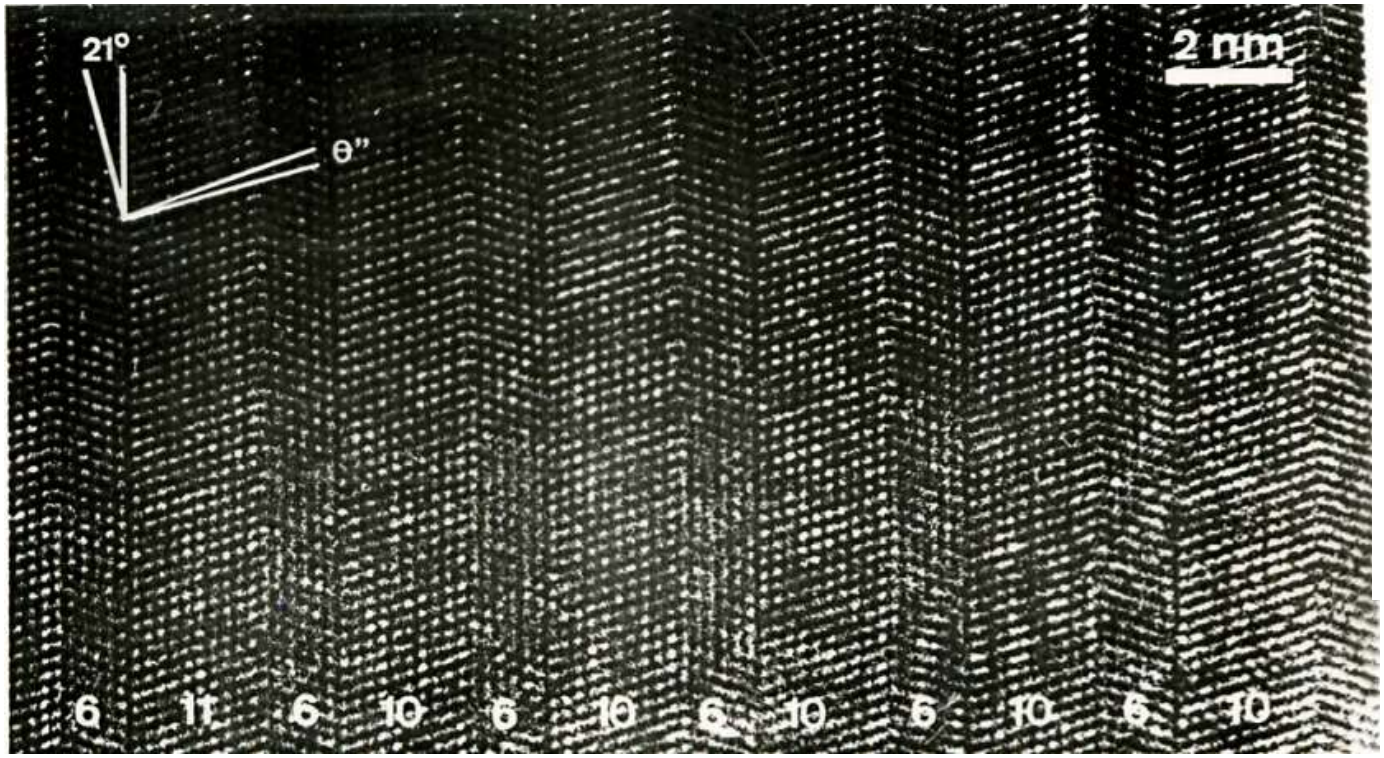
For cubic to orthorhombic (e.g. CuAlNi) $N = 6$ and

