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Interfaces and hysteresis in solid phase transformations

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

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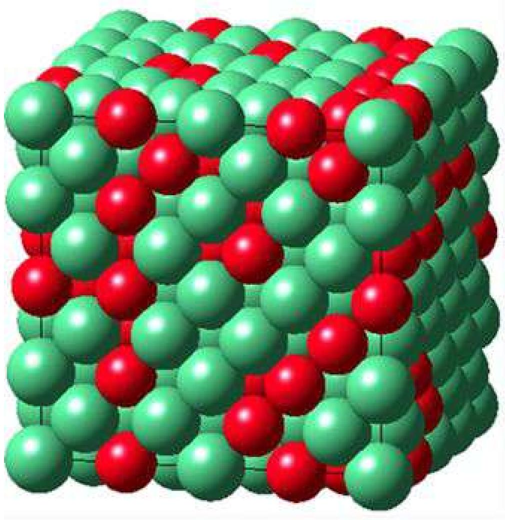
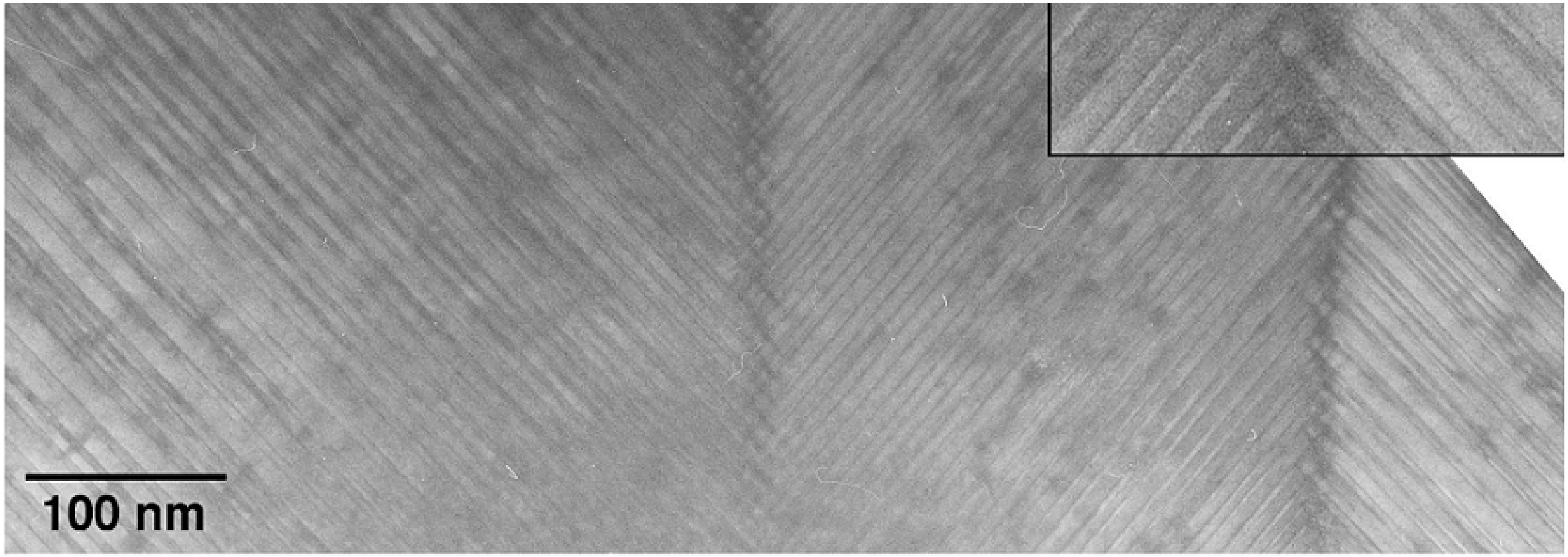
Metallic alloys comprise a mixture of different elements forming a crystal lattice.

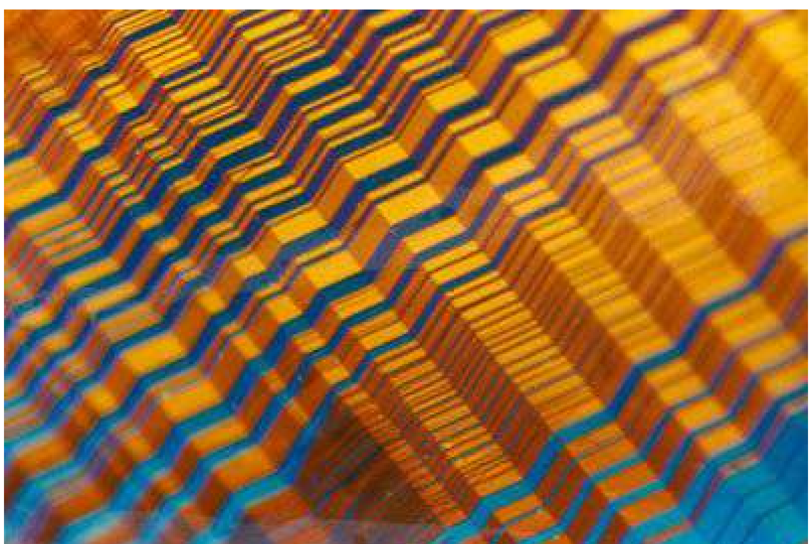


This course is about martensitic phase transformations. These are solid-solid phase transformations in which the underlying crystal lattice of an alloy changes shape as the temperature is reduced through a critical temperature.

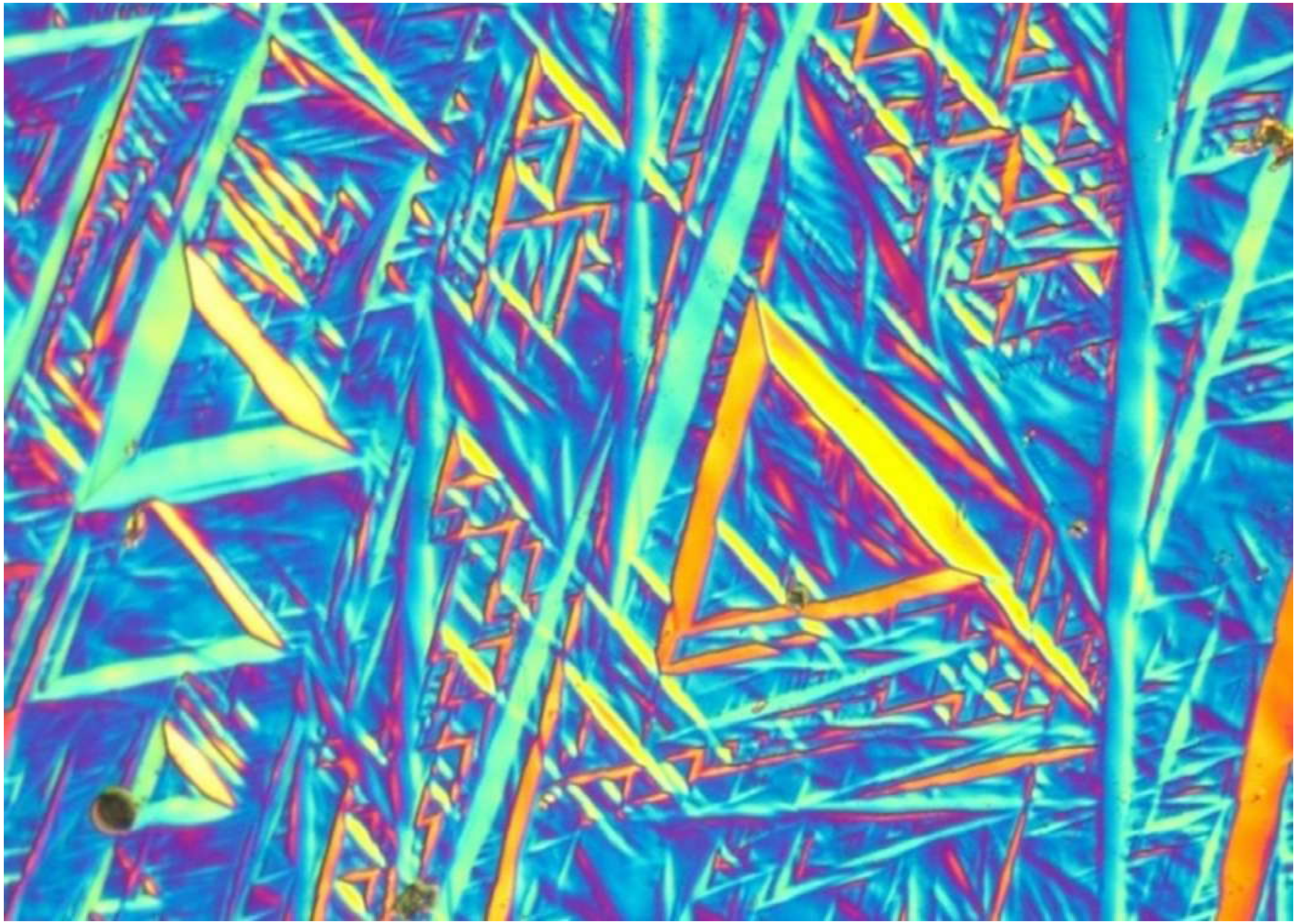
It turns out that there are different possible symmetry related variants of the low temperature phase, and the crystal has to deform in such a way that these different variants are geometrically compatible. This leads to remarkable patterns of microstructure that determine how the alloy behaves macroscopically.



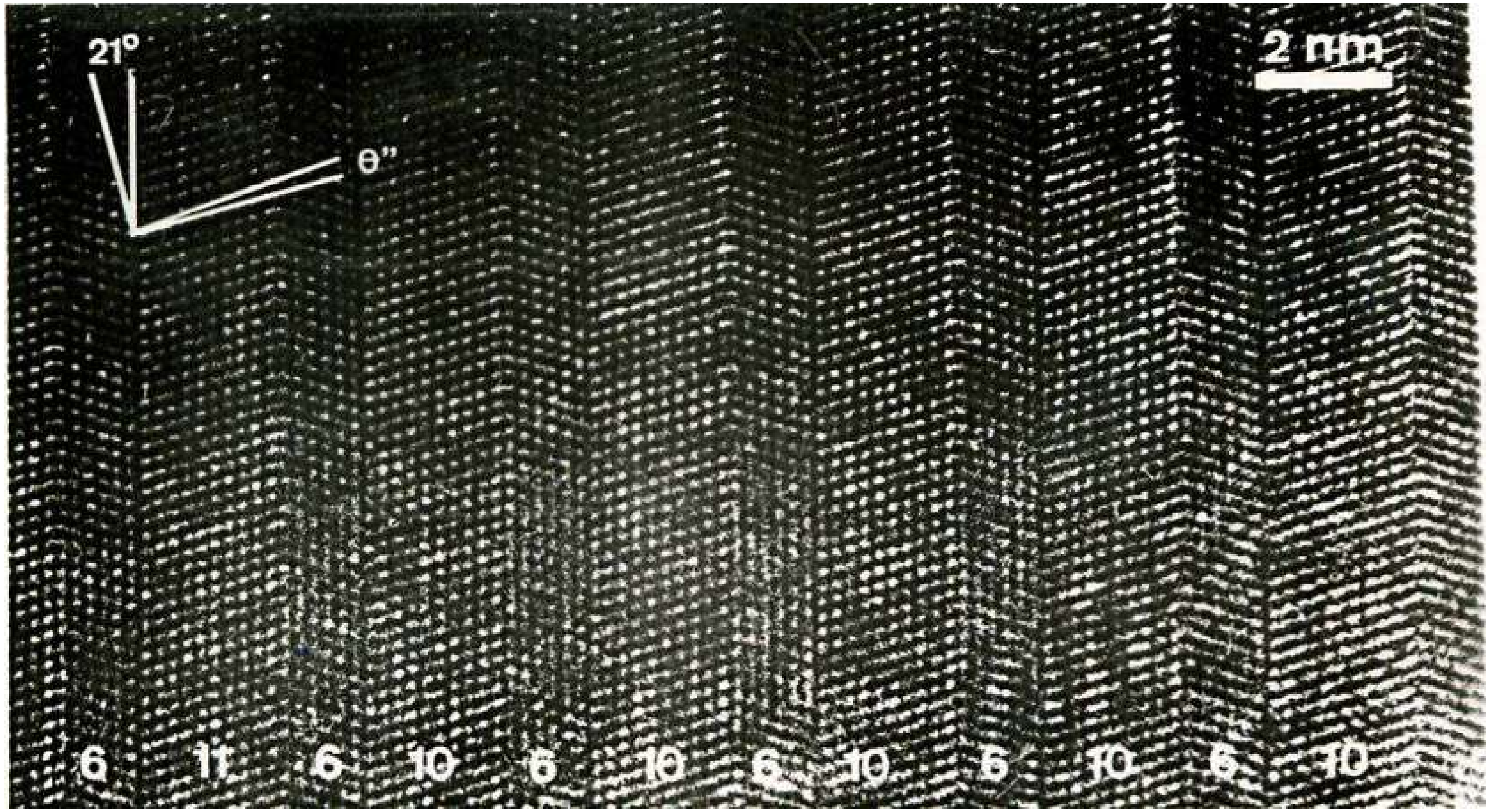
$Ni_{65}Al_{35}$ (Boullay/Schryvers)



CuAlNi (Chu/James)



β-titanium (T. Inamura, M. Ii, N. Kamioka, M. Tahara, H. Hosoda, S. Miyazaki)



NiMn (Baele, van Tendeloo, Amelinckx)

Questions

1. What exactly are we seeing in these micrographs?

2. What is a good mathematical model?

3. Can we predict the microstructure morphology?

4. Why is the microstructure so fine (i.e. the length-scale so small)?

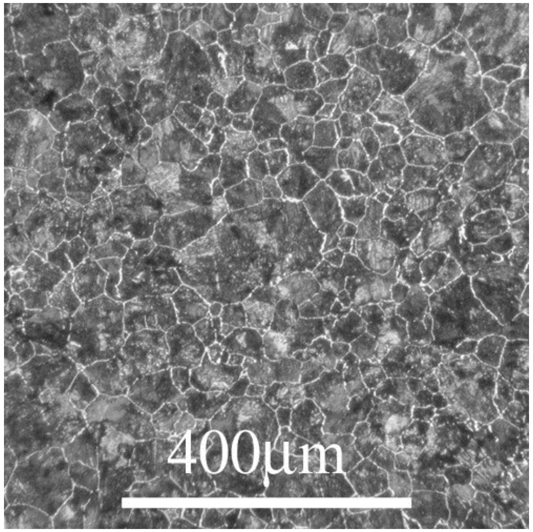
Topics

1. Nonlinear elastostatics.
2. Existence of minimizers and analysis tools.
3. Martensitic phase transformations.
4. Microstructure.
5. Austenite-martensite interfaces.
6. Complex interfaces.
7. Incompatibility induced metastability and nucleation of austenite.
8. Remarks on polycrystals.
9. Local minimizers with and without interfacial energy.

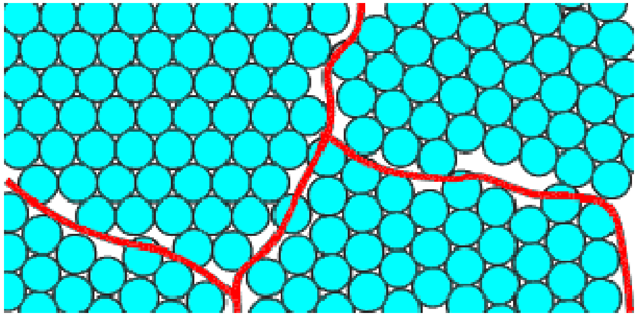
1. Nonlinear elastostatics

The central model of solid mechanics. Rubber, metals (and alloys), rock, wood, bone … can all be modelled as elastic materials, even though their chemical compositions are very different.

For example, metals and alloys are crystalline, with grains consisting of regular arrays of atoms.

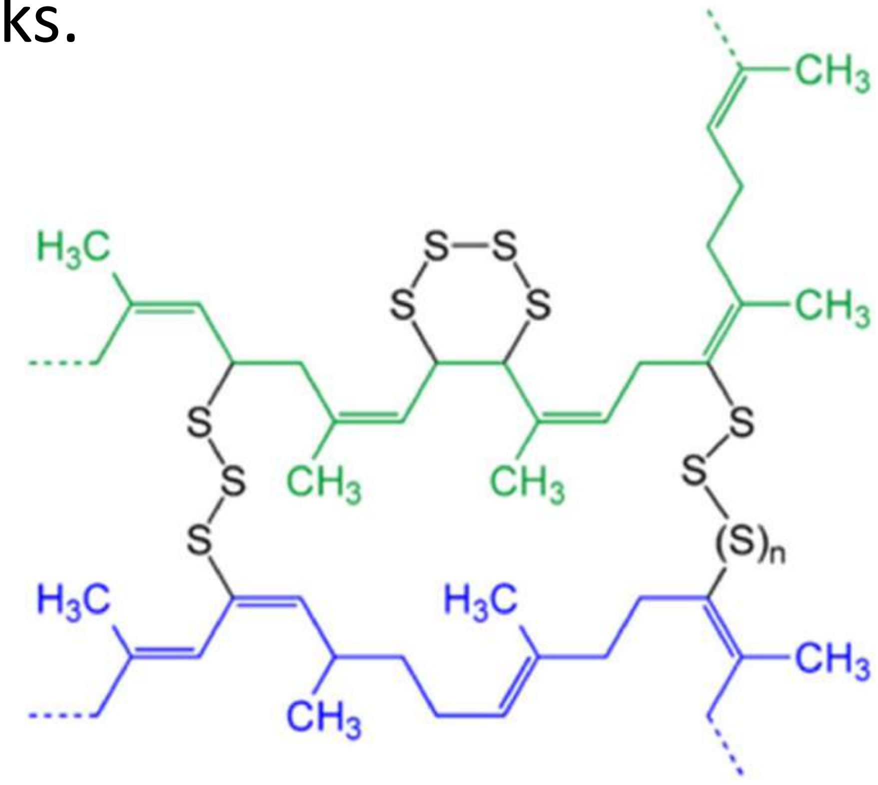


Iron carbon alloy, showing grain structure



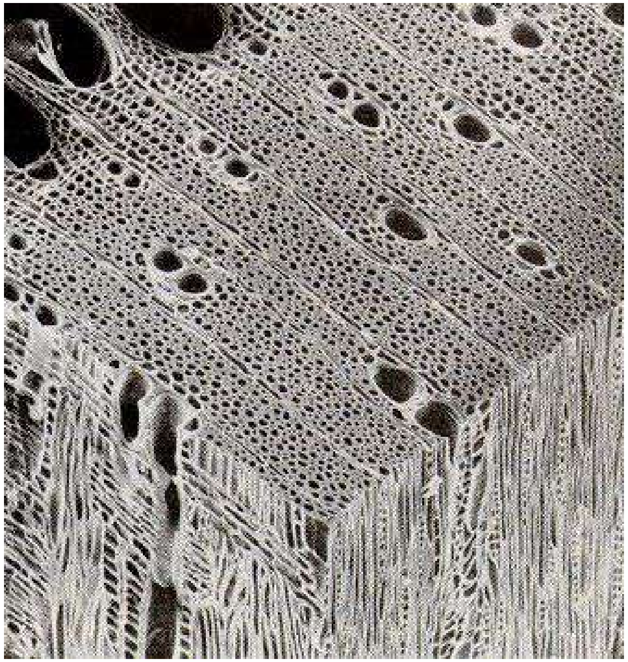
http://www.doitpoms.ac.uk

Polymers (such as rubber) consist of long chain molecules that are wriggling in thermal motion, often joined to each other by chemical bonds called crosslinks.



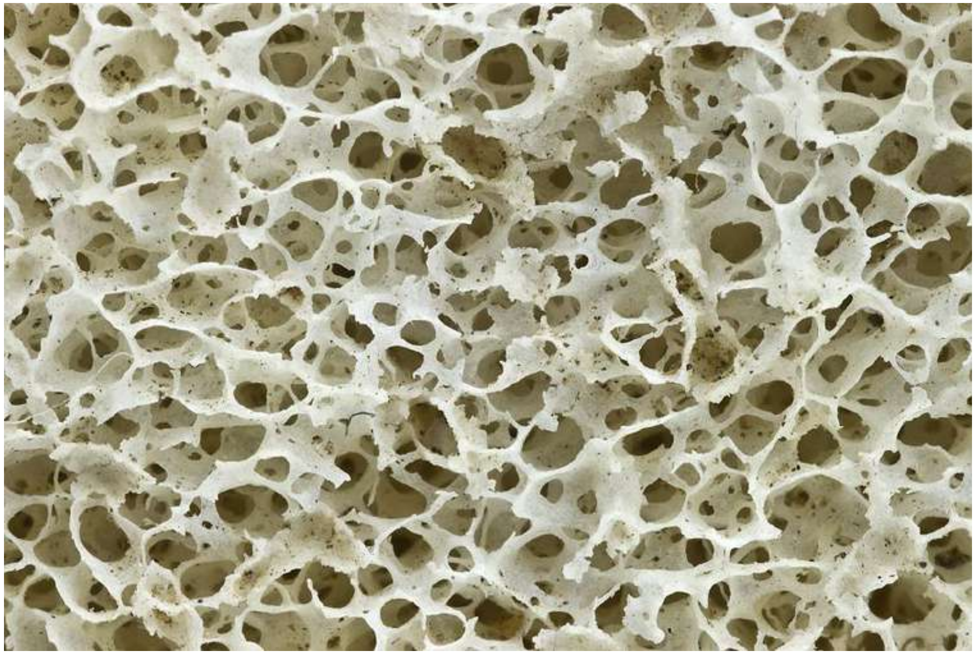
Schematic presentation of two strands (blue and green) of natural rubber after vulcanization with sulphur. (Wikipedia)

Wood and bone have a cellular structure.