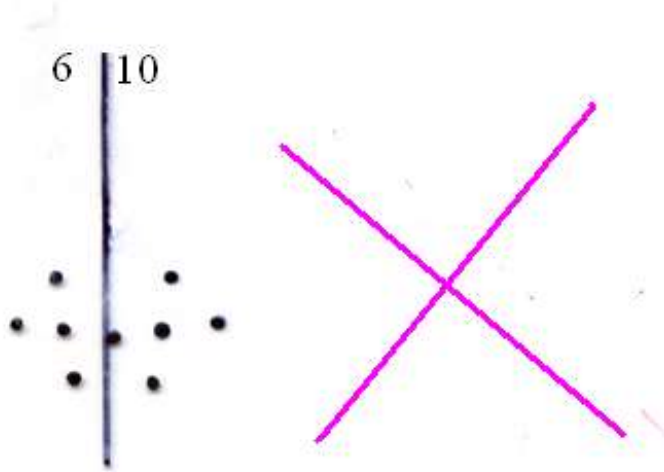
$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \mathbf{U}_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2}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

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

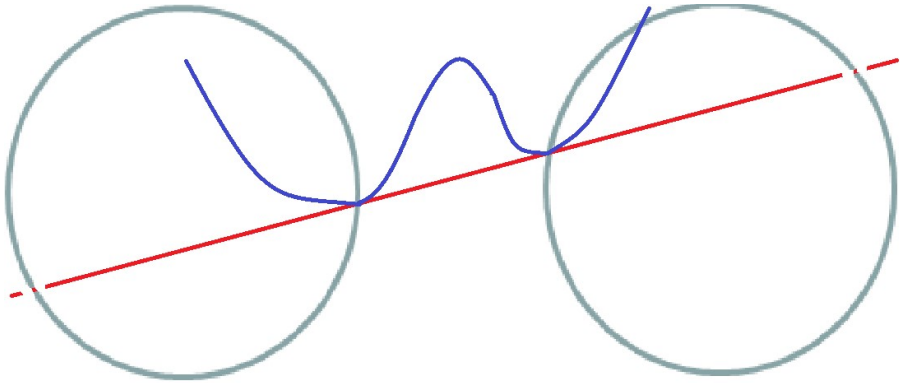
where $\alpha = \alpha(\theta) > 0, \beta = \beta(\theta) > 0, \gamma = \gamma(\theta) > 0$ are distinct.

There are rank-one connections between the martensitic energy wells that are twins, and they can be calculated explicitly. For example, for cubic to tetragonal the twins have normals parallel to $\mathbf{e}_i \pm \mathbf{e}_j$ for $i \neq j$.





NiMn, Baele, van Tenderloo, Amelinckx



The existence of these rank-one connections implies that $\psi(\cdot, \theta)$ is not *rank-one convex*, that is not convex in the direction of matrices of rank-one.

The central convexity condition of the multi-dimensional calculus of variations is *quasiconvexity* (in the sense of Morrey (1950)), which is roughly speaking necessary and sufficient for the existence of minimizers for general boundary conditions.

But *quasiconvexity implies rank-one convexity* (the converse is false due to a famous counterexample of Šverák), and so $\psi(\cdot, \theta)$ is not quasiconvex.

Thus we don't expect energy-minimizing configurations to exist in this model (!!), and this can be viewed as an explanation for why we see extremely fine microstructures.

In contrast there are good models for rubber for which $\psi(\cdot, \theta)$ *is* quasiconvex, and for which there exist energy minimizers.

By definition the function $g = g(D\mathbf{y})$ is quasiconvex if

$$\fint_Q g(D\mathbf{z}(\mathbf{x}))\, d\mathbf{x} \geq g(\mathbf{A})$$

whenever $\mathbf{z}$ is smooth with $\mathbf{z}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ for $\mathbf{x} \in \partial Q$, where $Q = (0,1)^3$.

Unfortunately quasiconvexity is poorly understood, and there is no known general way of deciding whether a given g is quasiconvex. In particular Kristensen (1999) showed that quasiconvexity is not a local condition.

Even though $\psi(\cdot, \theta)$ is not quasiconvex, quasiconvexity is crucial for understanding microstructure. For example, suppose $\theta < \theta_c$, so that

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

Then the set of *macroscopic* deformation gradients corresponding to zero-energy microstructures, i.e. gradients of (weak) limits of minimizing sequences, is given by the *quasiconvex hull* of $K(\theta)$

$$K(\theta)^{\text{qc}} := \{\mathbf{B} \in GL^+(3, \mathbb{R}) : g(\mathbf{B}) \leq \max_{\mathbf{A} \in K(\theta)} g(\mathbf{A}) \ \forall \text{ quasiconvex } g\}.$$

Largely because we do not have a tractable characterization of quasiconvexity, we do not know how to calculate this set when $N \geq 3$.

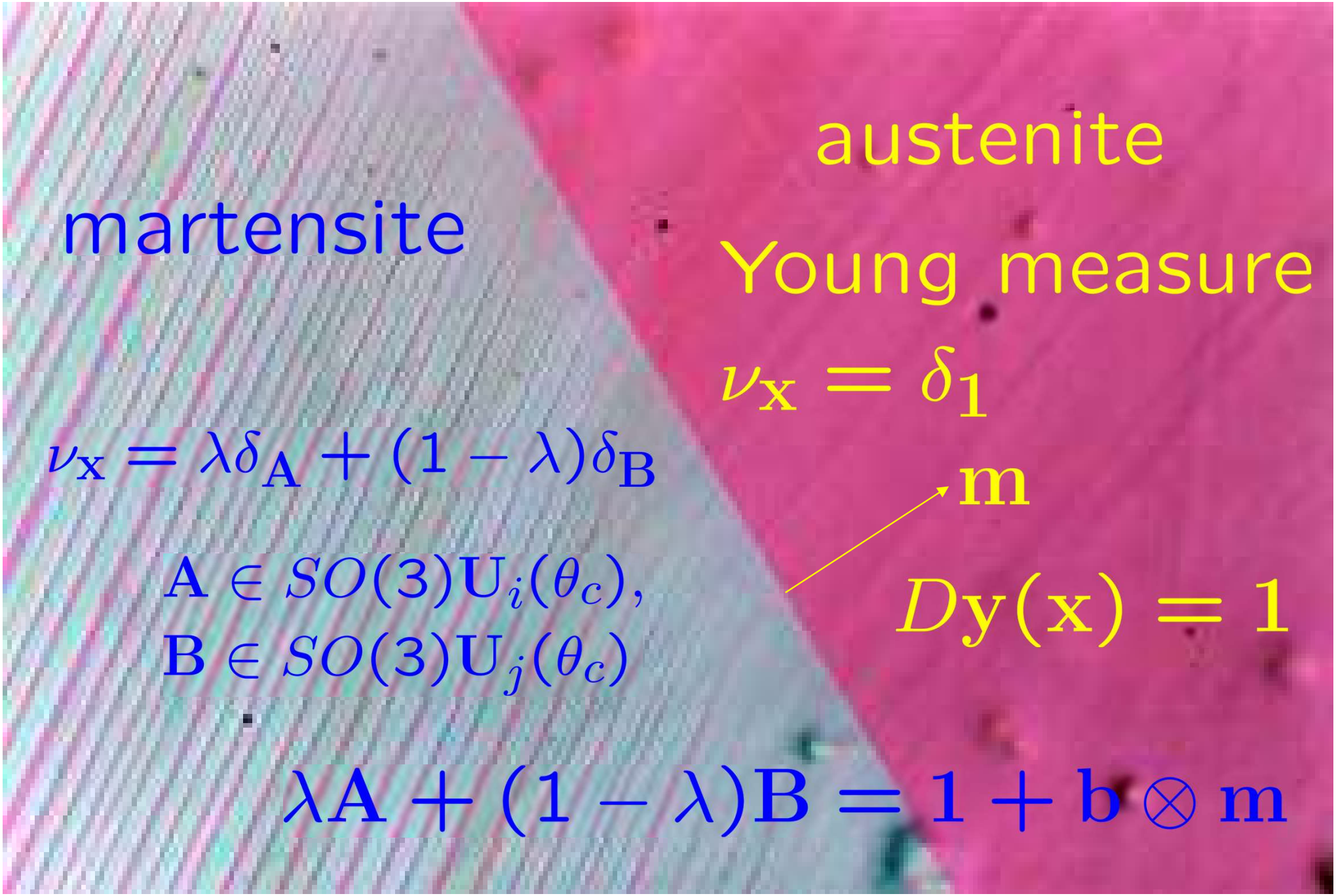
How does austenite transform to martensite as the temperature θ is reduced through θ_c?