White ash

http://classes.mst.edu/civeng120/lessons/wood/cell_structure/index.html



Human hip bone

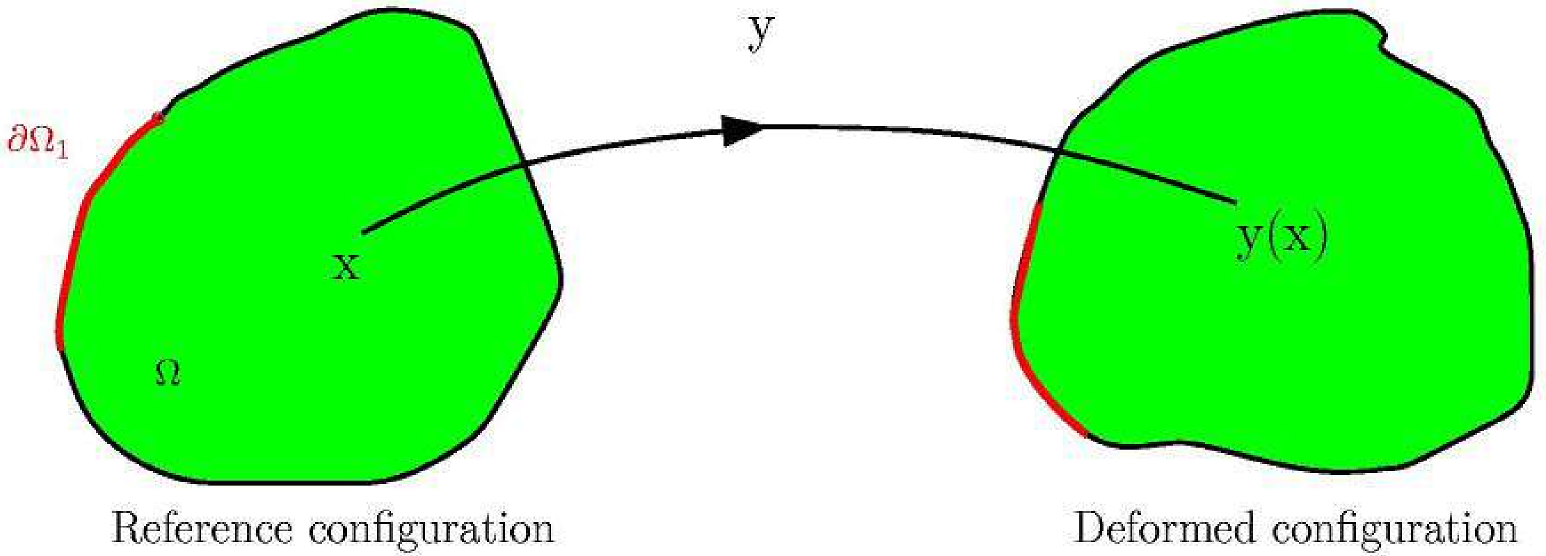
Patrick Siemer, San Francisco, USA

A brief history

1678 Hooke's Law
1705 Jacob Bernoulli
1742 Daniel Bernoulli
1744 L. Euler *elastica* (elastic rod)
1821 Navier, special case of linear elasticity via molecular model
(Dalton's atomic theory was 1807)
1822 Cauchy, stress, *nonlinear* and linear elasticity

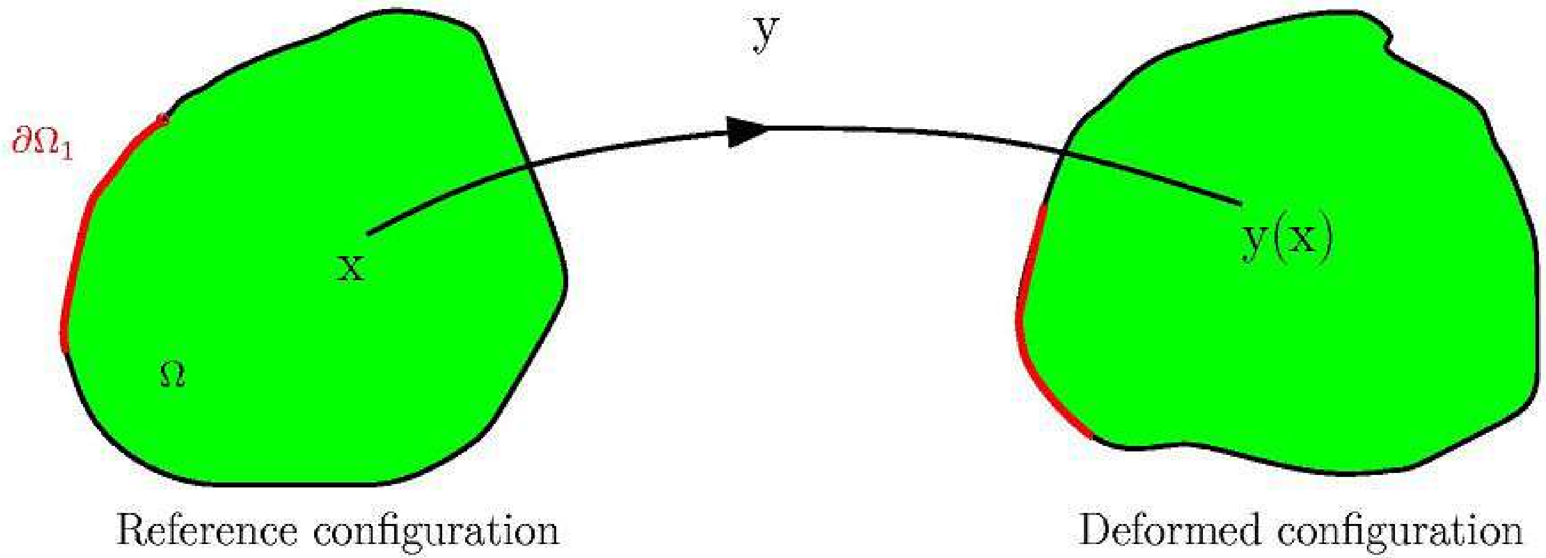
For a long time the nonlinear theory was ignored/forgotten.
1927 A.E.H. Love, Treatise on linear elasticity
1950's R. Rivlin, Exact solutions in *incompressible* nonlinear elasticity (rubber)
1960 - 80 Nonlinear theory clarified by J.L. Ericksen, C. Truesdell …
1980 - Mathematical developments, applications to materials, biology …

Description of deformation



$\Omega \subset \mathbb{R}^3$ bounded domain with closure $\bar{\Omega}$ and (Lipschitz) boundary $\partial\Omega$.

Label the material points of the body by the positions $x \in \Omega$ they occupy in the reference configuration.



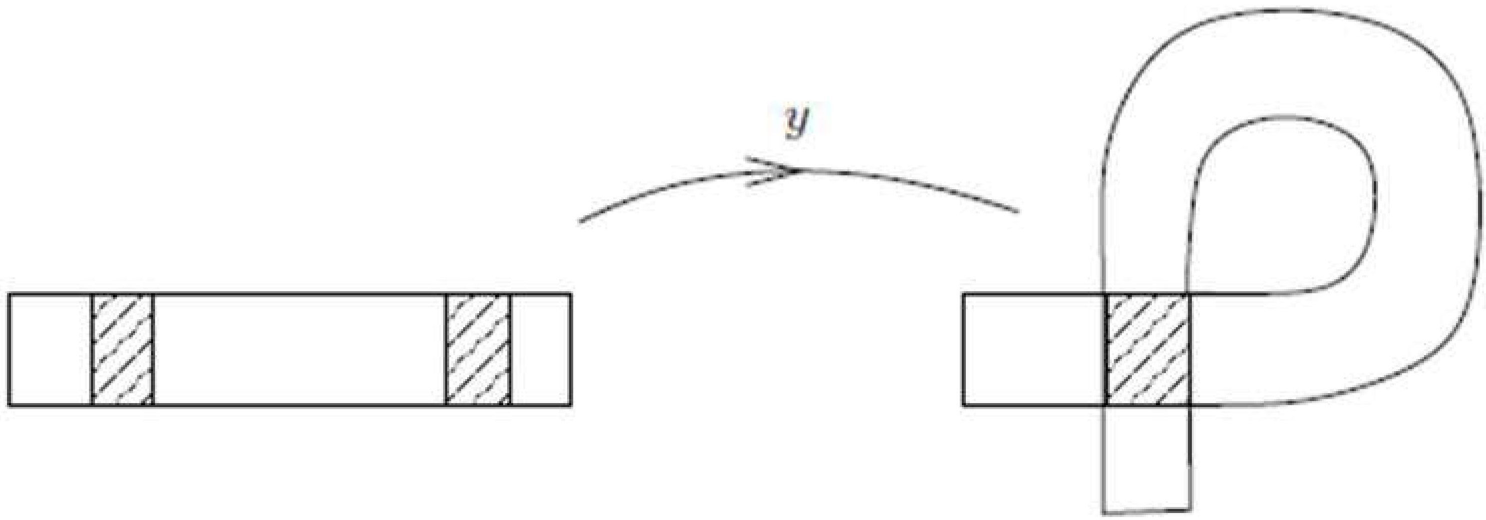
A typical deformation is described by a map $y : \bar{\Omega} \to \mathbb{R}^3$.

For the time being we suppose that y is smooth with deformation gradient

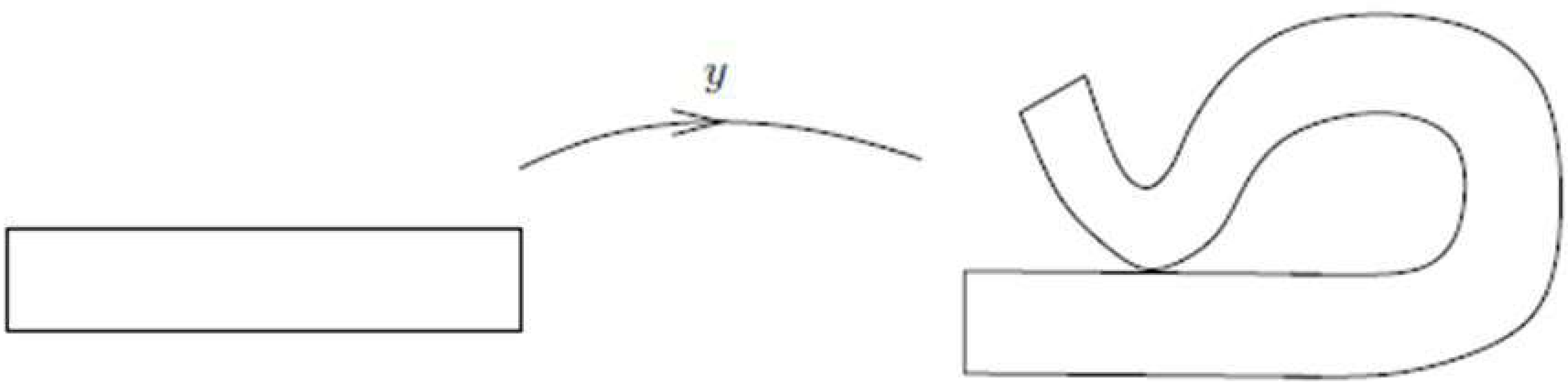
$$F = Dy(x), \ F_{i\alpha} = \frac{\partial y_i}{\partial x_\alpha}.$$

To avoid interpenetration of matter, $y : \Omega \to \mathbb{R}^3$ should be invertible.

Examples.



locally invertible but not globally invertible



invertible on Ω
not on $\overline{\Omega}$

How can we ensure invertibility?

For C^1 maps we can use:

Theorem. Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary $\partial\Omega$ (in particular Ω lies on one side of $\partial\Omega$ locally). Let $y \in C^1(\bar{\Omega}; \mathbb{R}^3)$ with

$$\det Dy(x) > 0 \text{ for all } x \in \bar{\Omega} \qquad (*)$$

and $y|_{\partial\Omega}$ one-to-one. Then y is invertible on $\bar{\Omega}$.

(The proof uses degree theory. See, for example, Meisters & Olech, Duke Math. J. 30 (1963) 63-80.)

When y is not smooth, or is not prescribed on the whole of $\partial\Omega$, things are more complicated. For the rest of this course we ignore issues of invertibility, but we will assume that $(*)$ holds in some sense.

Notation

$$\begin{aligned} M^{3\times 3} &= \{\text{real } 3\times 3 \text{ matrices}\} \\ M^{3\times 3}_{+} &= \{F \in M^{3\times 3} : \det F > 0\} \\ SO(3) &= \{R \in M^{3\times 3}_{+} : R^T R = 1\} \\ &= \{\text{rotations}\}. \end{aligned}$$

If $a \in \mathbb{R}^3$, $b \in \mathbb{R}^3$, the tensor product $a \otimes b$ is the matrix with the components

$$(a \otimes b)_{ij} = a_i b_j.$$

[Thus $(a \otimes b)c = (b \cdot c)a$ if $c \in \mathbb{R}^3$.]

Theorem (Square root theorem) Let C be a positive symmetric 3×3 matrix. Then there is a unique positive definite symmetric 3×3 matrix U such that $C = U^2$. If C has spectral decomposition $C = \sum_{i=1}^{3} \lambda_i \hat{e}_i \otimes \hat{e}_i$, then $U = \sum_{i=1}^{3} \lambda_i^{1/2} \hat{e}_i \otimes \hat{e}_i$. (We write $U = C^{\frac{1}{2}}$.)

Theorem (Polar decomposition)
Let $F \in M_+^{3\times 3}$. Then there exist positive definite symmetric U, V and $R \in SO(3)$ such that

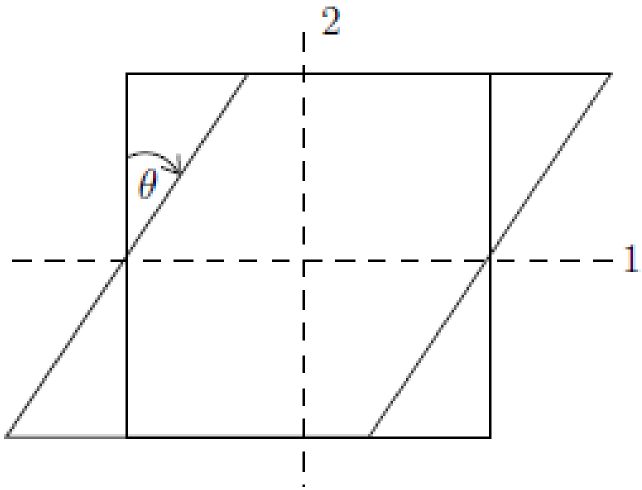
$$F = RU = VR,$$

and $U = (F^T F)^{\frac{1}{2}}, V = (FF^T)^{\frac{1}{2}}$.
These representations are unique.

Because $V = RUR^T$ the strictly positive eigenvalues v_1, v_2, v_3 of U and V are the same. They are called the *singular values* of F, or the *principal stretches*.

Exercise: simple shear

$$y(x) = (x_1 + \gamma x_2, x_2, x_3).$$



$\gamma = \tan\theta$

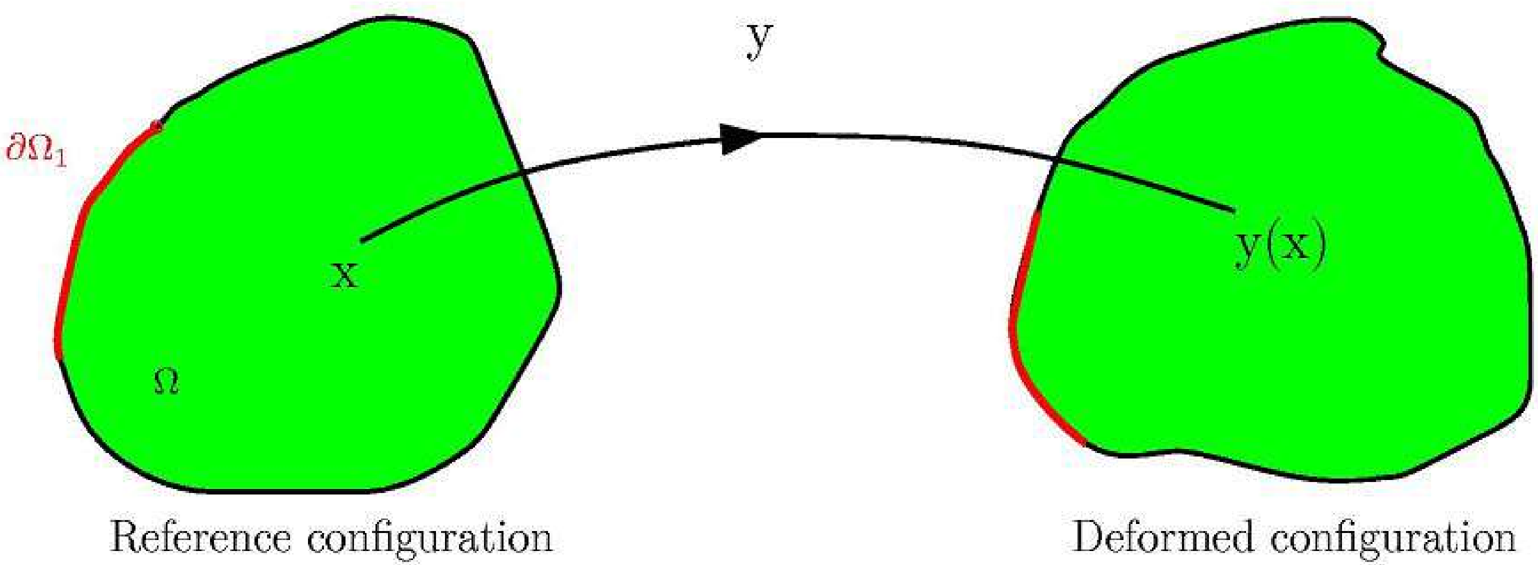
$\theta =$ angle of shear

Show that

$$F = \begin{pmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\psi & \sin\psi & 0 \\ \sin\psi & \frac{1+\sin^2\psi}{\cos\psi} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$\tan\psi = \frac{\gamma}{2}$. As $\gamma \to 0+$ the eigenvectors of U and V tend to $\frac{1}{\sqrt{2}}(e_1 + e_2), \frac{1}{\sqrt{2}}(e_1 - e_2), e_3$.

Variational formulation of nonlinear elasticity



Find a deformation $y = y(x)$ minimizing the total free energy given by

$$I(y) = \int_\Omega \psi(Dy(x))\,dx$$

subject to suitable boundary conditions, for example $y|_{\partial\Omega_1} = \bar{y}$, where $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$ is given.

Properties of the free-energy density ψ.

Assume

(H1) $\psi(\cdot) : M_+^{3\times 3} \to [0,\infty)$ is C^1.

(H2) $\psi(F) \to \infty$ as $\det F \to 0+$.

(H3) (Frame indifference) $\psi(QF) = \psi(F)$ for all $Q \in SO(3)$, $F \in M_+^{3\times 3}$.

Hence $\psi(F) = \psi(RU) = \psi(U)$.

The *Piola-Kirchhoff stress tensor* is given by

$$T_R(Dy) = D\psi(Dy).$$

Material symmetry

Some materials have a mechanical response that depends on how they are oriented in the reference configuration. To make this precise we ask the question as to which initial linear deformations $H \in M_+^{3\times 3}$ do not change ψ? That is, for which H do we have

$$\psi(F) = \psi(FH) \qquad \text{for all } F \in M_+^{3\times 3}?$$

These H form a subgroup $\mathcal{S}$ of $M_+^{3\times 3}$, the *symmetry group* of ψ. For example, if ψ has cubic symmetry we can take

$$\mathcal{S} = P^{24} = \{\text{rotations of a cube}\}.$$

Isotropic materials

These are materials for which all rotations are in the symmetry group, i.e. $SO(3) \subset \mathcal{S}$.

Theorem
ψ is isotropic iff $\psi(F) = \Phi(v_1, v_2, v_3)$ for some Φ that is symmetric with respect to permutations of v_1, v_2, v_3.

Examples of isotropic ψ are given by the Ogden models of rubber:

$$\Phi = \sum_{i=1}^{N} \alpha_i (v_1^{p_i} + v_2^{p_i} + v_3^{p_i} - 3) + \sum_{i=1}^{M} \beta_i ((v_2 v_3)^{q_i} + (v_3 v_1)^{q_i} + (v_1 v_2)^{q_i} - 3) + h(v_1 v_2 v_3)$$

where $\alpha_i, \beta_i, p_i, q_i$ are constants and $h(\delta) \to \infty$ as $\delta \to 0+$.

Why do we minimize energy?

This is a deep question, the rough answer being the Second Law of Thermodynamics.

Under suitable mechanical and thermal boundary conditions the Second Law endows (Duhem, Ericksen) the equations of dynamic (thermo)elasticity with a Lyapunov function

$$\int_\Omega \left(\frac{1}{2}\rho_R|y_t|^2 + \epsilon(Dy,\theta) - \theta_0\eta(Dy,\theta)\right)\,dx$$

entropy

density

velocity

internal energy

temperature

constant boundary temperature

and we expect $y_t \to 0$, $\theta \to \theta_0$ as $t \to \infty$. Thus we expect the dynamics to generically give minimizing sequences for $\int_\Omega \psi(Dy(x))\,dx$, where $\psi(Dy) = \epsilon(Dy,\theta_0) - \theta_0\eta(Dy,\theta_0)$.

2. Existence of minimizers and analysis tools

L^p spaces

All mappings, sets assumed measurable, all integrals Lebesgue integrals.

Let $1 \leq p \leq \infty$.

$$L^p(\Omega) = \{u : \Omega \to \mathbb{R} : \|u\|_p < \infty\},$$

where

$$\|u\|_p = \begin{cases} \left(\int_\Omega |u(x)|^p \, dx\right)^{\frac{1}{p}} & \text{if } 1 \leq p < \infty \\ \operatorname{ess\,sup}_{x\in\Omega} |u(x)| & \text{if } p = \infty \end{cases}$$

$$L^p(\Omega; \mathbb{R}^n) = \{u = (u_1, \ldots, u_n) : u_i \in L^p(\Omega)\}.$$

$u^{(j)} \to u$ in L^p if $\|u^{(j)} - u\|_p \to 0$.

The Sobolev space $W^{1,p}$

$W^{1,p} = \{y : \Omega \to \mathbb{R}^3 : \|y\|_{1,p} < \infty\}$, where

$$\|y\|_{1,p} = \begin{cases} \left(\int_\Omega [|y(x)|^p + |Dy(x)|^p]\, dx\right)^{1/p} & \text{if } 1 \le p < \infty \\ \operatorname{ess\,sup}_{x\in\Omega} (|y(x)| + |Dy(x)|) & \text{if } p = \infty \end{cases}$$

i.e. $y \in L^p(\Omega; \mathbb{R}^3), Dy \in L^p(\Omega; M^{3\times 3})$.