In order for there to be a rank-one connection between $SO(3)$ (the austenite energy well at $\theta = \theta_c$) and $SO(3)\mathbf{U}_i(\theta_c)$ we have seen that it is necessary and sufficient that $\mathbf{U}_i(\theta_c)$ has middle eigenvalue one, which is not usually the case.

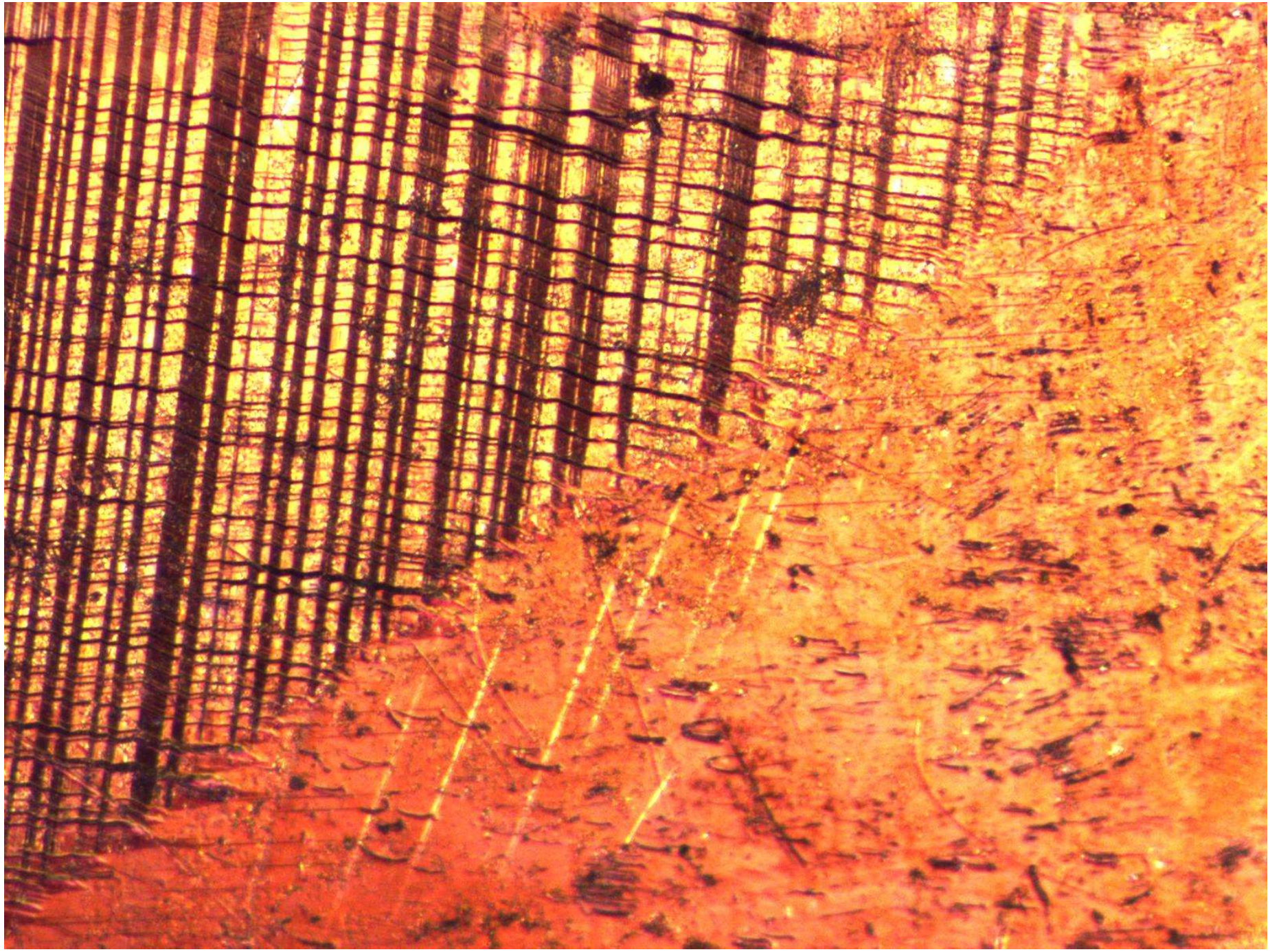
Instead the martensite is typically nucleated by a (classical) austenite-martensite interface separating the austenite ($D\mathbf{y}(\mathbf{x}) = \mathbf{1}$ say) from a finely-twinned martensitic laminate, whose macroscopic deformation gradient $\mathbf{F}$ is compatible with the austenite, i.e.