Dy is interpreted in the weak (or distributional) sense, so that

$$\int_\Omega \frac{\partial y_i}{\partial x_\alpha} \varphi \, dx = -\int_\Omega y_i \frac{\partial \varphi}{\partial x_\alpha} \, dx$$

for all $\varphi \in C_0^\infty(\Omega)$.

Weak convergence

$=$ convergence of averages

$u^{(j)}$ converges *weakly* to u (or weak* if $p = \infty$) in L^p, written $u^{(j)} \rightharpoonup u$ (or $u^{(j)} \overset{*}{\rightharpoonup} u$ if $p = \infty$) if

$$\int_\Omega u^{(j)} \varphi \, dx \to \int_\Omega u \varphi \, dx \text{ for all } \varphi \in L^{p'},$$

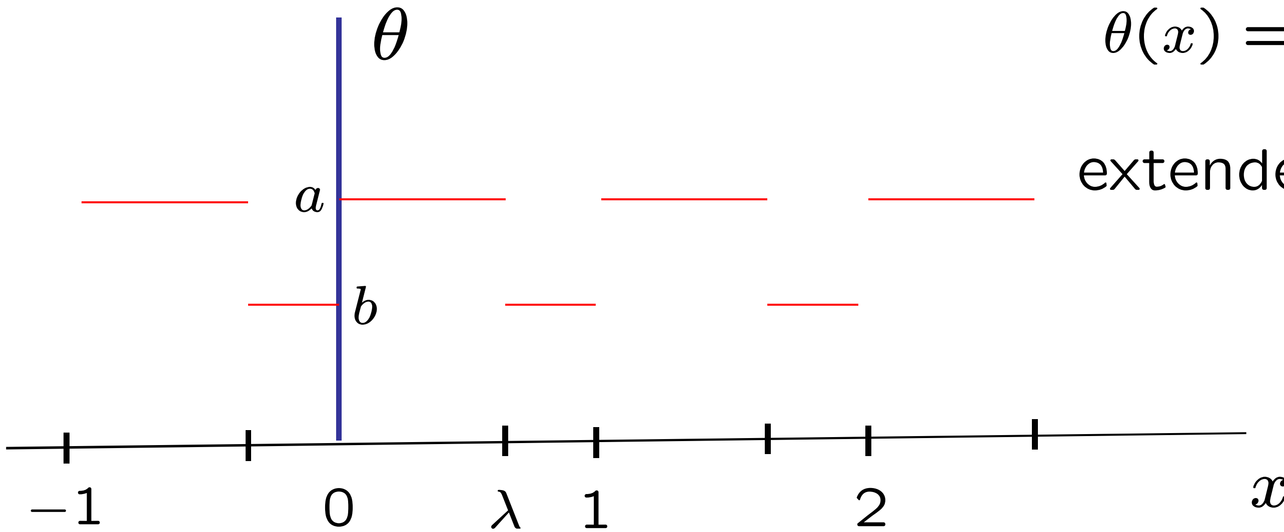
where $\frac{1}{p} + \frac{1}{p'} = 1$.

The importance of weak convergence for nonlinear PDE comes from the fact that if $1 < p \leq \infty$ then any bounded sequence in L^p has a weakly convergent subsequence (weak* if $p = \infty$).

If the bounded sequence is a sequence of approximating solutions to the PDE (e.g. coming from some numerical method, or a minimizing sequence for a variational problem), then the weak limit is a candidate solution.

But then we need somehow to pass to the limit in nonlinear terms using weak convergence.

Example: Rademacher functions.



$$\theta(x) = \begin{cases} a & \text{if } 0 < x \leq \lambda \\ b & \text{if } \lambda < x \leq 1 \end{cases}$$

extended periodically to $\mathbb{R}$.

Exercise. Define $\theta^{(j)}(x) = \theta(jx)$.

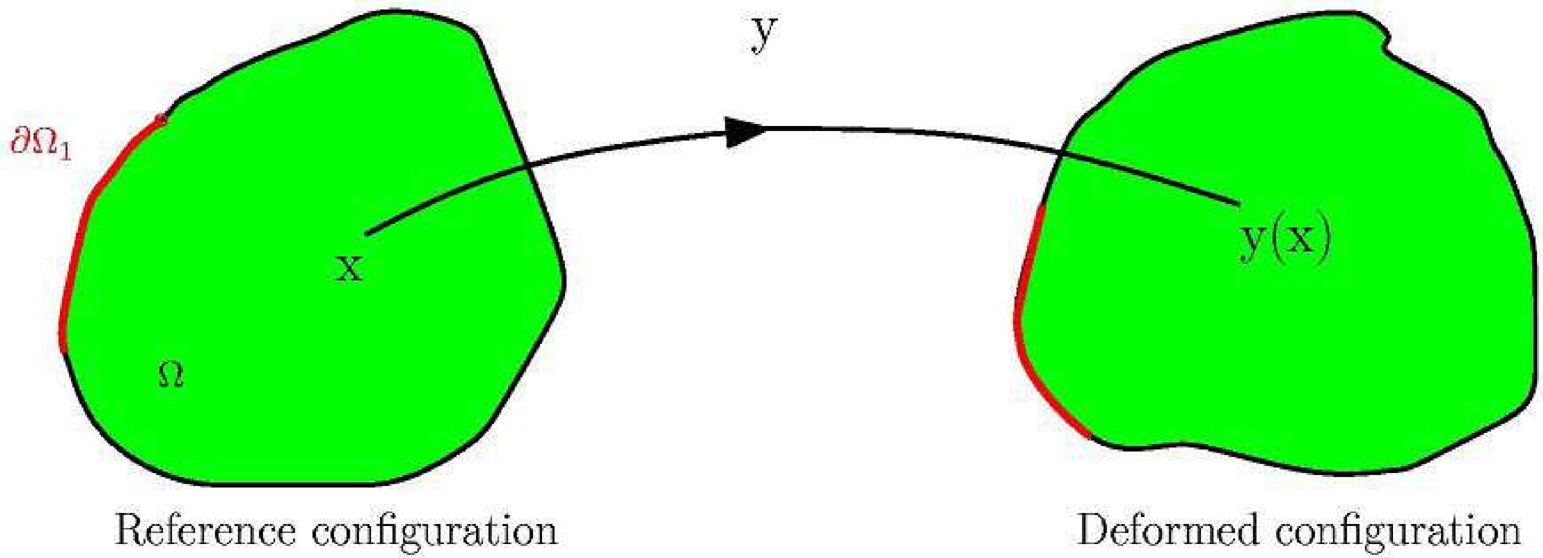
(i) Prove that $\theta^{(j)} \overset{*}{\rightharpoonup} \lambda a + (1-\lambda)b$ in $L^\infty(0,1)$

(ii) Deduce that if $f : \mathbb{R} \to \mathbb{R}$ is continuous and such that $u^{(j)} \overset{*}{\rightharpoonup} u$ in L^∞ implies $f(u^{(j)}) \overset{*}{\rightharpoonup} f(u)$ in L^∞ then f is *affine*, i.e. $f(v) = \alpha v + \beta$ for constants α, β.

We say that $y^{(j)} \rightharpoonup y$ in $W^{1,p}$ if $y^{(j)} \rightharpoonup y$ in L^p and $Dy^{(j)} \rightharpoonup Dy$ in L^p ($\rightharpoonup$ replaced by $\overset{*}{\rightharpoonup}$ if $p = \infty$).

Question: for what continuous $f : M^{3\times 3} \to \mathbb{R}$ does $y^{(j)} \overset{*}{\rightharpoonup} y$ in $W^{1,\infty}$ imply $f(Dy^{(j)}) \overset{*}{\rightharpoonup} f(Dy)$ in L^∞?

Answering this turns out to be a key to proving the existence of minimizers for a realistic class of materials.



$\Omega \subset \mathbb{R}^3$ bounded domain with Lipschitz boundary $\partial\Omega$, $\partial\Omega_1 \subset \partial\Omega$ relatively open, $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$.

We want to minimize

$$I(y) = \int_\Omega \psi(Dy)\, dx$$

in the set of admissible mappings

$$\mathcal{A} = \{y \in W^{1,1} : \det Dy(x) > 0 \text{ a.e.}, \ y|_{\partial\Omega_1} = \bar{y}\}.$$

(Note that we have replaced the invertibility condition by the local condition $\det Dy(x) > 0$ a.e., which is easier to handle.)

So far we have assumed that

(H1) $\qquad \psi : M^{3\times 3}_{+} \to [0,\infty)$ is C^1,

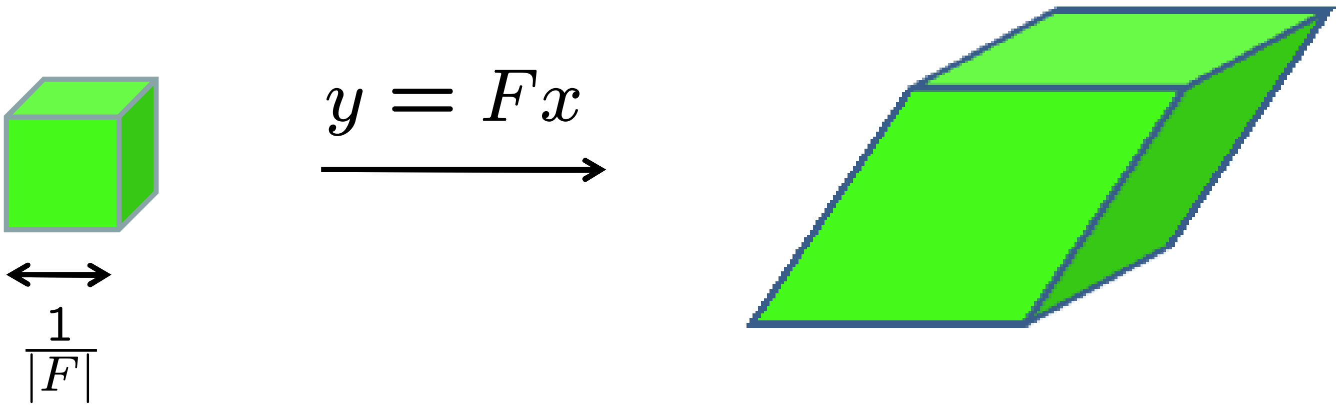
(H2) $\qquad \psi(F) \to \infty$ as $\det F \to 0+$,

so that setting $\psi(F) = \infty$ if $\det F \leq 0$, we have that $\psi : M^{3\times 3} \to [0,\infty]$ is continuous, and that ψ is *frame-indifferent*, i.e.

(H3) $\qquad \psi(RF) = \psi(F)$ for all $R \in \mathrm{SO}(3), F \in M^{3\times 3}$.

(In fact (H3) plays no direct role in the existence theory.)

Growth condition



$$\lim_{|F| \to \infty} \frac{\psi(F)}{|F|^3} = \infty$$

says that you can't get a finite line segment from an infinitesimal cube with finite energy.

We will use growth conditions a little weaker than this. Note that if

$$\psi(F) \geq C(1 + |F|^{3+\varepsilon})$$

for some $\varepsilon > 0$ then any deformation with finite elastic energy

$$\int_\Omega \psi(Dy(x))\, dx$$

and satisfying suitable boundary conditions is in $W^{1,3+\varepsilon}$ and so is continuous by the Sobolev embedding theorem.

Convexity conditions

The key difficulty is that ψ is never convex

(Recall that ψ is convex if

$$\psi(\lambda F + (1-\lambda)G) \leq \lambda\psi(F) + (1-\lambda)\psi(G)$$

for all F, G and $0 \leq \lambda \leq 1$.)

Reasons

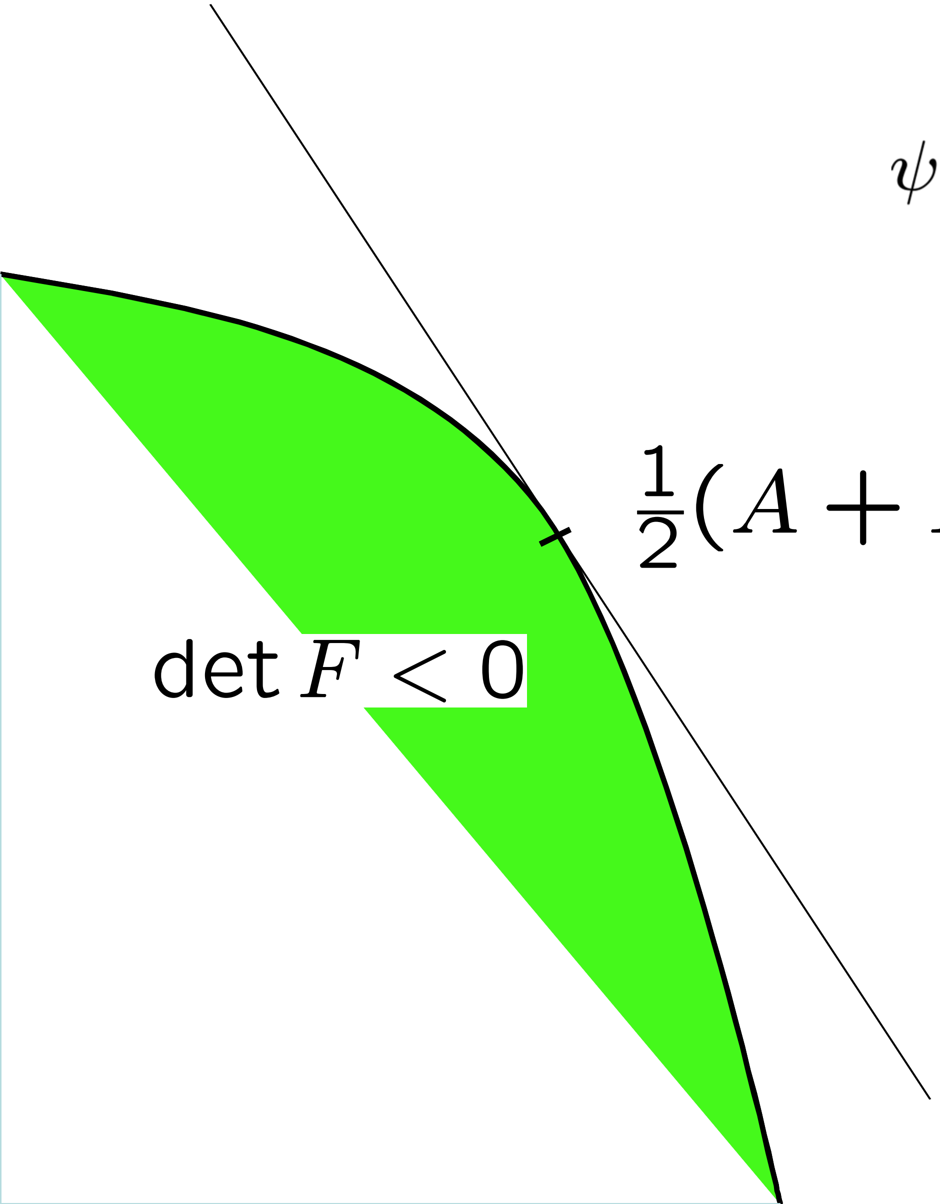
1. Convexity of ψ is inconsistent with (H2) because $M_+^{3\times 3}$ is not convex.

Remark: $M_+^{3\times 3}$ is not simply-connected.

$A = \text{diag}\,(1,1,1)$

$$\psi(\tfrac{1}{2}(A+B)) = \infty$$
$$> \tfrac{1}{2}\psi(A) + \tfrac{1}{2}\psi(B)$$

$\frac{1}{2}(A+B) = \text{diag}\,(0,0,1)$



det $F > 0$

$B = \text{diag}\,(-1,-1,1)$

2. If ψ is convex, then any equilibrium solution (solution of the EL equations) is an absolute minimizer of the elastic energy

$$I(y) = \int_\Omega \psi(Dy)\, dx.$$

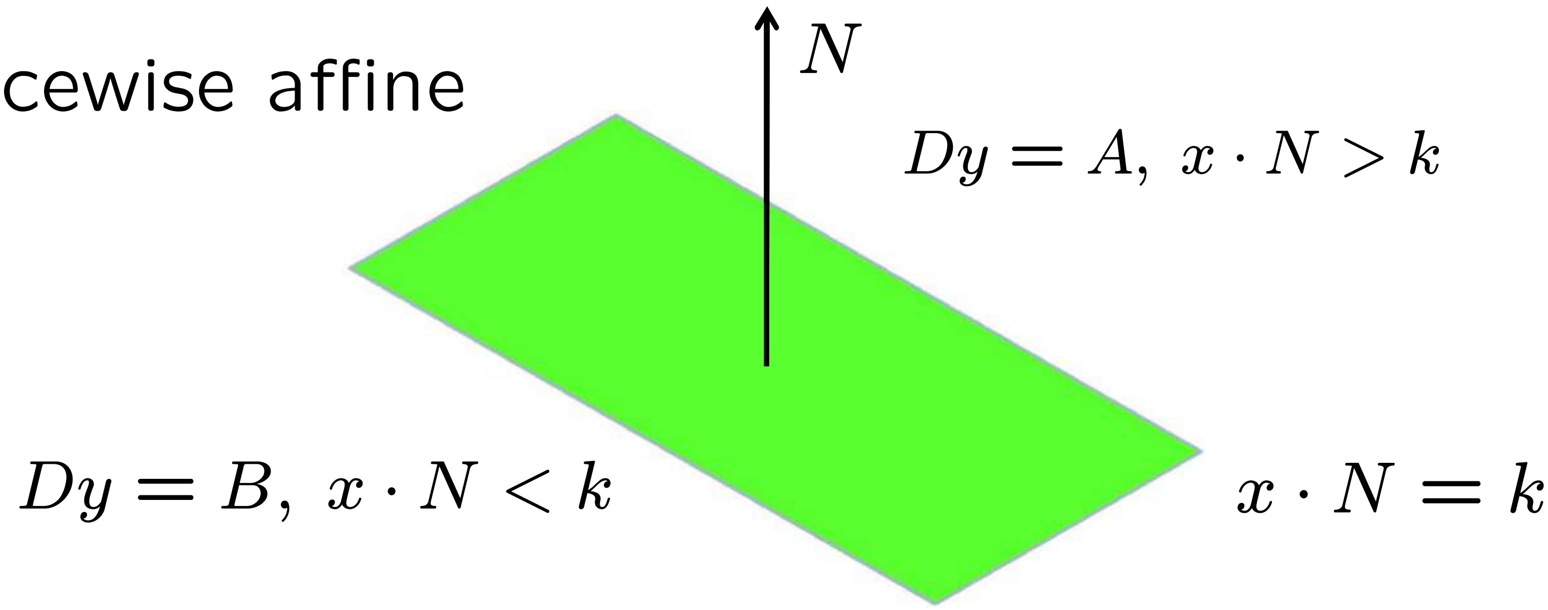
Proof.

$$I(z) = \int_\Omega \psi(Dz)\, dx \geq$$
$$\int_\Omega [\psi(Dy) + D\psi(Dy) \cdot (Dz - Dy)]\, dx = I(y).$$

This contradicts common experience of nonunique equilibria, e.g. buckling.

Rank-one matrices and the Hadamard jump condition

y piecewise affine

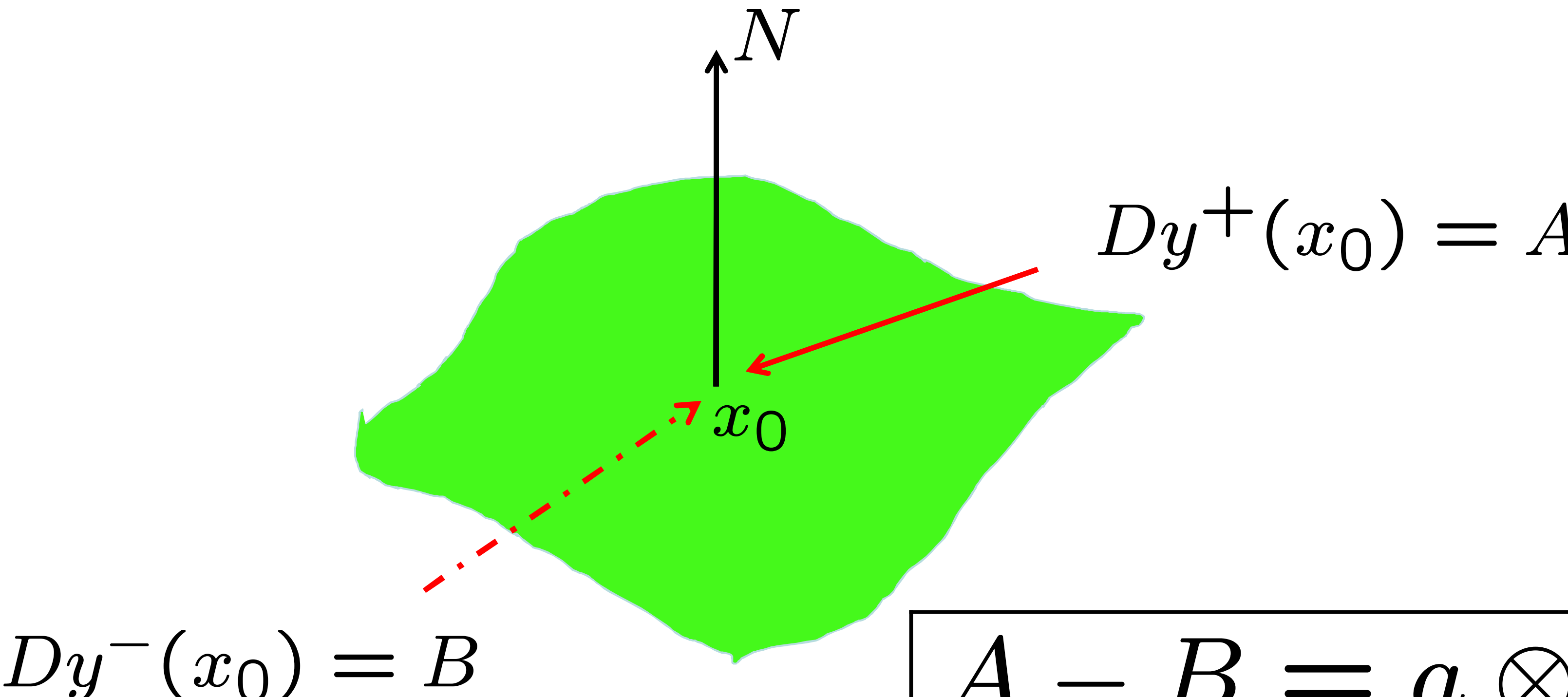


Let $C = A - B$. Then $Cx = 0$ if $x \cdot N = 0$. Thus $C(z - (z \cdot N)N) = 0$ for all z, and so $Cz = (CN \otimes N)z$. Hence

$$\boxed{A - B = a \otimes N}$$

Hadamard jump condition

More generally this holds for y piecewise C^1, with Dy jumping across a C^1 surface.



$$\boxed{A - B = a \otimes N}$$

Exercise: prove this by blowing up around x using $y_\varepsilon(x) = \varepsilon y(\frac{x - x_0}{\varepsilon})$.

(See later for generalizations when y not piecewise C^1.)

Rank-one convexity

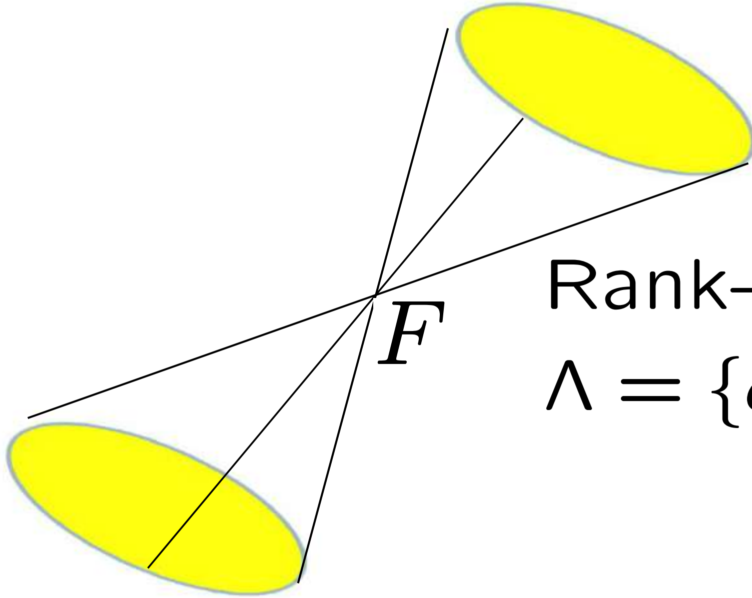
ψ is *rank-one convex* if the map $t \mapsto \psi(F + ta \otimes N)$ is convex for each $F \in M^{3\times 3}$ and $a \in \mathbb{R}^3, N \in \mathbb{R}^3$.

(Same definition for $M^{m\times n}$.)

Equivalently ψ is rank-one convex if

$$\psi(\lambda F + (1-\lambda)G) \leq \lambda\psi(F) + (1-\lambda)\psi(G)$$

if $F, G \in M^{3\times 3}$ with $F - G = a \otimes N$ and $\lambda \in (0,1)$.



Rank-one cone

$\Lambda = \{a \otimes N : a, N \in \mathbb{R}^3\}$

Rank-one convexity is consistent with (H2) because $\det(F + ta \otimes N)$ is linear in t, so that $M_+^{3\times3}$ is rank-one convex (i.e. if $F, G \in M_+^{3\times3}$ with $F - G = a \otimes N$ then $\lambda F + (1-\lambda)G \in M_+^{3\times3}$.)

If $\psi \in C^2(M_+^{3\times 3})$ then ψ is rank-one convex iff

$$\frac{d^2}{dt^2}\psi(F + ta \otimes N)|_{t=0} \geq 0,$$

for all $F \in M_+^{3\times 3}, a, N \in \mathbb{R}^3$, or equivalently

$$D^2\psi(F)(a \otimes N, a \otimes N) = \frac{\partial^2 \psi(F)}{\partial F_{i\alpha} \partial F_{j\beta}} a_i N_\alpha a_j N_\beta \geq 0,$$

(Legendre-Hadamard condition).

Quasiconvexity (C.B. Morrey,1952)

Let $\psi : M^{m\times n} \to [0,\infty]$ be continuous. ψ is said to be *quasiconvex at* $F \in M^{m\times n}$ if the inequality

$$\int_\Omega \psi(F + D\varphi(x))\,dx \geq \int_\Omega \psi(F)\,dx$$

definition independent of Ω

holds for any $\varphi \in W_0^{1,\infty}(\Omega;\mathbb{R}^m)$, and is *quasiconvex* if it is quasiconvex at every $F \in M^{m\times n}$.

Could replace by $C_0^\infty(\Omega;\mathbb{R}^m)$

Here $\Omega \subset \mathbb{R}^n$ is any bounded open set with Lipschitz boundary, and $W_0^{1,\infty}(\Omega;\mathbb{R}^m)$ is the set of those $y \in W^{1,\infty}(\Omega;\mathbb{R}^m)$ which are zero on $\partial\Omega$ (in the sense of trace).

Setting $m = n = 3$ we see that ψ is quasiconvex if for any $F \in M^{3\times 3}$ the pure displacement problem to minimize

$$I(y) = \int_\Omega \psi(Dy(x))\, dx$$

subject to the linear boundary condition

$$y(x) = Fx,\ x \in \partial\Omega,$$

has $y(x) = Fx$ as a minimizer.

Theorem

If ψ is continuous and quasiconvex then ψ is rank-one convex.

Corollary If $m = 1$ or $n = 1$ then a continuous $\psi : M^{m\times n} \to [0, \infty]$ is quasiconvex iff it is convex.

Proof.

If $m = 1$ or $n = 1$ then rank-one convexity is the same as convexity. If ψ is convex then by Jensen's inequality:

$$\frac{1}{\operatorname{meas}\Omega}\int_\Omega \psi(F + D\varphi)\,dx$$
$$\geq \psi\left(\frac{1}{\operatorname{meas}\Omega}\int_\Omega (F + D\varphi)\,dx\right) = \psi(F).$$

Theorem (van Hove)

Let $\psi(F) = c_{ijkl}F_{ij}F_{kl}$ be quadratic. Then ψ is rank-one convex $\Leftrightarrow$ ψ is quasiconvex.

Proof.

Let ψ be rank-one convex. Since for any $\varphi \in W_0^{1,\infty}$

$$\int_\Omega [\psi(F + D\varphi) - \psi(F)]\, dx = \int_\Omega c_{ijkl}\varphi_{i,j}\varphi_{k,l}\, dx$$

we just need to show that the RHS is ≥ 0.

Extend φ by zero to the whole of $\mathbb{R}^n$ and take Fourier transforms.

By the Plancherel formula

$$
\begin{aligned}
\int_\Omega c_{ijkl}\varphi_{i,j}\varphi_{k,l}\,dx &= \int_{\mathbb{R}^n} c_{ijkl}\varphi_{i,j}\varphi_{k,l}\,dx \\
&= 4\pi^2 \int_{\mathbb{R}^n} \mathrm{Re}\,[c_{ijkl}\widehat{\varphi}_i\xi_j\bar{\widehat{\varphi}}_k\xi_l]\,d\xi \\
&\geq 0
\end{aligned}
$$

as required.

Null Lagrangians

When does equality hold in the quasiconvexity condition? That is, for what L is

$$\int_\Omega L(F + D\varphi(x))\,dx = \int_\Omega L(F)\,dx$$

for all $\varphi \in W_0^{1,\infty}(\Omega;\mathbb{R}^m)$? We call such L *quasiaffine*.

Theorem (Landers, Morrey, Reshetnyak ...)
If $L : M^{3\times 3} \to \mathbb{R}$ is continuous then the following are equivalent:

(i) L is quasiaffine.

(ii) L is a (smooth) *null Lagrangian*, i.e. the Euler-Lagrange equations $\mathrm{Div}\, D_F L(Du) = 0$ hold for *all* smooth u.

(iii) $L(F) = \text{const.} + C \cdot F + D \cdot \operatorname{cof} F + e \det F$.

(iv) $u \mapsto L(Du)$ is sequentially weakly continuous from $W^{1,p} \to L^1$ for sufficiently large p ($p > 3$ will do).

Proof that $u \mapsto \operatorname{cof} Du$ is sequentially weakly continuous.

Consider, for example, $J(Du) = u_{1,1}u_{2,2} - u_{1,2}u_{2,1}$.

Let $u^{(j)} \rightharpoonup u$ in $W^{1,p}$, $p > 2$. Then $J(Du^{(j)})$ is bounded in $L^{p/2}$ and so we can suppose that $J(Du^{(j)}) \rightharpoonup \chi$ in L^1.

Let $\varphi \in C_0^\infty(\Omega)$. For smooth v we have the identity

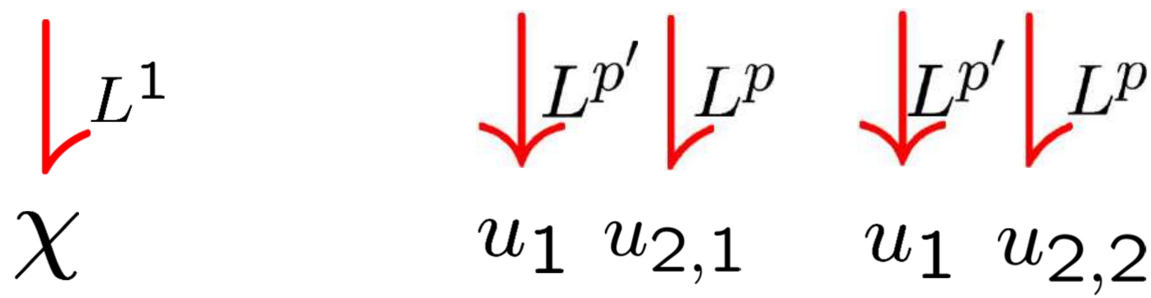
$$J(Dv) = (v_1 v_{2,2})_{,1} - (v_1 v_{2,1})_{,2}.$$

Thus, approximating $v \in W^{1,2}$ by smooth mappings we find that

$$\int_\Omega J(Dv)\varphi \, dx = \int_\Omega [v_1 v_{2,1}\varphi_{,2} - v_1 v_{2,2}\varphi_{,1}] \, dx.$$

Setting $v = u^{(j)}$ we get

$$\int_\Omega J(Du^{(j)})\varphi\, dx = \int_\Omega [u_1^{(j)} u_{2,1}^{(j)} \varphi_{,2} - u_1^{(j)} u_{2,2}^{(j)} \varphi_{,1}]\, dx.$$



So

$$\begin{aligned}\int_\Omega \chi\varphi\, dx &= \int_\Omega [u_1 u_{2,1}\varphi_{,2} - u_1 u_{2,2}\varphi_{,1}]\, dx \\ &= \int_\Omega J(Du)\varphi\, dx.\end{aligned}$$

Hence $\chi = J(Du)$ as required.

Polyconvexity

Definition

ψ is *polyconvex* if there exists a convex function $g : M^{3\times 3} \times M^{3\times 3} \times \mathbb{R} \to (-\infty, \infty]$ such that

$$\psi(F) = g(F, \text{cof}\, F, \det F) \text{ for all } F \in M^{3\times 3}.$$

Theorem

Let ψ be polyconvex, with g lower semicontinuous. Then ψ is quasiconvex.

Proof. Writing $\mathbf{J}(F) = (F, \operatorname{cof} F, \det F)$ and

$$\fint_\Omega f\,dx = \frac{1}{\operatorname{meas}\Omega}\int_\Omega f\,dx,$$

$$\begin{aligned}
\fint_\Omega \psi(F + D\varphi(x))\,dx &= \fint_\Omega g(\mathbf{J}(F + D\varphi(x)))\,dx \\
&\overset{\text{Jensen}}{\geq} g\left(\fint_\Omega \mathbf{J}(F + D\varphi)\,dx\right) \\
&= g(\mathbf{J}(F)) \\
&= \psi(F).
\end{aligned}$$

Remark

There are quadratic rank-one convex ψ that are not polyconvex. Such ψ cannot be written in the form

$$\psi(F) = Q(F) + \sum_{l=1}^{N} \alpha_l J_2^{(l)}(F),$$

where $Q \geq 0$ is quadratic and the $J_2^{(l)}$ are 2×2 minors (Terpstra, D. Serre).

Examples and counterexamples

We have shown that

$$\psi \text{ convex} \underset{\not\Leftarrow}{\Rightarrow} \psi \text{ polyconvex} \underset{\not\Leftarrow \text{ Zhang}}{\Rightarrow} \psi \text{ quasiconvex}$$

$\psi = \det$

$$\underset{\not\Leftarrow \text{ Šverák}}{\Rightarrow} \psi \text{ rank-one convex.}$$

The reverse implications are all false.

So is there a tractable characterization of quasiconvexity? This is the main road-block of the subject.

Theorem (Kristensen 1999)
There is no local condition equivalent to quasiconvexity (for example, no condition involving ψ and any number of its derivatives at an arbitrary matrix F).

This might lead one to think that it is not possible to characterize quasiconvexity. On the other hand Kristensen also proved

Theorem (Kristensen)
Polyconvexity is not a local condition.

For example, one might contemplate a characterization of the type

ψ quasiconvex $\Leftrightarrow$ ψ is the supremum of a family of special quasiconvex functions (including null Lagrangians).

Quasiconvexity is essentially both necessary and sufficient for the existence of minimizers (for the sufficiency under suitable growth conditions on ψ).

However, as well as being a practically unverifiable condition, the existence theorems based on quasiconvexity (still) do not really apply to elasticity because they assume that ψ is everywhere finite, whereas this is contradicted by (H2).

However we will show that it is possible to prove the existence of minimizers for mixed boundary value problems if we assume ψ is polyconvex and satisfies (H2) and appropriate growth conditions. Furthermore the hypotheses are satisfied by various commonly used models of natural rubber and other materials (but not, as we see later, for materials undergoing martensitic phase transformations).

Theorem (Müller, Qi &Yan 1994, following JB 1977)
Suppose that ψ satisfies (H1), (H2) and
(H4) $\psi(F) \geq c_0(|F|^2+|\text{cof}\, F|^{3/2})-c_1$ for all $F \in M^{3\times 3}$,
where $c_0 > 0$,
(H5) ψ is *polyconvex*, i.e. $\psi(F) = g(F, \text{cof}\, F, \det F)$ for all $F \in M^{3\times 3}$ for g continuous and convex.
Let

$$I(y) = \int_\Omega \psi(Dy(x))\, dx.$$

Assume that there exists some y in

$$\mathcal{A} = \{y \in W^{1,1}(\Omega; \mathbb{R}^3) : y|_{\partial\Omega_1} = \bar{y}\}$$

with $I(y) < \infty$, where $\mathcal{H}^2(\partial\Omega_1) > 0$ and $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$.
Then there exists a global minimizer y^* of I in $\mathcal{A}$.

The theorem applies to the Ogden materials:

$$\Phi = \sum_{i=1}^{N} \alpha_i(v_1^{p_i} + v_2^{p_i} + v_3^{p_i} - 3)$$

$$+ \sum_{i=1}^{M} \beta_i((v_2v_3)^{q_i} + (v_3v_1)^{q_i} + (v_1v_2)^{q_i} - 3)$$

$$+h(v_1v_2v_3)$$

where $\alpha_i, \beta_i, p_i, q_i$ are constants and h is convex, $h(\delta) \to \infty$ as $\delta \to 0+$, $\frac{h(\delta)}{\delta} \to \infty$ as $\delta \to \infty$, under appropriate conditions on the constants.

Sketch of proof

Let's make the slightly stronger hypothesis that

$$g(F, H, \delta) \geq c_0(|F|^p + |H|^{p'} + |\delta|^q) - c_1,$$

for all $F \in M^{3\times 3}$, where $p \geq 2$, $\frac{1}{p} + \frac{1}{p'} = 1$, $c_0 > 0$ and $q > 1$.

Let $l = \inf_{y\in\mathcal{A}} I(y) < \infty$ and let $y^{(j)}$ be a minimizing sequence for I in $\mathcal{A}$, so that

$$\lim_{j\to\infty} I(y^{(j)}) = l.$$

Then we may assume that for all j

$$
\begin{aligned}
l+1 \geq \quad & I(y^{(j)}) \\
\geq \quad & \int_\Omega \Big(c_0[|Dy^{(j)}|^p + |\mathrm{cof}\, Dy^{(j)}|^{p'} \\
& \qquad + |\det Dy^{(j)}|^q] - c_1\Big)\, dx.
\end{aligned}
$$

Lemma

There exists a constant $d > 0$ such that

$$
\int_\Omega |z|^p dx \leq d \left(\int_\Omega |Dz|^p dx + \left| \int_{\partial\Omega_1} z\, dA \right|^p \right)
$$

for all $z \in W^{1,p}(\Omega;\mathbb{R}^3)$.

By the Lemma $y^{(j)}$ is bounded in $W^{1,p}$ and so we may assume $y^{(j)} \rightharpoonup y^*$ in $W^{1,p}$ for some y^*.

But also we have that $\operatorname{cof} Dy^{(j)}$ is bounded in $L^{p'}$ and that $\det Dy^{(j)}$ is bounded in L^q. So we may assume that $\operatorname{cof} Dy^{(j)} \rightharpoonup H$ in $L^{p'}$ and that $\det Dy^{(j)} \rightharpoonup \delta$ in L^q.

By the results on the weak continuity of minors we deduce that $H = \operatorname{cof} Dy^*$ and $\delta = \det Dy^*$.

Let $u^{(j)} = (Dy^{(j)}, \operatorname{cof} Dy^{(j)}, \det Dy^{(j)})$, $u = (Dy^*, \operatorname{cof} Dy^*, \det Dy^*))$. Then

$$u^{(j)} \rightharpoonup u \text{ in } L^1(\Omega; \mathbb{R}^{19}).$$

But g is convex, and so (e.g. using Mazur's theorem),

$$\begin{aligned} I(y^*) = \int_\Omega g(u)\, dx &\le \liminf_{j\to\infty} \int_\Omega g(u^{(j)})\, dx \\ &= \lim_{j\to\infty} I(y^{(j)}) = l. \end{aligned}$$

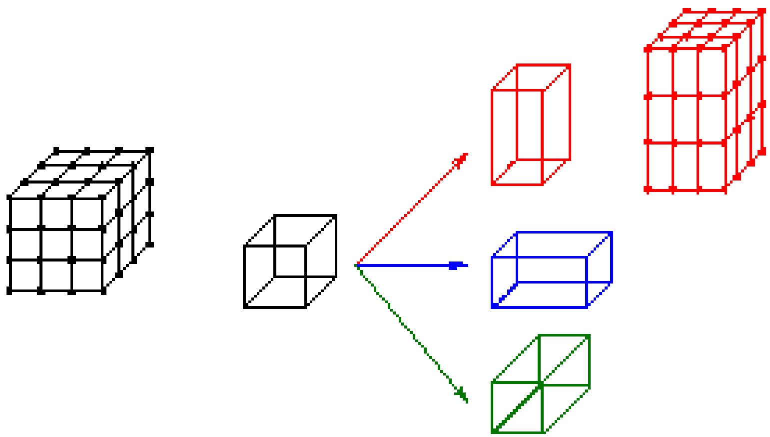
But $y^{(j)}|_{\partial\Omega_1} = \bar{y} \rightharpoonup y^*|_{\partial\Omega_1}$ in $L^1(\partial\Omega_1; \mathbb{R}^3)$ and so $y^* \in \mathcal{A}$ and y^* is a minimizer.

3. Martensitic phase transformations

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

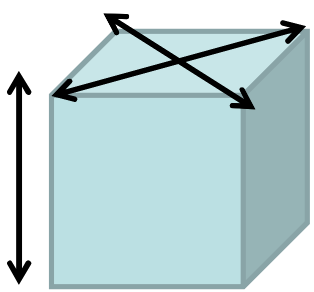
e.g. cubic to tetragonal

$\theta > \theta_c$
cubic
austenite

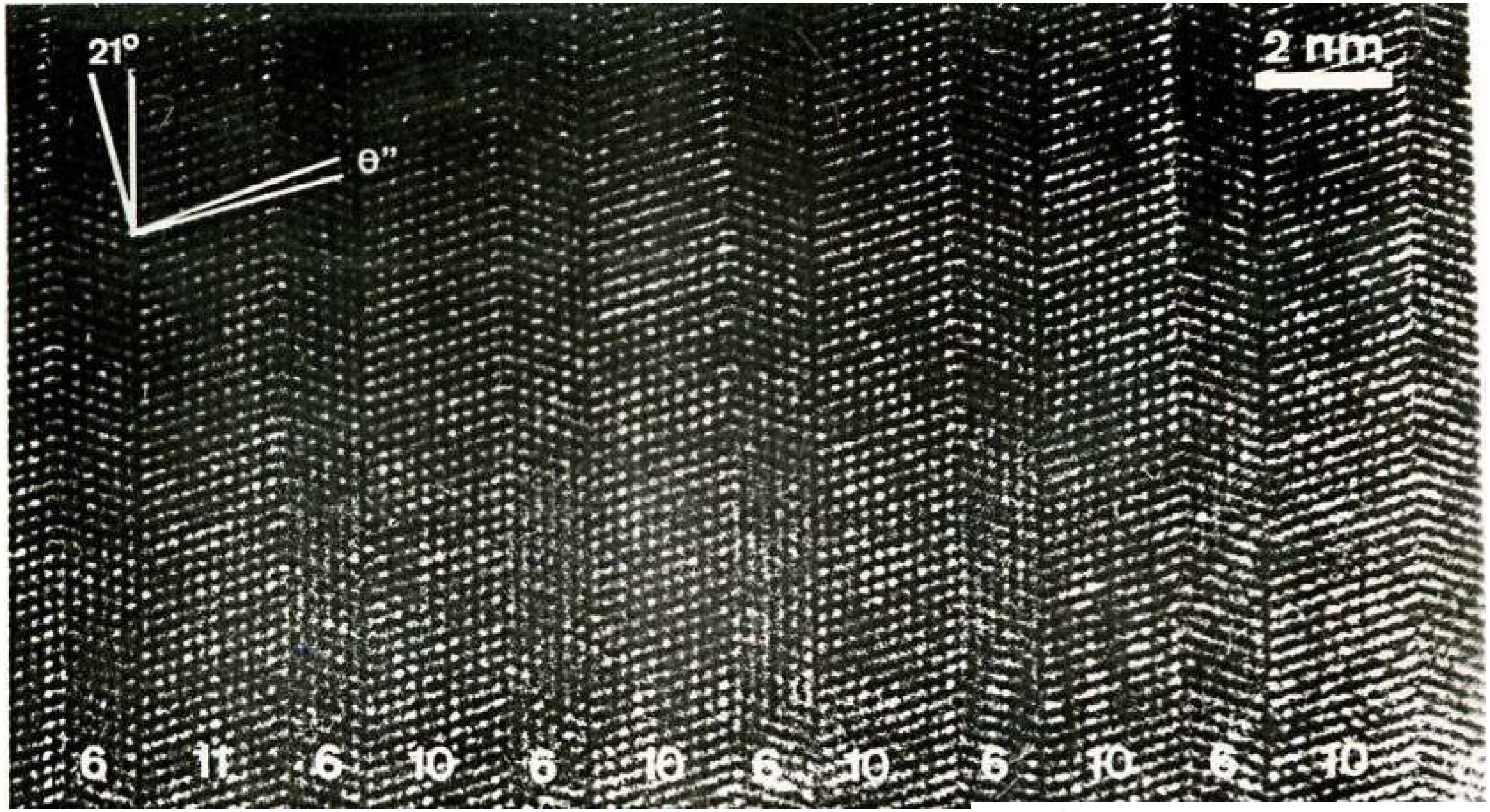


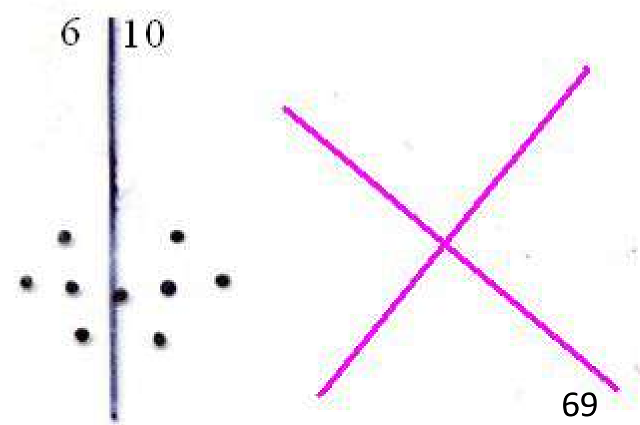
$\theta < \theta_c$
three tetragonal variants
of martensite

cubic to
orthorhombic
(e.g. CuAlNi)



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





Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

Baele, van Tenderloo, Amelinckx

Energy minimization problem for single crystal

Minimize $I_\theta(y) = \int_\Omega \psi(Dy(x), \theta)\, dx$

subject to suitable boundary conditions, for example

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

$\theta =$ temperature,

$\psi = \psi(A, \theta) =$ free-energy density of crystal, defined for $A \in M_+^{3\times 3}$.