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

for some $\mathbf{b} \in \mathbb{R}^3$ and habit plane normal $\mathbf{m}$.



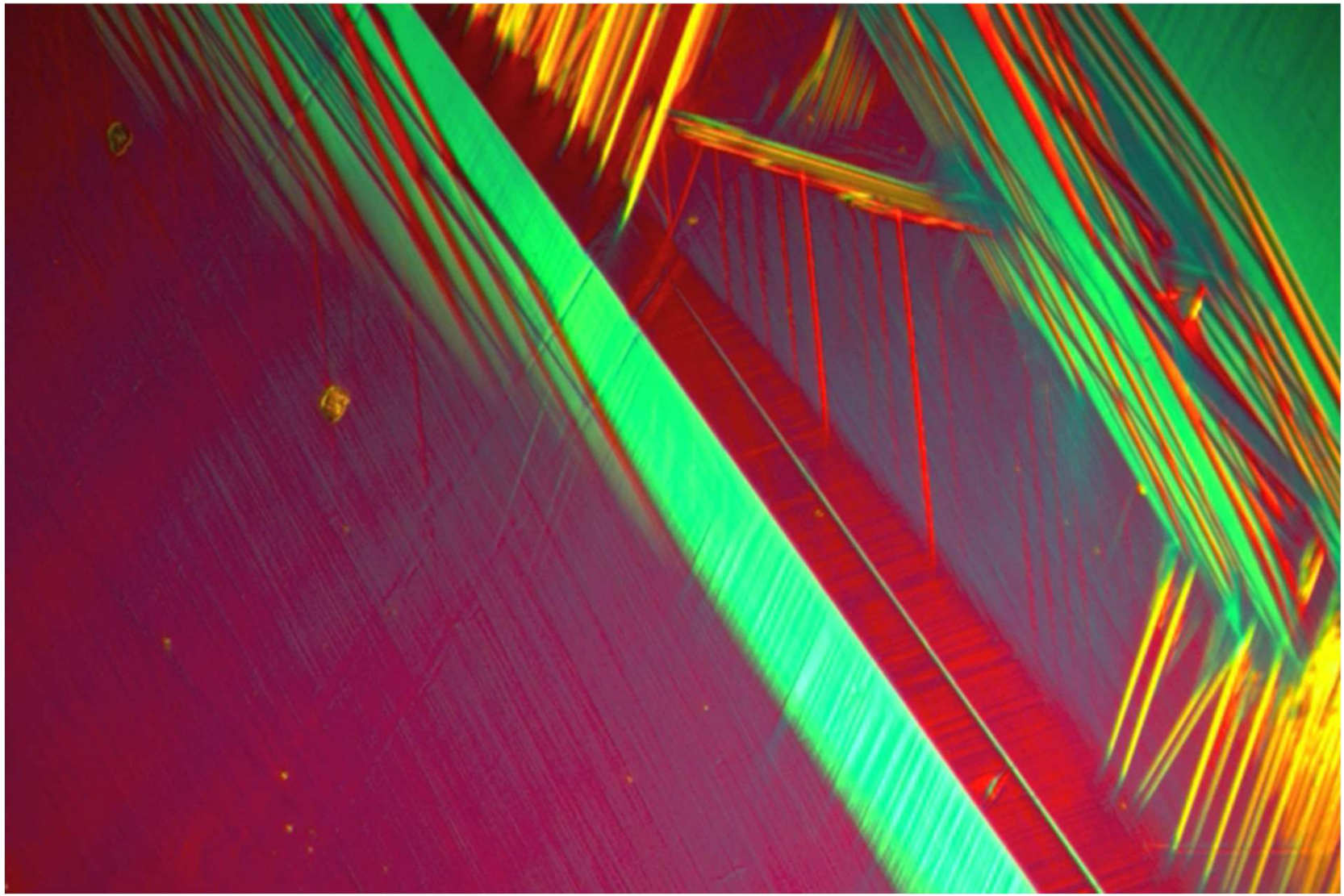
Austenite-martensite interface in CuAlNi (Chu & James)