Energy-well structure

$$K(\theta) = \{A \in M_+^{3\times 3} \text{ that minimize } \psi(A,\theta)\}$$

Assume

austenite

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

$$\alpha(\theta_c) = 1$$

martensite

The $U_i(\theta)$ are the distinct matrices $QU_1(\theta)Q^T$ for $Q \in P^{24}$ = cubic group.

For cubic to tetragonal $N = 3$ and

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

For cubic to orthorhombic $N = 6$ and

$$U_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix},\quad U_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix},\quad U_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},$$
$$U_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},\quad U_5 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix},\quad U_6 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}.$$

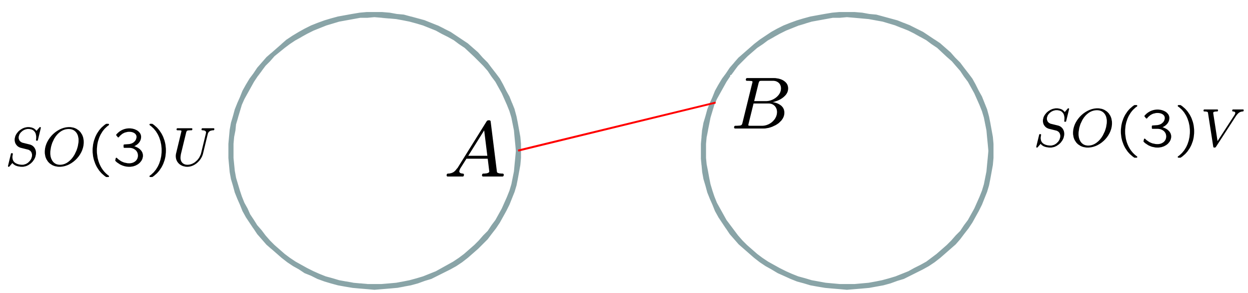
By the Hadamard jump condition, interfaces correspond to pairs of matrices A, B with

$$A - B = a \otimes N,$$

where N is the interface normal. At minimum energy $A, B \in K(\theta)$.

From the form of $K(\theta)$, we need to know what the rank-one connections are between two given energy wells $SO(3)U$, $SO(3)V$.

$$A - B = a \otimes N \neq 0$$



Theorem

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

$$U^2 - V^2 = c(M \otimes N + N \otimes M) \qquad (*)$$

for unit vectors M, N and some $c \neq 0$.
If $M \neq \pm N$ there are exactly two rank-one connections between V and $\mathrm{SO}(3)\,U$ given by

$$RU = V + a \otimes N, \quad \tilde{R}U = V + \tilde{a} \otimes M,$$

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

Corollaries.

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

Proof. In this case $U = V$, contradicting $c \neq 0$.

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

Proof. Clearly $\det(U_i^2 - U_j^2) = 0$ is necessary, since the matrix on the RHS of (*) is of rank at most 2.

Conversely suppose that $\det(U_i^2 - U_j^2) = 0$. Then $U_i^2 - U_j^2$ has the spectral decomposition

$$U_i^2 - U_j^2 = \lambda e \otimes e + \mu \hat{e} \otimes \hat{e},$$

and since $U_j = R U_i R^T$ for some $R \in P^{24}$ it follows that $\operatorname{tr}(U_i^2 - U_j^2) = 0$. Hence $\mu = -\lambda$ and

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

as required.

Remark: Another equivalent condition due to Forclaz is that $\det(U_i - U_j) = 0$. This is because of the surprising identity (not valid in higher dimensions)

$$\det(U_i^2 - U_j^2) = (\lambda_1 + \lambda_2)(\lambda_2 + \lambda_3)(\lambda_3 + \lambda_1)\det(U_i - U_j).$$

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

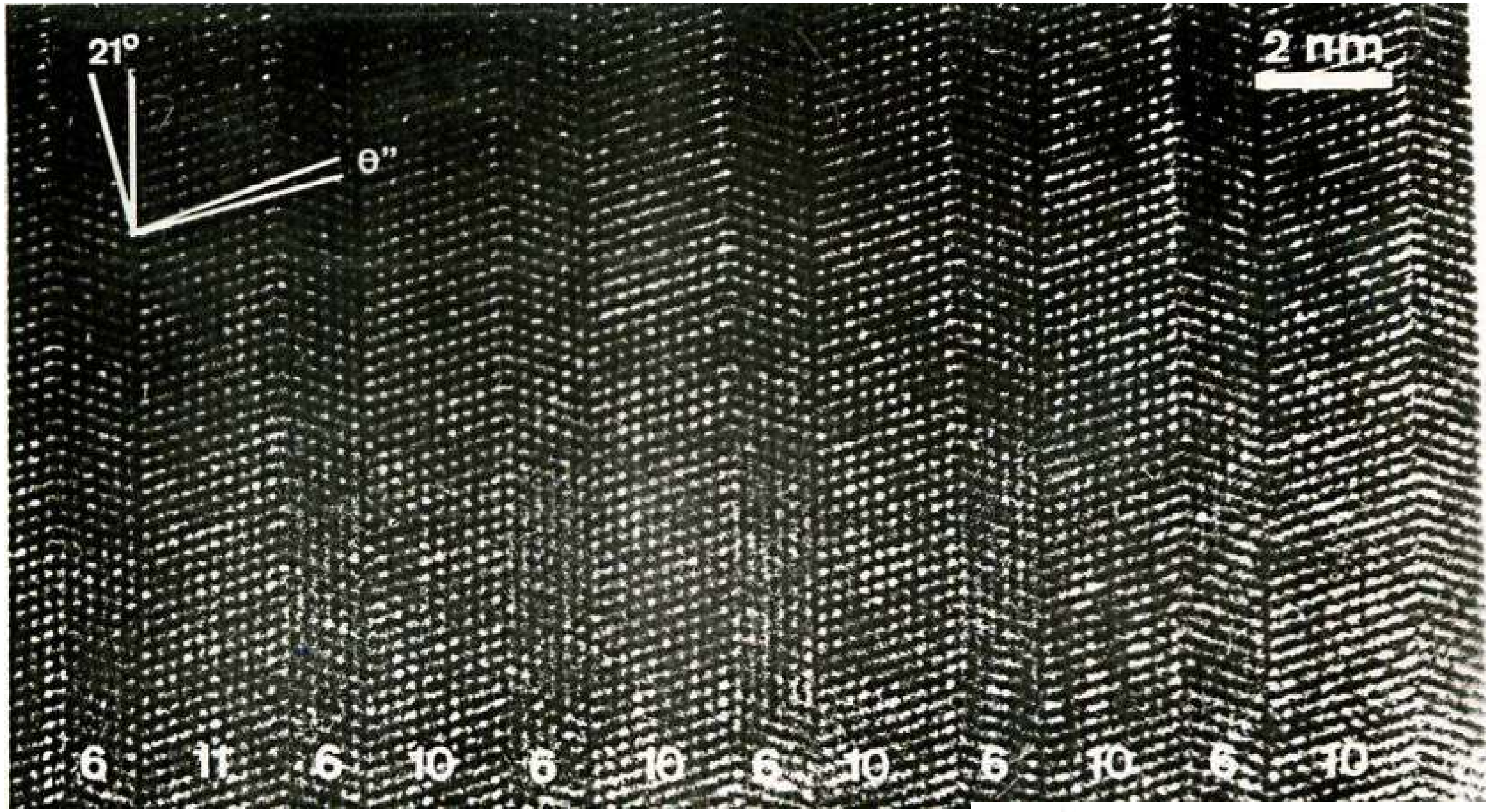
Proof. If there is a rank-one connection then 1 is an eigenvalue since $\det(U_i^2 - 1) = 0$.

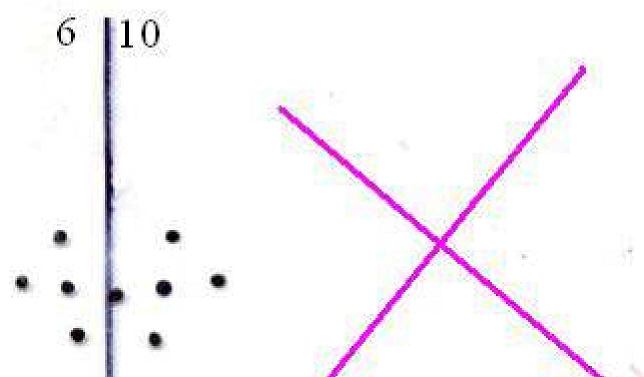
Choosing e with $M\cdot e > 0, N\cdot e > 0$ and $M\cdot e > 0$, $N\cdot e < 0$, we see that 1 is the middle eigenvalue. Conversely, if 1 is the middle eigenvalue

$$\begin{aligned} U_i^2 - 1 &= (\lambda_1^2 - 1)e_1 \otimes e_1 + (\lambda_3^2 - 1)e_3 \otimes e_3 \\ &= \frac{\lambda_3^2 - \lambda_1^2}{2}((\alpha e_1 + \beta e_3) \otimes (-\alpha e_1 + \beta e_3) \\ &\quad + (-\alpha e_1 + \beta e_3) \otimes (\alpha e_1 + \beta e_3)), \end{aligned}$$

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

Exercise Show that for a cubic-to-tetragonal transformation the possible twin planes are those with normals in the [110] family (i.e. $\frac{1}{\sqrt{2}}(1,1,0)$, $\frac{1}{\sqrt{2}}(0,1,1)$, $\frac{1}{\sqrt{2}}(1,0,1)$).





Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

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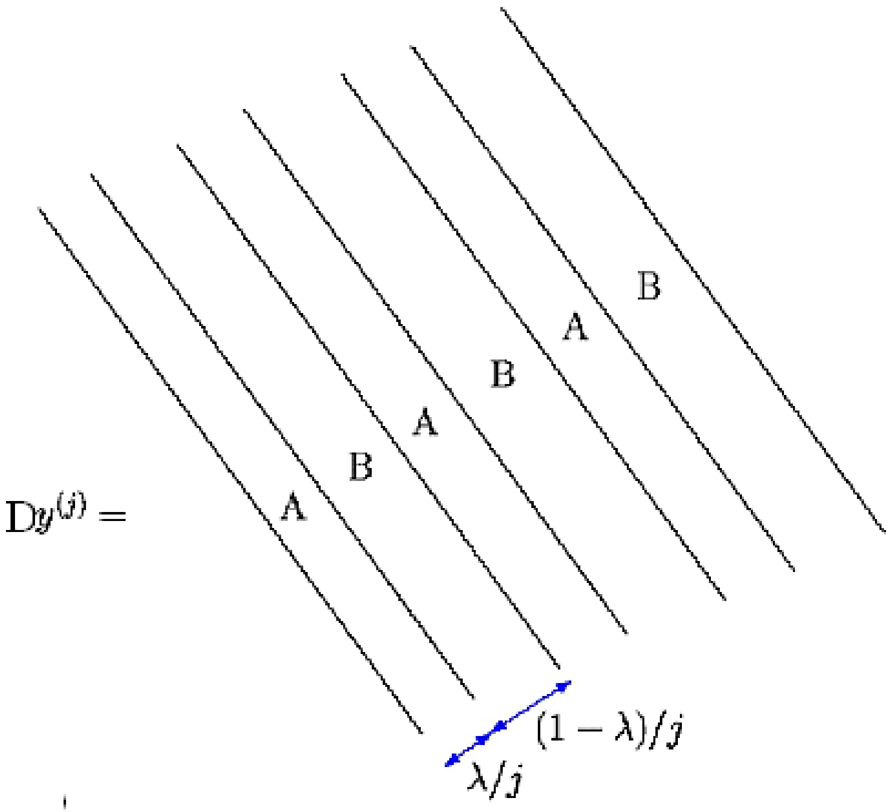
Layering twins



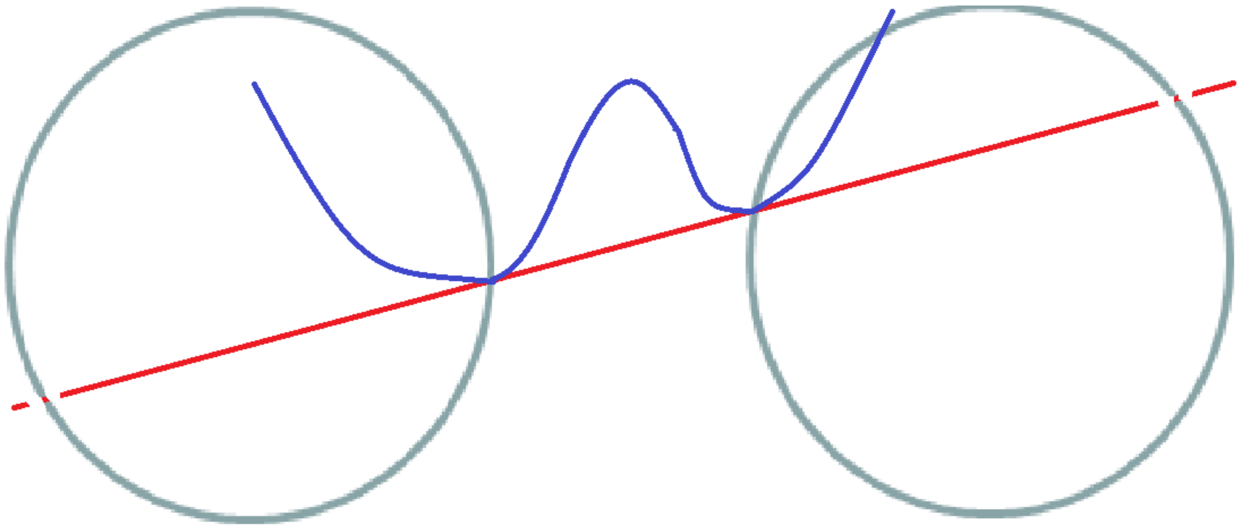
Simple laminate

$$A - B = c \otimes N$$

$$Dy^{(j)} \rightharpoonup Dy = \lambda A + (1-\lambda)B$$

4. Microstructure

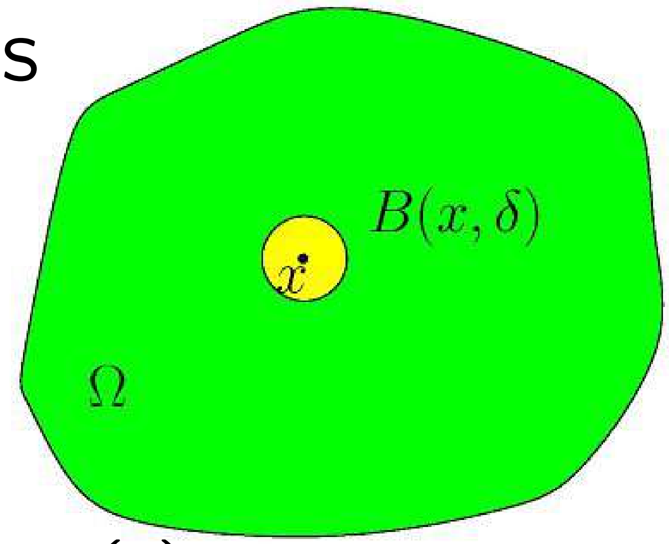
The free-energy function $\psi(\cdot, \theta)$ is not quasi-convex. This is because the existence of twins implies that $\psi(\cdot, \theta)$ is not rank-one convex.



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

Gradient Young measures

Given a sequence of gradients $Dy^{(j)}$, fix j, x, δ.



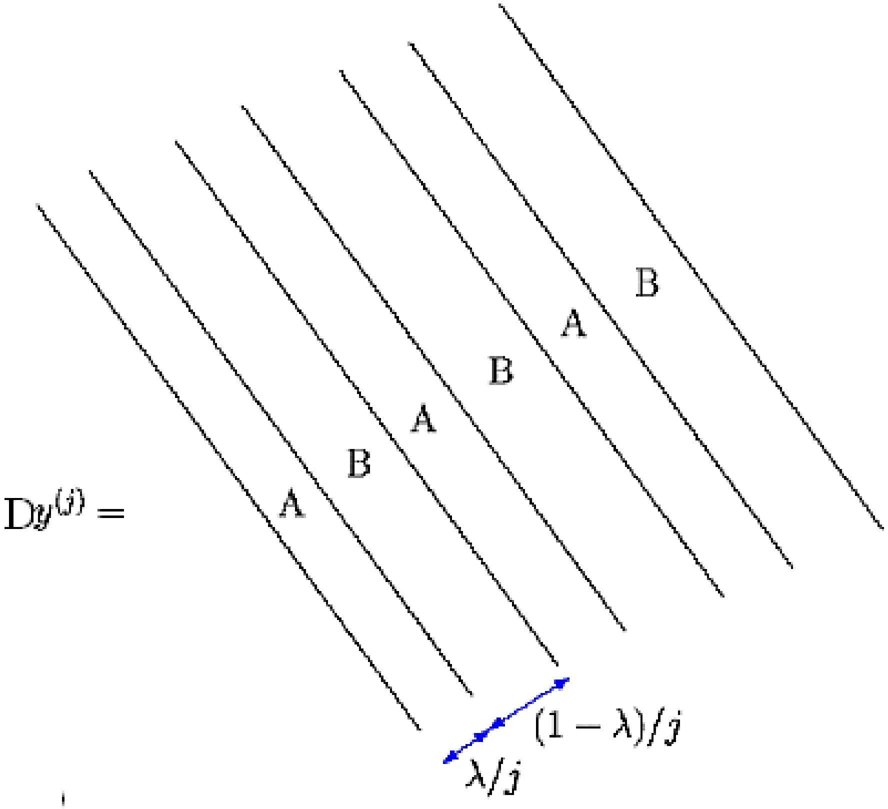
Let $E \subset M^{3\times 3}$, where $M^{3\times 3} = \{3 \times 3 \text{ matrices}\}$

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

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

is the gradient Young measure generated by $Dy^{(j)}$.

Gradient Young measure of simple laminate



$$\nu_x = \lambda \delta_A + (1-\lambda)\delta_B$$

Theorem. (Kinderlehrer/Pedregal) *A family of probability measures* $(\nu_x)_{x\in\Omega}$ *on* $M^{m\times n}$ *is the Young measure of a sequence of gradients* $Dy^{(j)}$ *bounded in* L^∞ *if and only if*

(i) $\bar{\nu}_x$ *is a gradient (*Dy*, the weak limit of* $Dy^{(j)}$*)*

(ii) $\langle \nu_x, f\rangle \geq f(\bar{\nu}_x)$ *for all quasiconvex* f*.*

Here

$$\bar{\nu}_x = \int_{M^{m\times n}} A\, d\nu_x(A)$$

and

$$\langle \nu_x, f\rangle = \int_{M^{m\times n}} f(A)\, d\nu_x(A)$$

Quasiconvexification

Of functions:

$$W^{\text{qc}} = \sup\{g \text{ quasiconvex} : g \leq W\}.$$

Of sets:

A subset $E \subset M^{3\times3}$ if $E = g^{-1}(0)$ for some non-negative quasiconvex function g.

Let $K \subset M^{3\times3}$ be compact,

e.g. $K = \bigcup_{i=1}^{N} SO(3)U_i(\theta)$.

$$
\begin{aligned}
K^{\mathrm{qc}} &= \text{quasiconvexification of } K \\
&= \bigcap \{E : K \subset E,\ E \text{ quasiconvex}\} \\
&= \{\bar{\nu} : \nu \text{ gradient Young measure },\\
&\qquad\qquad \operatorname{supp}\nu \subset K\} \\
&= \{F \in M^{3\times 3} : g(F) \le \max_{A\in K} g(A) \\
&\qquad\qquad \text{for all quasiconvex } g\}.
\end{aligned}
$$

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

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

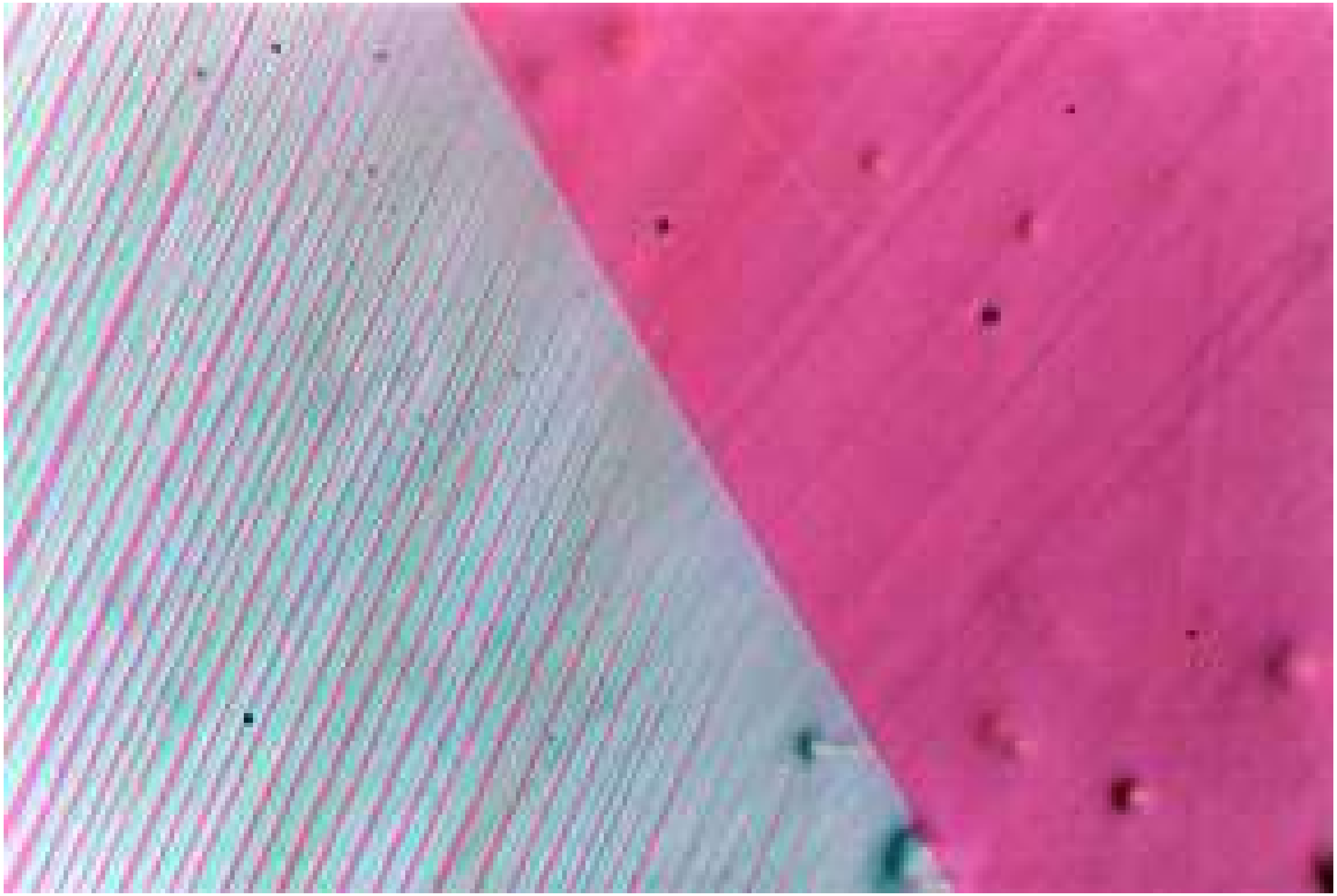
5. Austenite-martensite interfaces

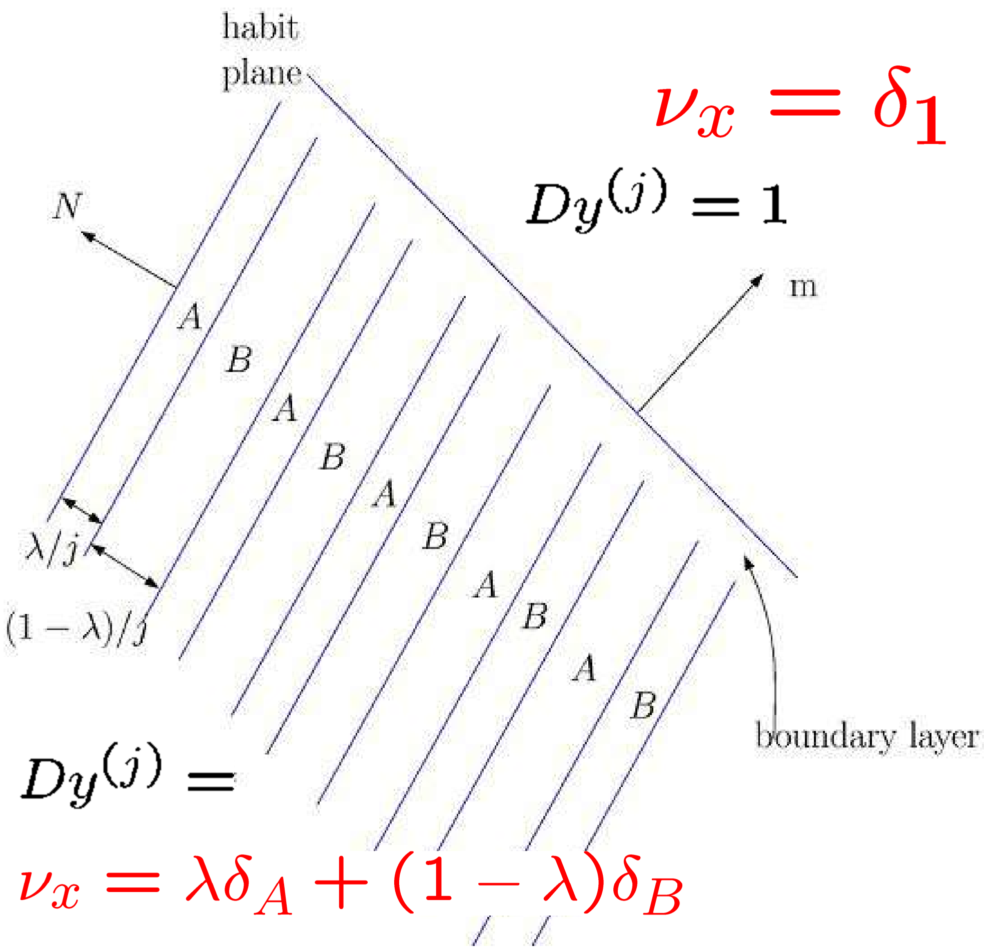
How does austenite transform to martensite as θ passes through θ_c?

It cannot do this by means of an exact interface between austenite and martensite, because this requires the middle eigenvalue of U_i to be one, which in general is not the case (but see studies of James et al on low hysteresis alloys).

So what does it do?

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





$$\nu_x = \delta_1$$

$$Dy^{(j)} = 1$$

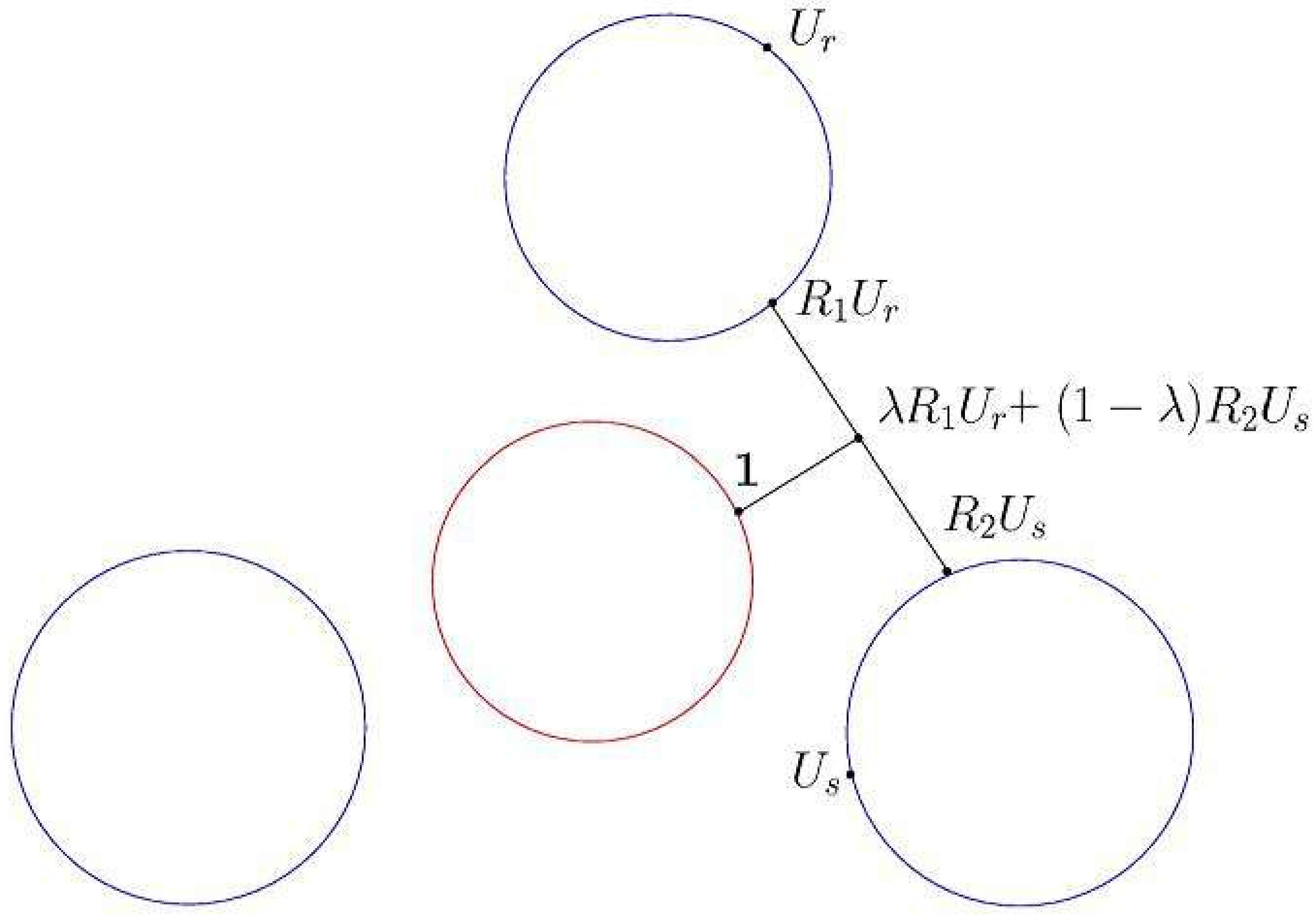
$$Dy^{(j)} =$$

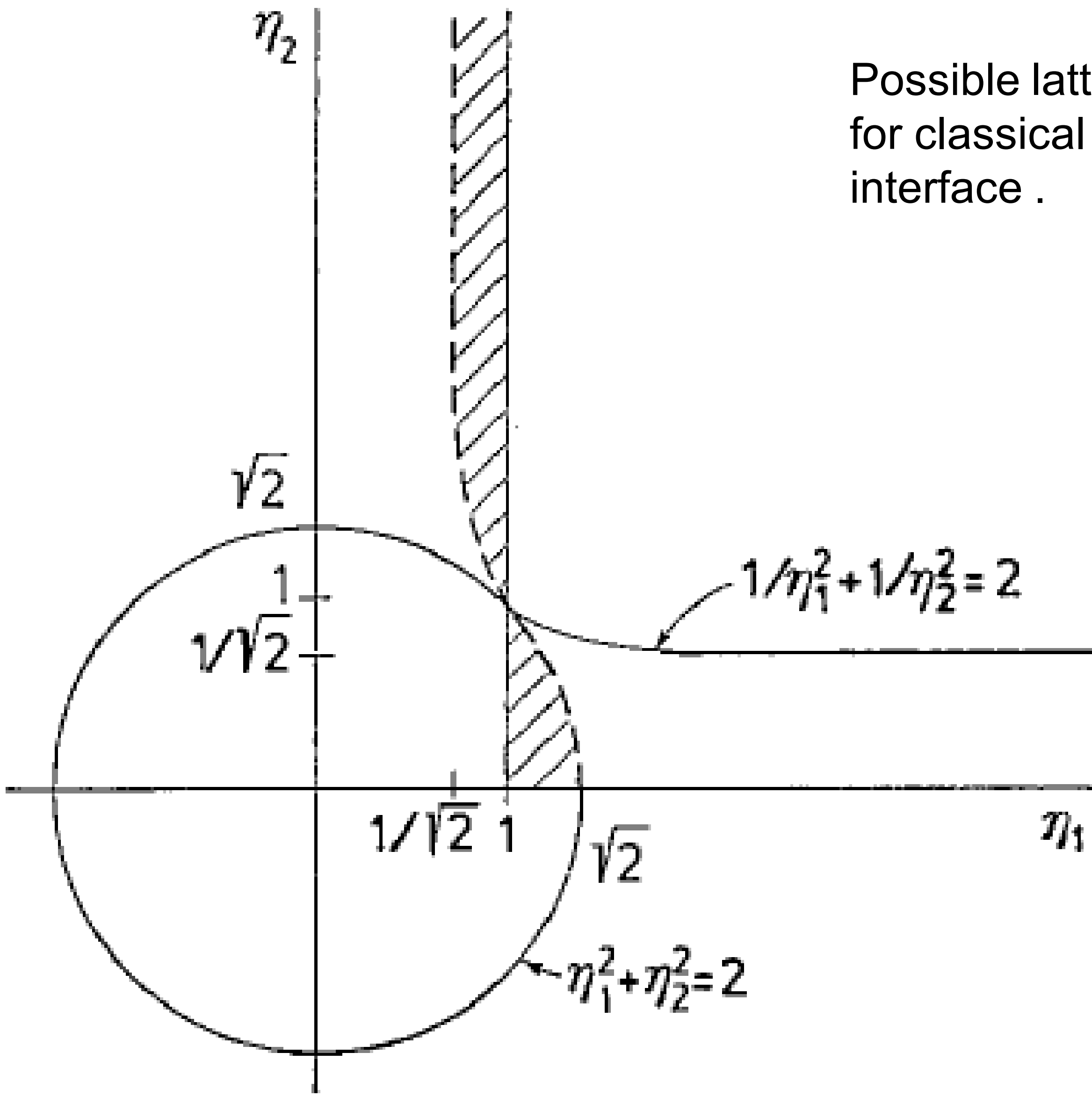
$$\nu_x = \lambda\delta_A + (1-\lambda)\delta_B$$

Gives formulae of the crystallographic theory of martensite (Wechsler, Lieberman, Read)

24 habit planes for cubic-to-tetragonal

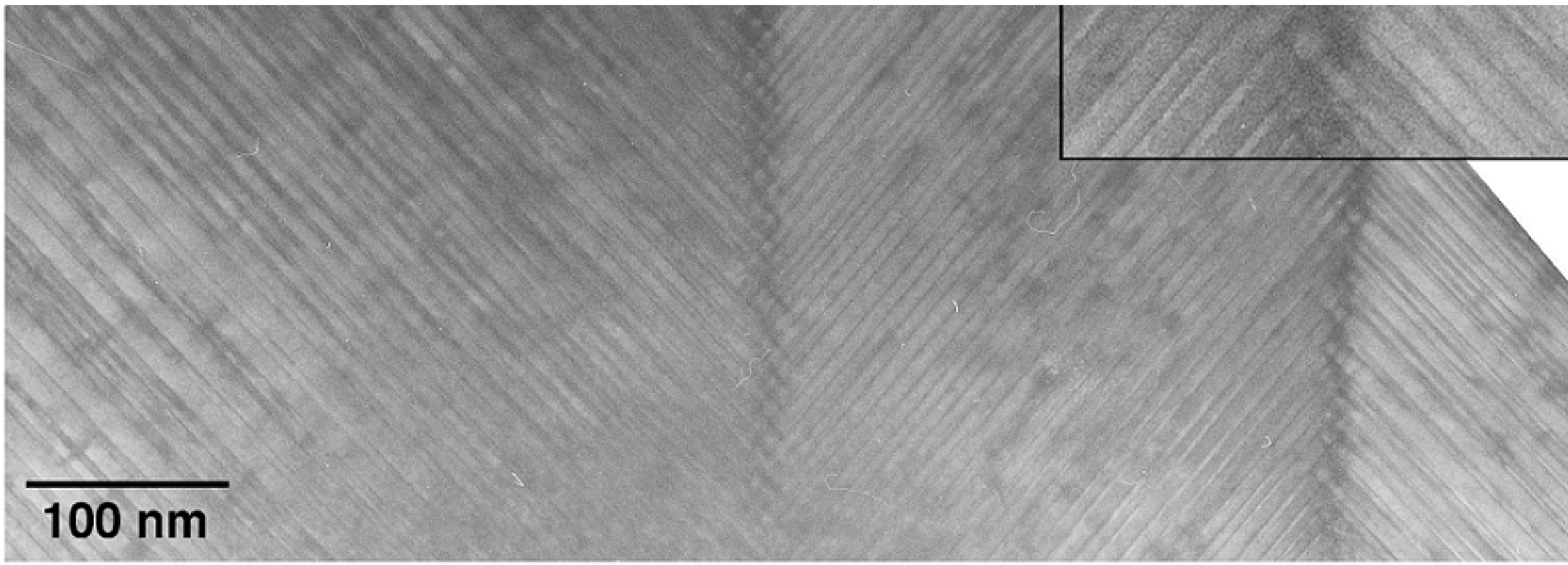
Rank-one connections for A/M interface



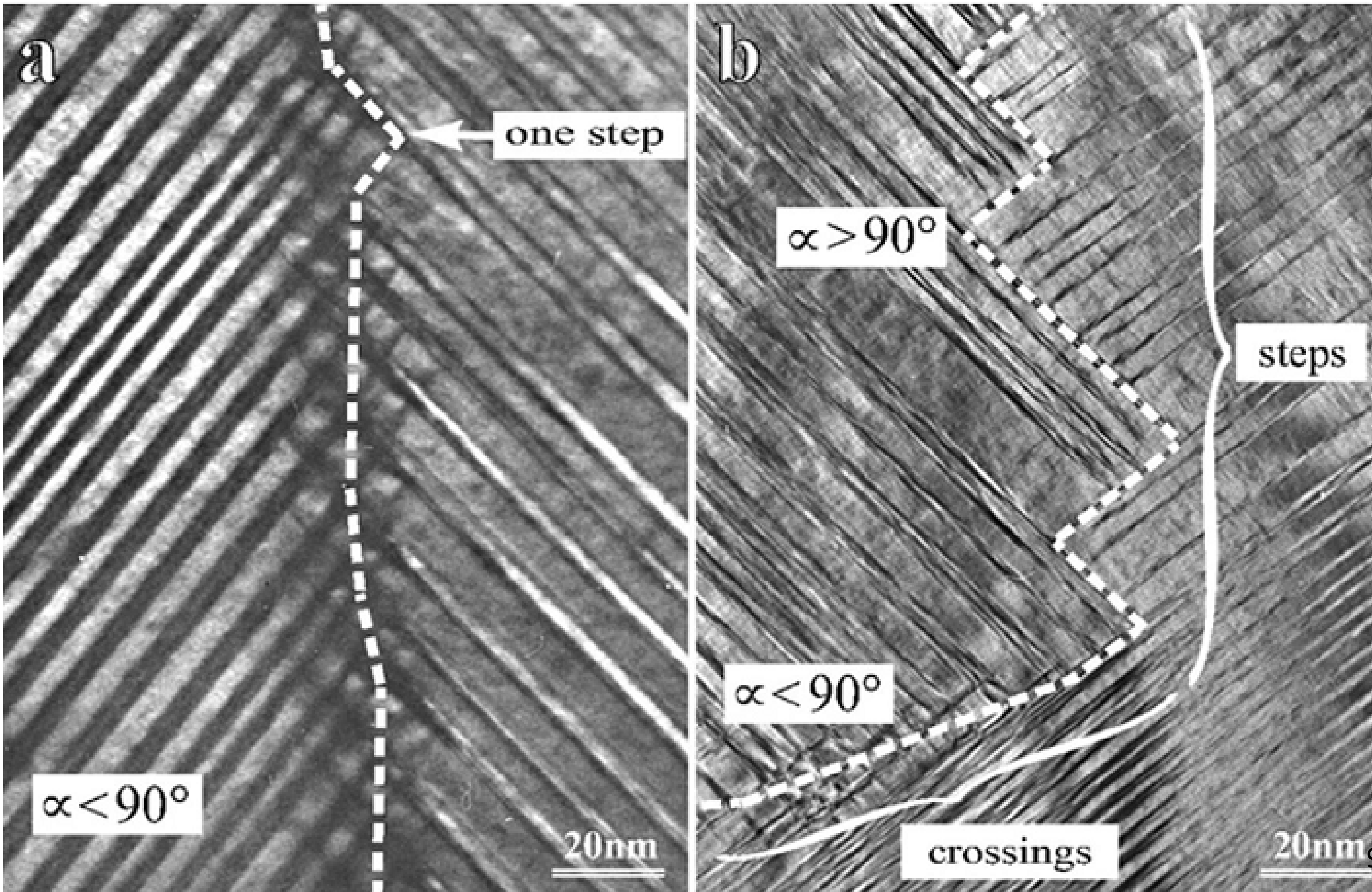


Possible lattice parameters for classical austenite-martensite interface .