Nonclassical austenite-martensite interface in CuAlNi (experiment of H. Seiner following theory of JB/Carstensen)

Nucleation of austenite in martensite (CuAlNi).
Experiment H.Seiner, theory Seiner/JB/Koumatos

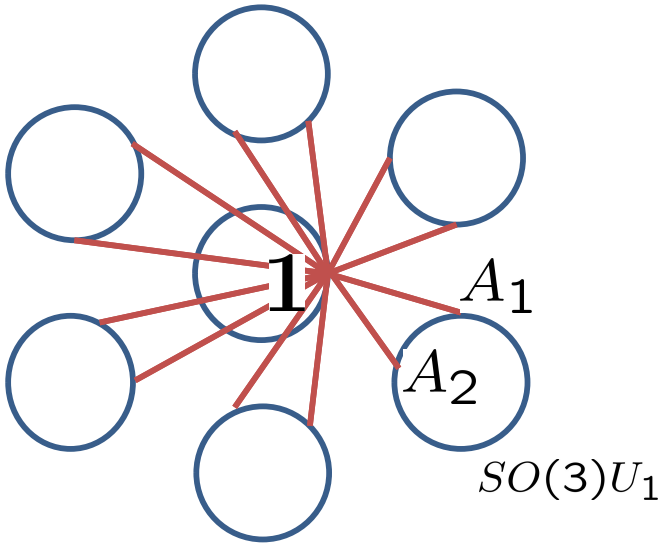
But what if the composition of the alloy is tuned so that the middle eigenvalue of $\mathbf{U}(\theta_c)$ equals one?