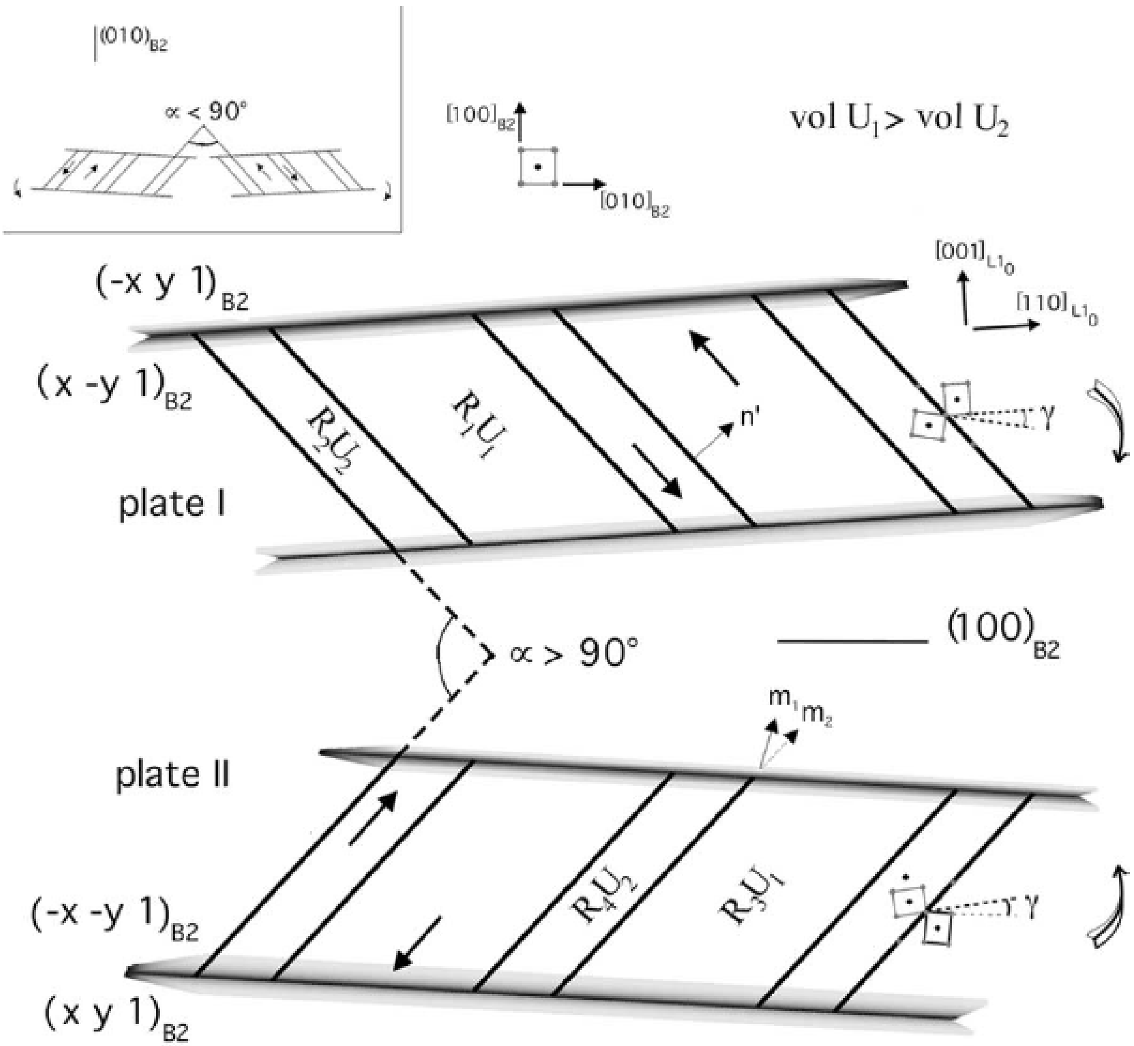
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)

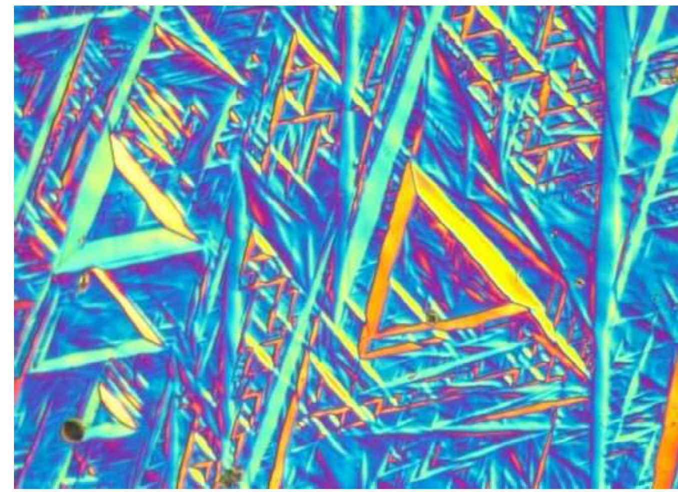


Crossings and steps



Macrotwin formation





Similar effects and analysis in β-titanium: T. Inamura, M. Ii, N. Kamioka, M. Tahara, H. Hosoda, S. Miyazaki ICOMAT 2014

Macroscopic deformation gradient in martensitic plate is

$$1 + b \otimes m$$

B/Schryvers 2003

Different martensitic plates never exactly compatible (Bhattacharya)

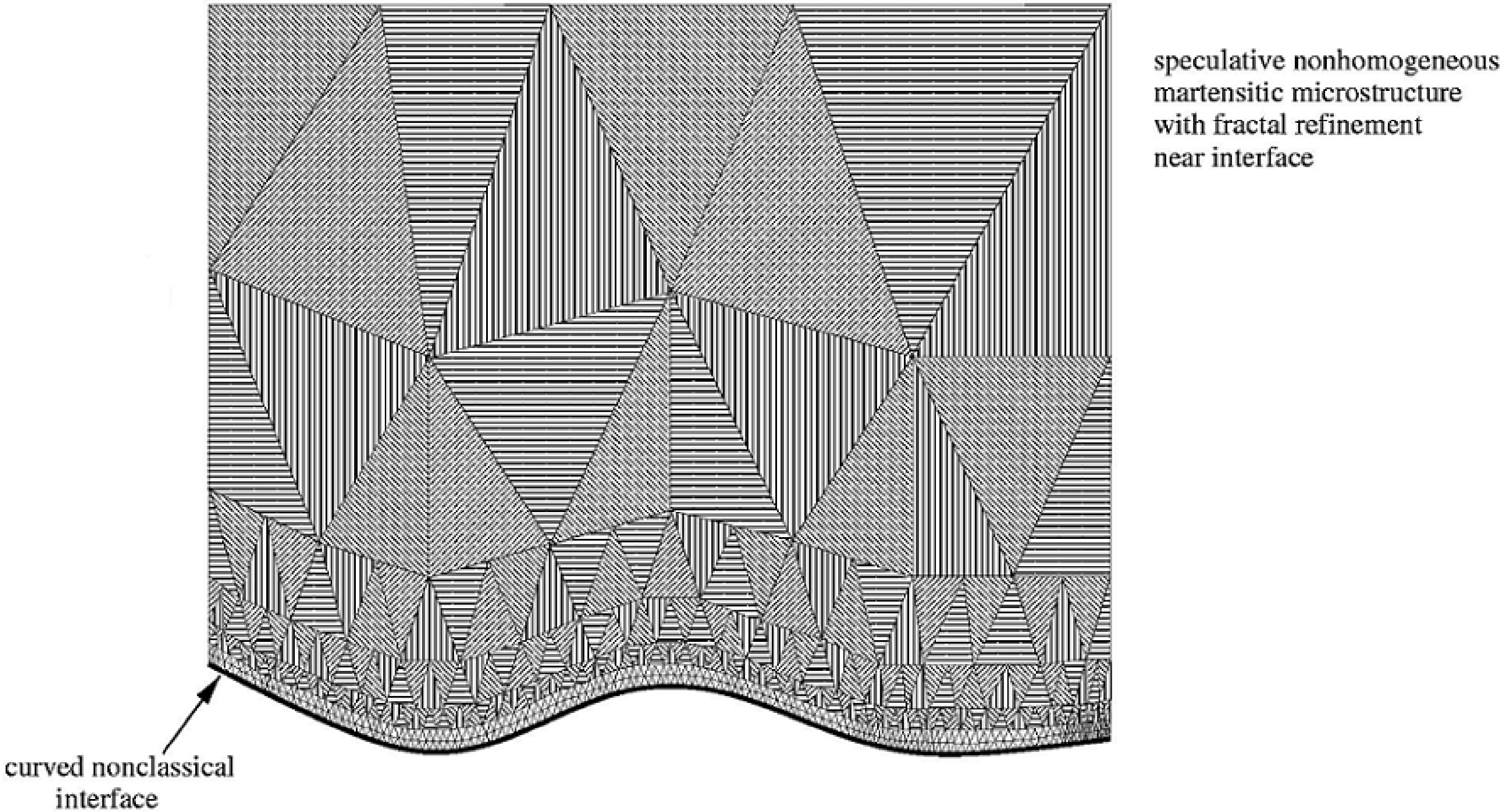
$$m = \left(\frac{1}{2}\chi(\delta + \nu\tau), \frac{1}{2}\chi\kappa(\nu\tau - \delta), 1\right)$$
$$b = \left(\frac{1}{2}\chi\zeta(\delta + \nu\tau), \frac{1}{2}\chi\zeta\kappa(\nu\tau - \delta), \beta\right)$$

where $\nu = 1$ for $\lambda = \lambda^*$, $\nu = -1$ for $\lambda = 1 - \lambda^*$, the microtwin planes have normals $(1, \kappa, 0)$ and $\chi = \pm 1$.

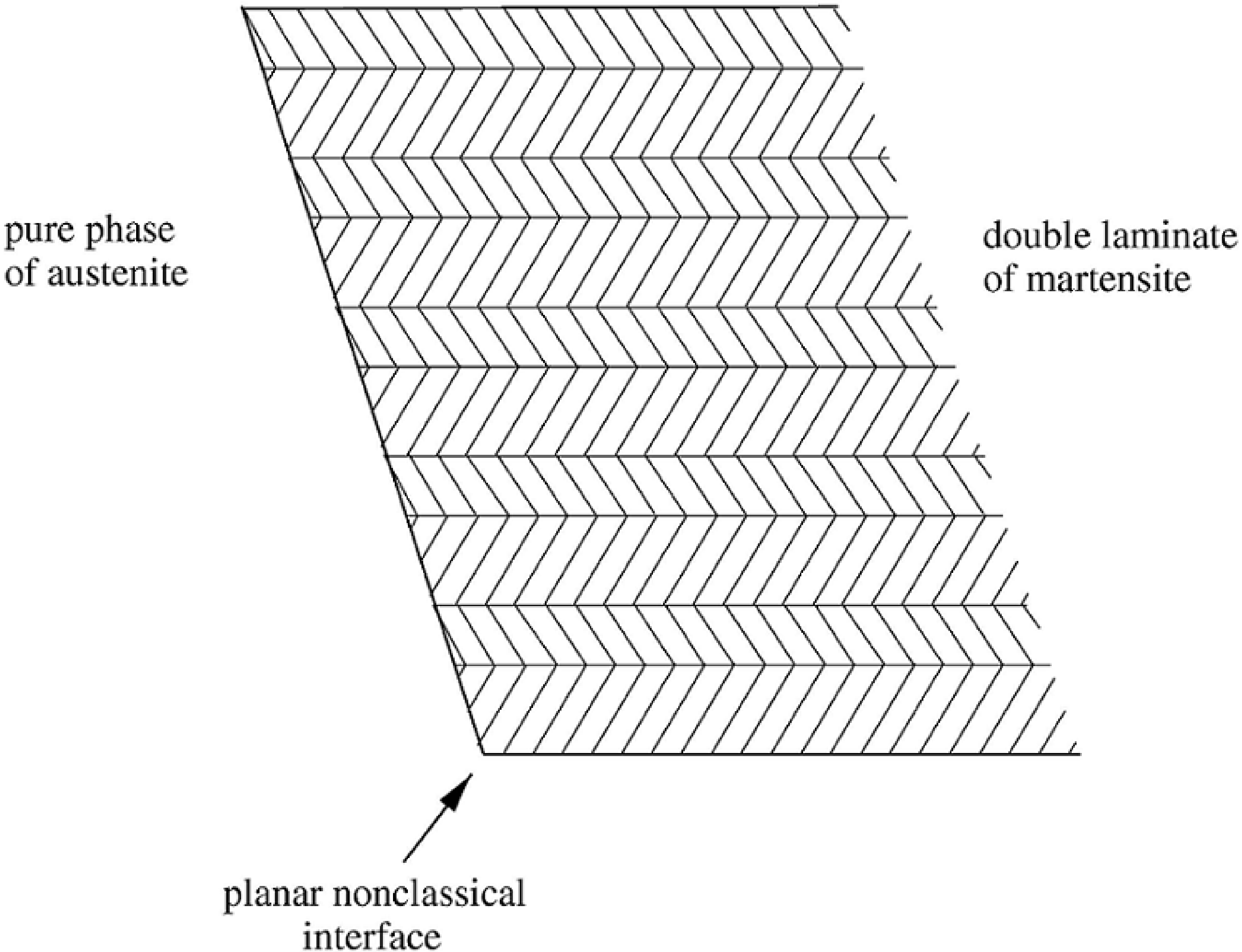
Table 1: Rotations Q_1 and Q_2 that bring Plate II into compatibility with Plate I ($\kappa_1 = \chi_1 = \nu_1 = 1$) and the corresponding macrotwin normals N_1 and N_2. The direction of rotation is that of a right-handed screw in the direction of the given axis. For the case $\kappa_2 = \nu_2 = 1, \chi_2 = -1$ see the text.

Parameter Values			Q_1			Q_2		
κ_2	χ_2	ν_2	Axis	Angle	N_1	Axis	Angle	N_2
-1	1	1	(.70,0,-.71)	1.64°	(0,1,0)	(.75,0,.66)	1.75°	(1,0,0)
-1	-1	1	(0,.99,.16)	7.99°	(1,0,0)	(0,.99,-.14)	7.99°	(0,1,0)
-1	1	-1	(.65,.48,-.59)	6.76°	(.59,-.81,0)	(.68,.50,.54)	6.91°	(-.81,-.59,0)
-1	-1	-1	(-.48,.65,.59)	6.76°	(-.81,-.59,0)	(-.50,.68,-.54)	6.91°	(.59,-.81,0)
1	1	-1	(-.54,.54,.64)	5.87°	$\frac{1}{\sqrt{2}}$(1,1,0)	(-.57,.57,-.59)	6.08°	$\frac{1}{\sqrt{2}}$(1,-1,0)
1	-1	-1	(.60,.60,-.52)	7.37°	$\frac{1}{\sqrt{2}}$(1,-1,0)	(.62,.62,.47)	7.47°	$\frac{1}{\sqrt{2}}$(1,1,0)

Nonclassical austenite-martensite interfaces (B/Carstensen 97)

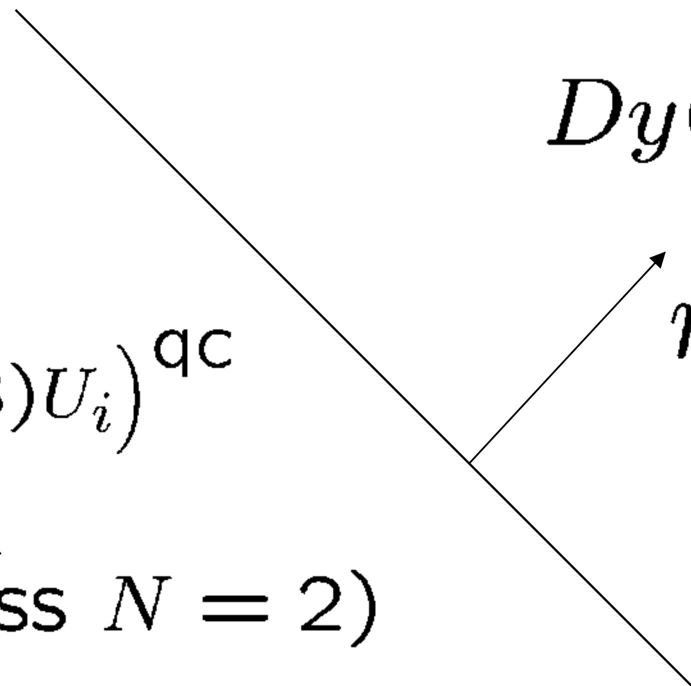


Nonclassical interface with double laminate



Nonclassical interface calculation

$$Dy(x) = 1$$



$$\nu_x = \delta_{\mathbf{1}}$$

$$Dy(x) = F = \bar{\nu}$$

$$F \in \left(\bigcup_{i=1}^{N} SO(3)U_i\right)^{\text{qc}}$$

(unknown unless $N = 2$)

$$\nu_x = \nu$$

$$\operatorname{supp} \nu \subset \bigcup_{i=1}^{N} SO(3)U_i$$

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

Two martensitic wells

Let $K = SO(3)U_1 \cup SO(3)U_2$, where

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

and the $\eta_i > 0$ (orthorhombic to monoclinic).

Theorem (Ball & James 92) K^{qc} consists of the matrices $F \in M_+^{3\times 3}$ such that

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

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

The proof is by calculating K^{pc} and showing by construction that any $F \in K^{pc}$ belongs to K^{qc}.

For a nonclassical interface we need that for some a, b, c satisfying these inequalities the middle eigenvalue of $F^T F$ is one, and we thus get (Ball & Carstensen 97) such an interface provided

$$\eta_2^{-1} \leq \eta_1 \leq 1 \text{ or } 1 \leq \eta_2^{-1} \leq \eta_1 \quad \text{if } \eta_3 < 1,$$

$$\eta_2 \leq \eta_1^{-1} \leq 1 \text{ or } 1 \leq \eta_2 \leq \eta_1^{-1} \quad \text{if } \eta_3 > 1.$$

More wells – necessary conditions

$$K = \bigcup_{i=1}^{N} SO(3)U_i$$

The martensitic variants U_i all have the same singular values (= eigenvalues) $0 < \eta_{\min} \leq \eta_{\text{mid}} \leq \eta_{\max}$.

Let $F \in K^{pc}$ have singular values

$$0 < \sigma_{\min}(F) \leq \sigma_{\text{mid}}(F) \leq \sigma_{\max}(F).$$

$$K^{pc} = \{F \in M^{m\times n} : \varphi(F) \le \max_{G\in K} \varphi(G)$$
$$\text{for all polyconvex } \varphi\}$$

First choose $\varphi(G) = \pm\det(G)$. Then

$$\det F = \sigma_{\min}(F)\sigma_{\mathrm{mid}}(F)\sigma_{\max}(F) = \eta_{\min}\eta_{\mathrm{mid}}\eta_{\max}.$$

Next choose $\varphi(G) = \sigma_{\max}(G) = \max_{|x|=1} |Gx|$, which is convex, hence polyconvex. Thus

$$\sigma_{\max}(F) \le \eta_{\max}.$$

Finally choose $\varphi(G) = \sigma_{\mathrm{max}}(\mathrm{cof}\, G)$, which is a convex function of $\mathrm{cof}\,(G)$ and hence polyconvex. Then

$$\sigma_{\mathrm{mid}}(F)\sigma_{\mathrm{max}}(F) \leq \eta_{\mathrm{mid}}\eta_{\mathrm{max}}$$

But $F = \mathbf{1} + b \otimes m$ implies $\sigma_{\mathrm{mid}}(F) = 1$.

Combining these inequalities we get that

$$\eta_{\mathrm{min}} \leq \eta_{\mathrm{mid}}^{-1} \leq \eta_{\mathrm{max}}.$$

For cubic to tetragonal we have that

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

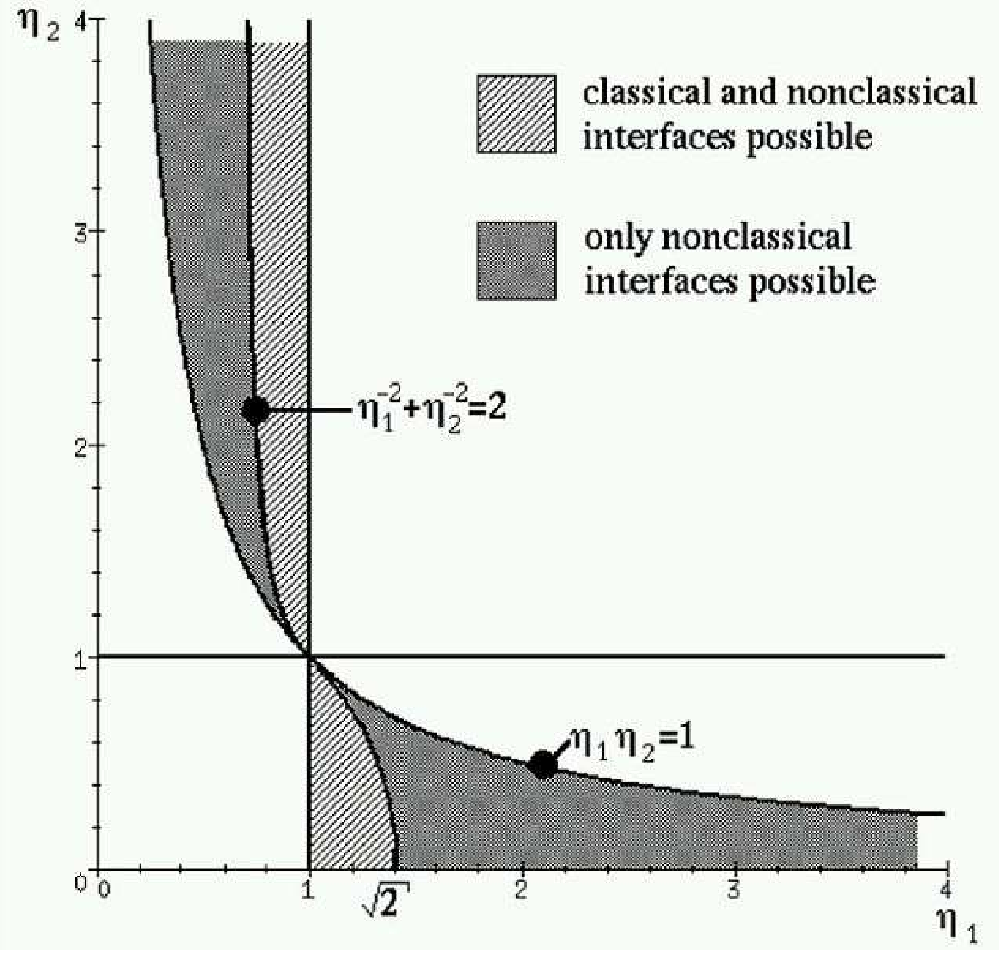
and the necessary conditions become

$$\eta_1 \le \eta_1^{-1} \le \eta_2 \text{ if } \eta_1 \le \eta_2,$$

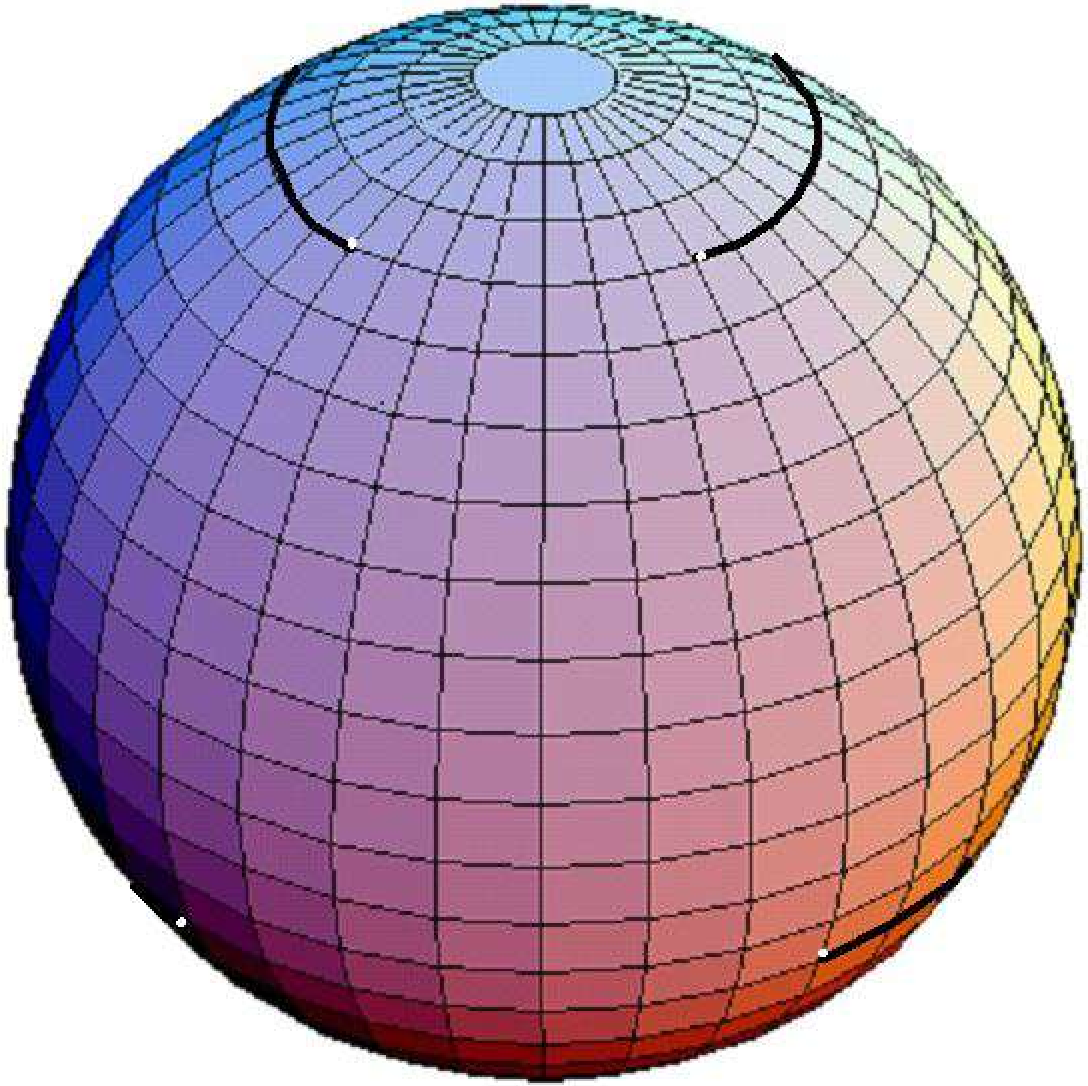
$$\eta_2 \le \eta_1^{-1} \le \eta_1 \text{ if } \eta_1 \ge \eta_2.$$