$Zn_{45}Au_{30}Cu_2$ ultra low hysteresis alloy

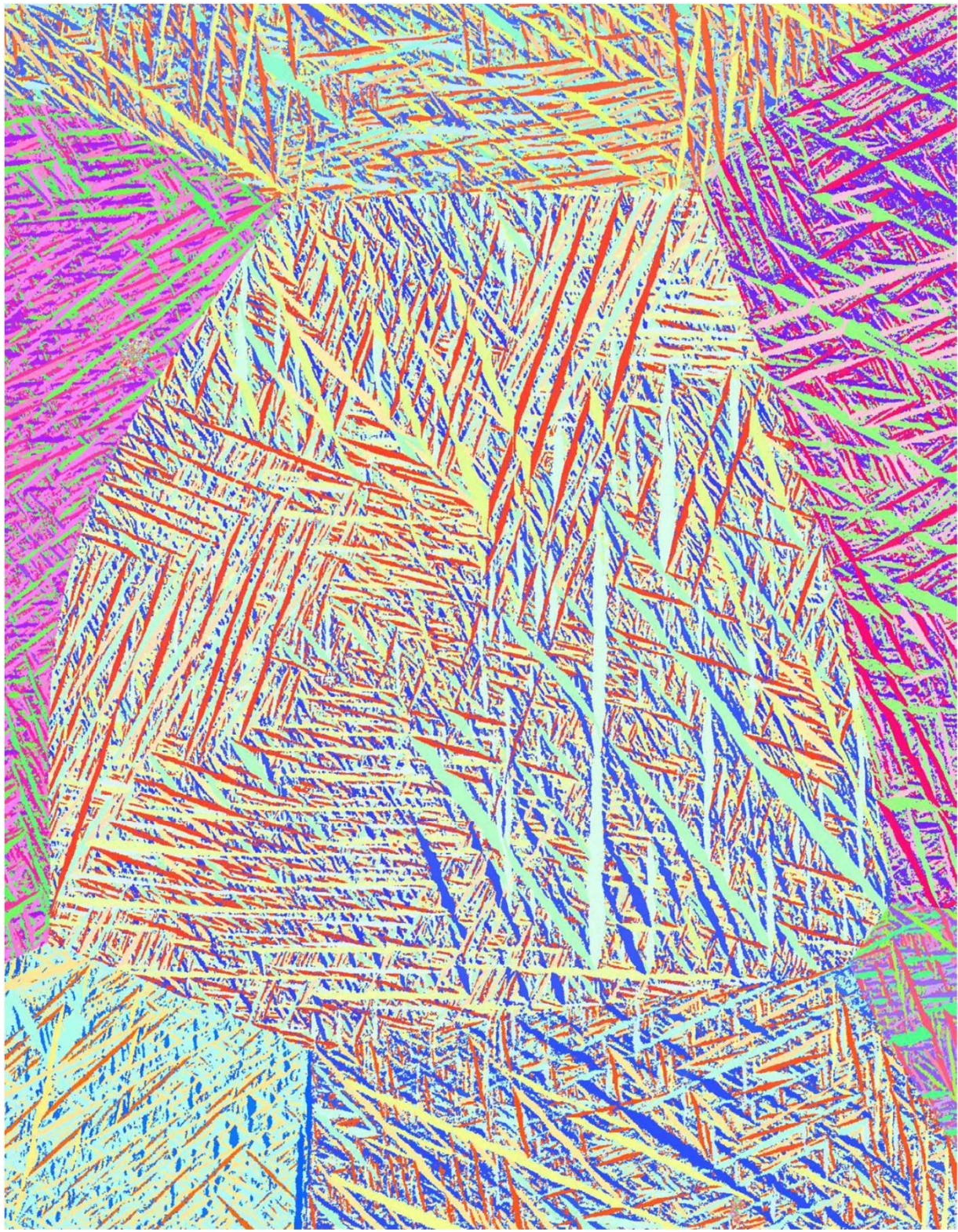
Yintao Song, Xian Chen, Vivekanand Dabade,
Thomas W. Shield, Richard D James, Nature, 502, 85–88 (03 October 2013)

$Ti_{76}Nb_{22}Al_2$ (T. Inamura)
theory JB/ Della Porta
Cubic to orthorhombic
$\lambda_2 = 1$



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

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



Summary

- Nonlinear elasticity gives rise to a successful mesoscopic theory of solid phase transformations and associated microstructures, explaining many observations.
- But it is handicapped by a lack of understanding of quasiconvexity.
- And it is not truly predictive – for that one would need a well-posed set of dynamic equations, a key issue being whether solutions could produce infinitely-fine microstructures in the limit $t \to \infty$.

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