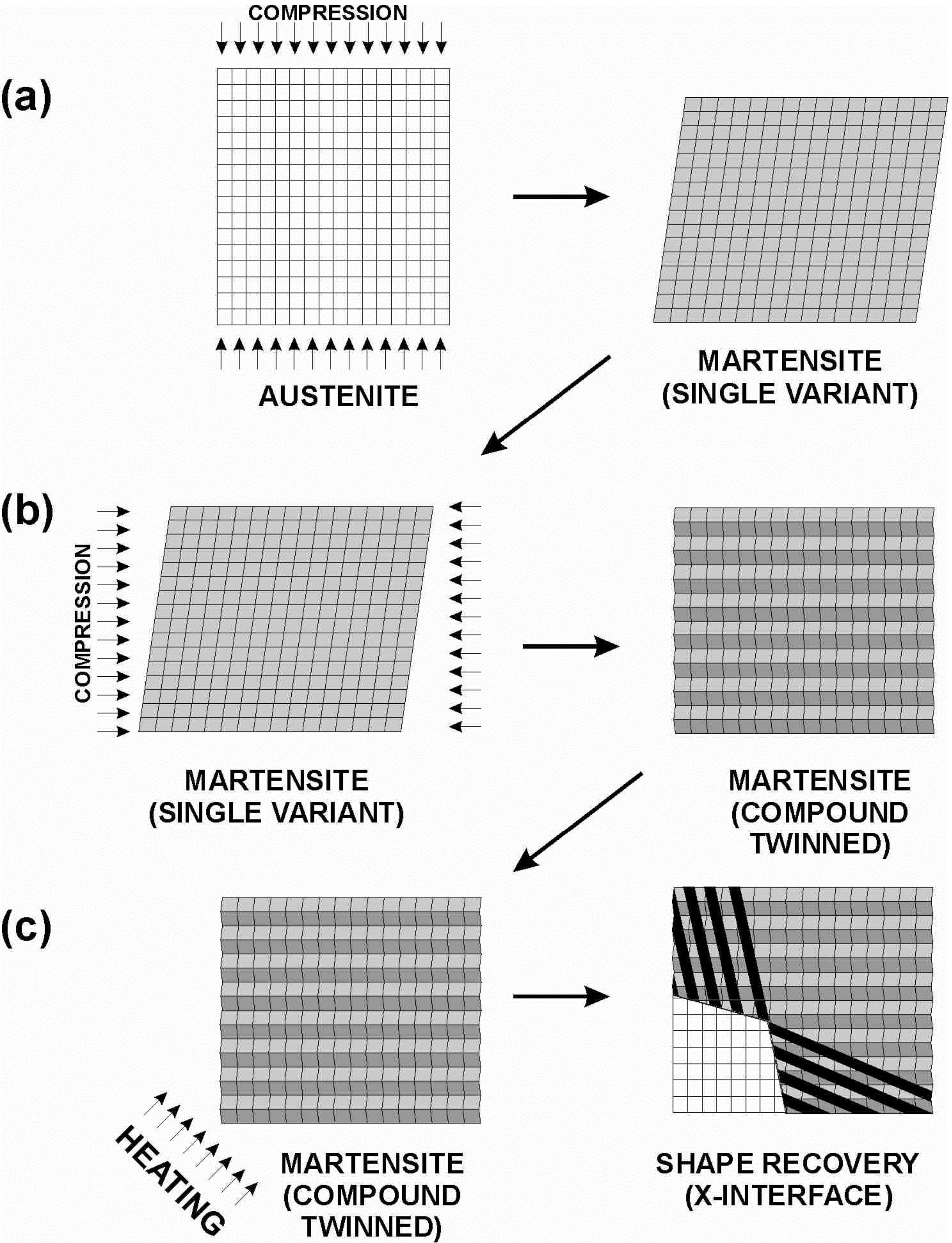
But these turn out to be exactly the conditions given by the two-well theorem to construct a rank-one connection from $(SO(3)U_1 \cup SO(3)U_2)^{qc}$ to the identity!
Hence the conditions are sufficient also.

Values of deformation parameters allowing classical and nonclassical austenite-martensite interfaces



Interface normals

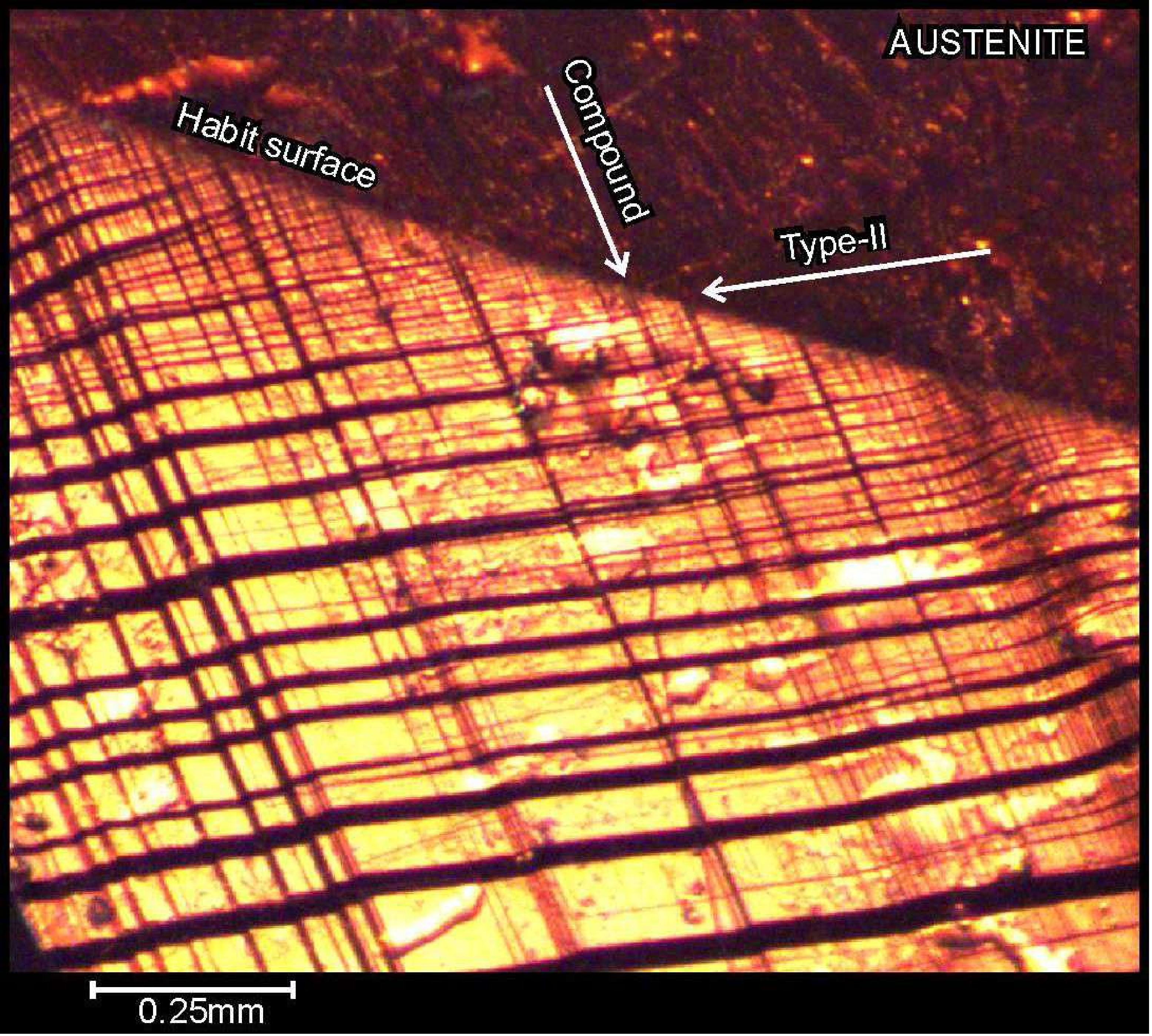




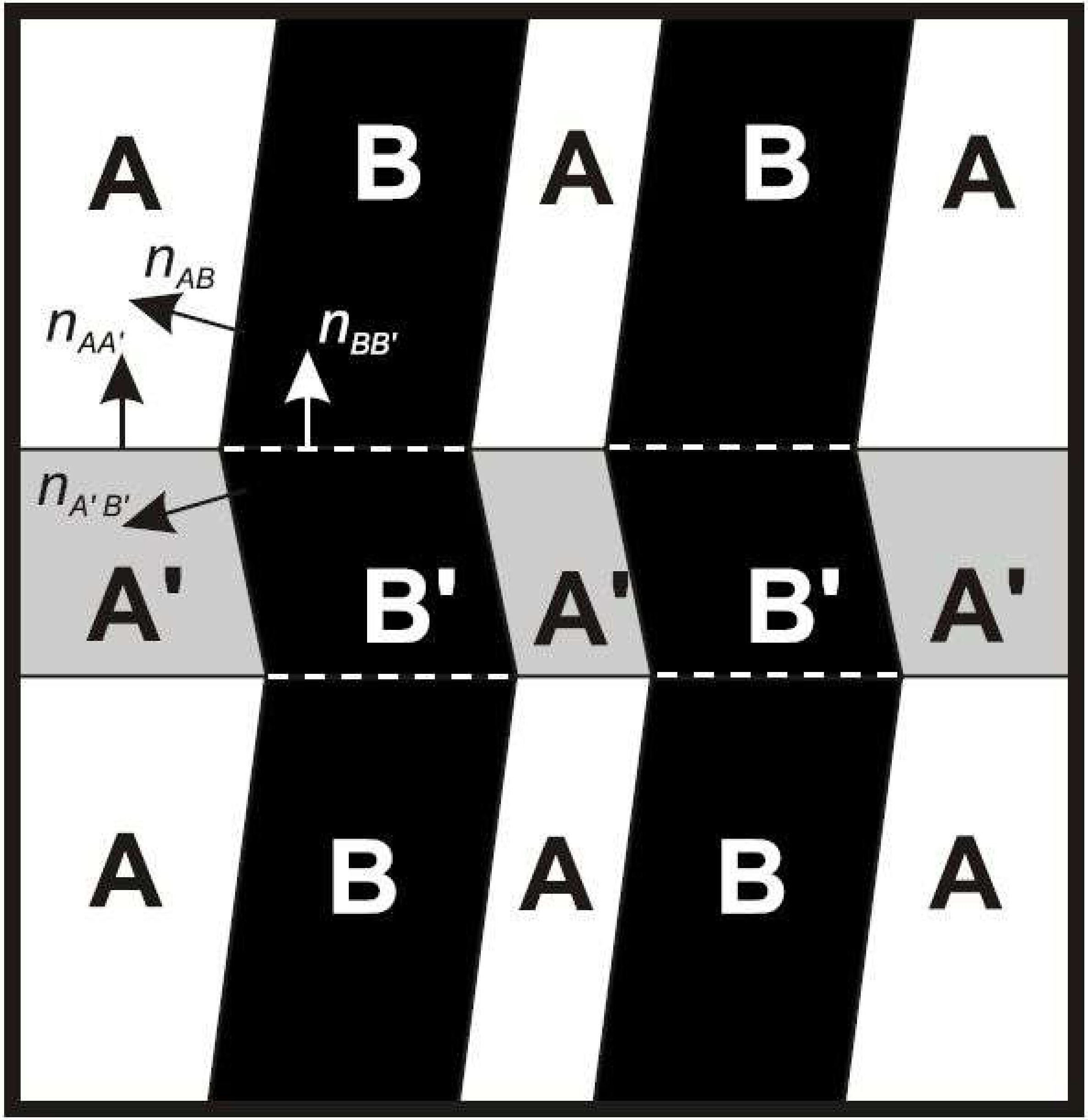
Experimental procedure (H. Seiner)

3.9×3.8×4.2mm CuAlNi single crystal

Theory JB/Koumatos, Seiner

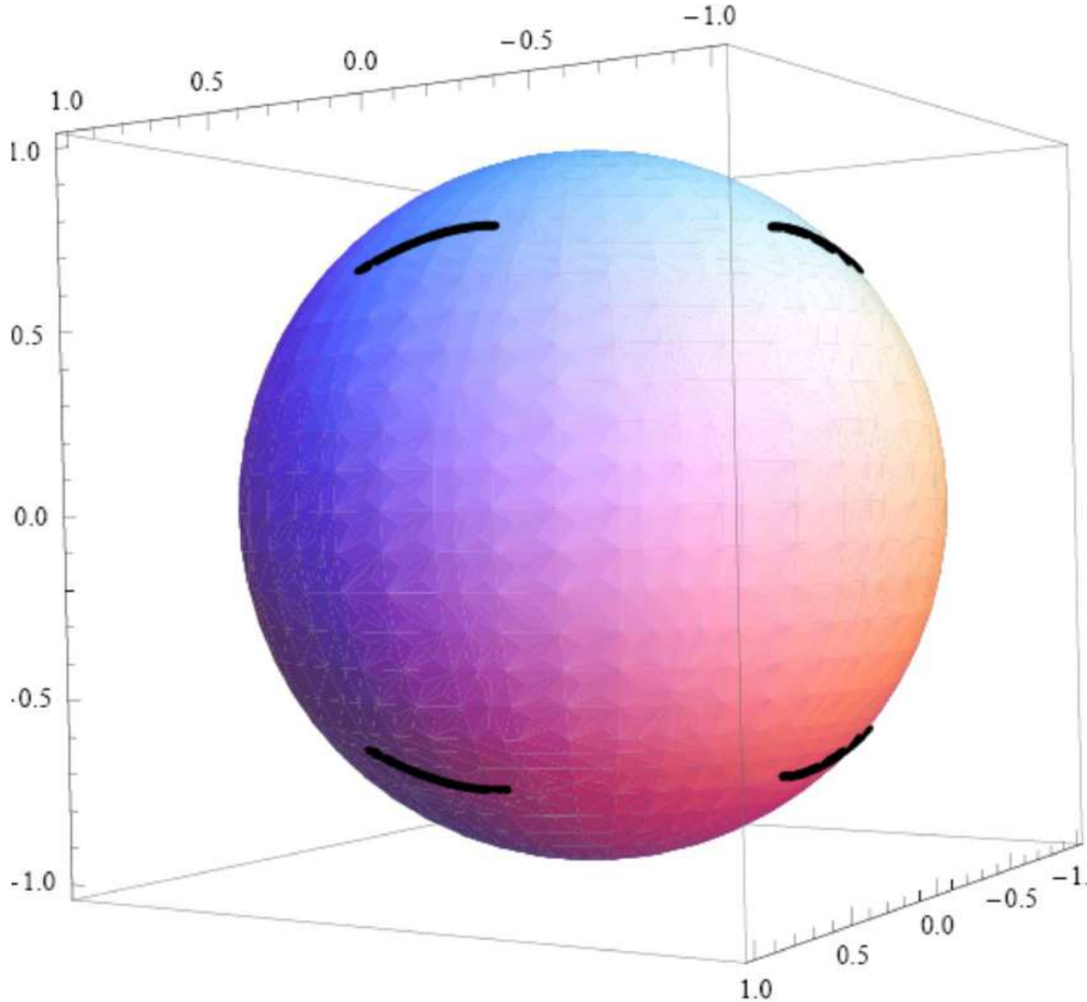


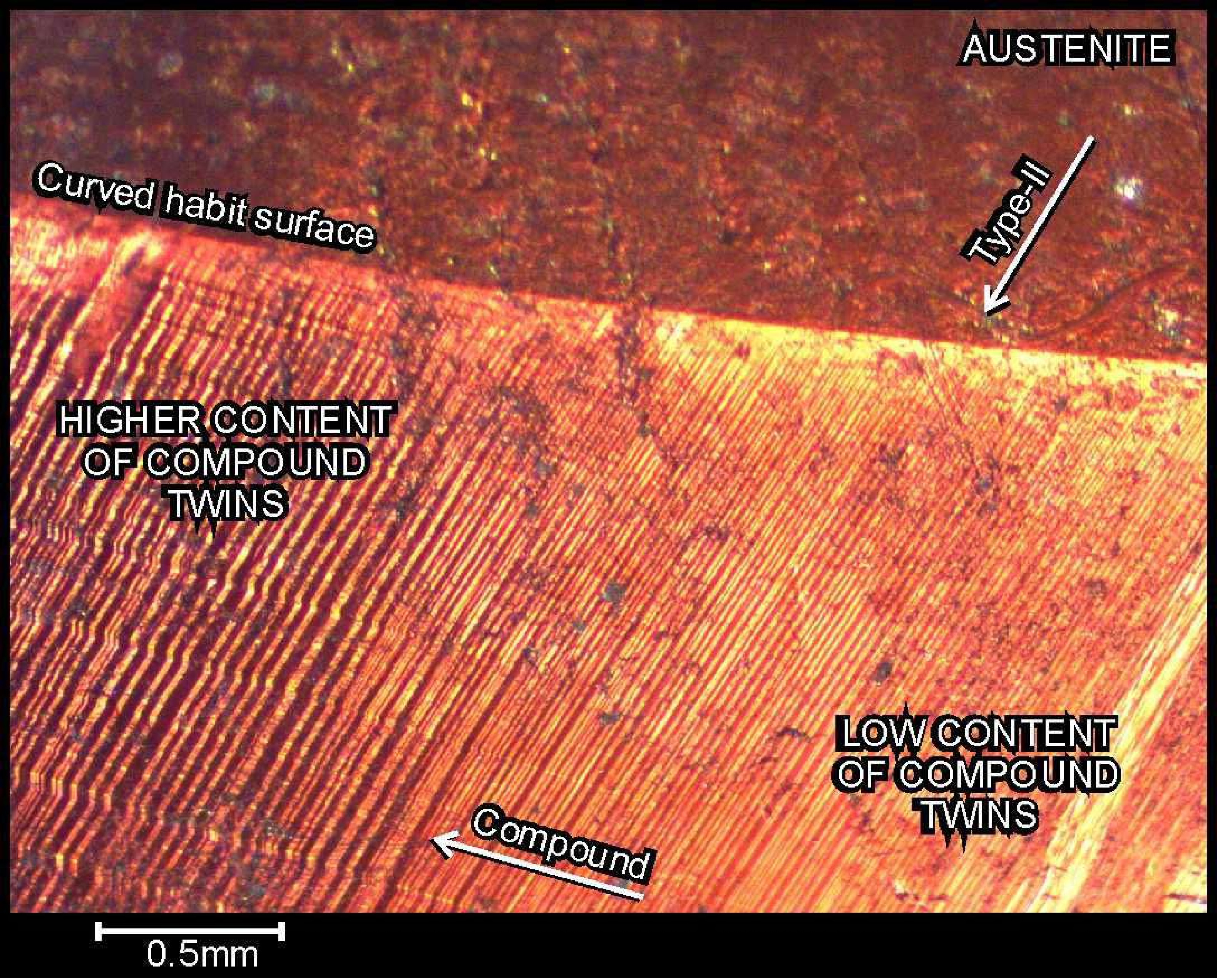
Optical micrograph (H. Seiner) of non-classical interface between austenite and a martensitic microstructure
.
The arrows indicate the orientations of twinning planes of Type-II and compound twinning systems



Twin crossing gradients

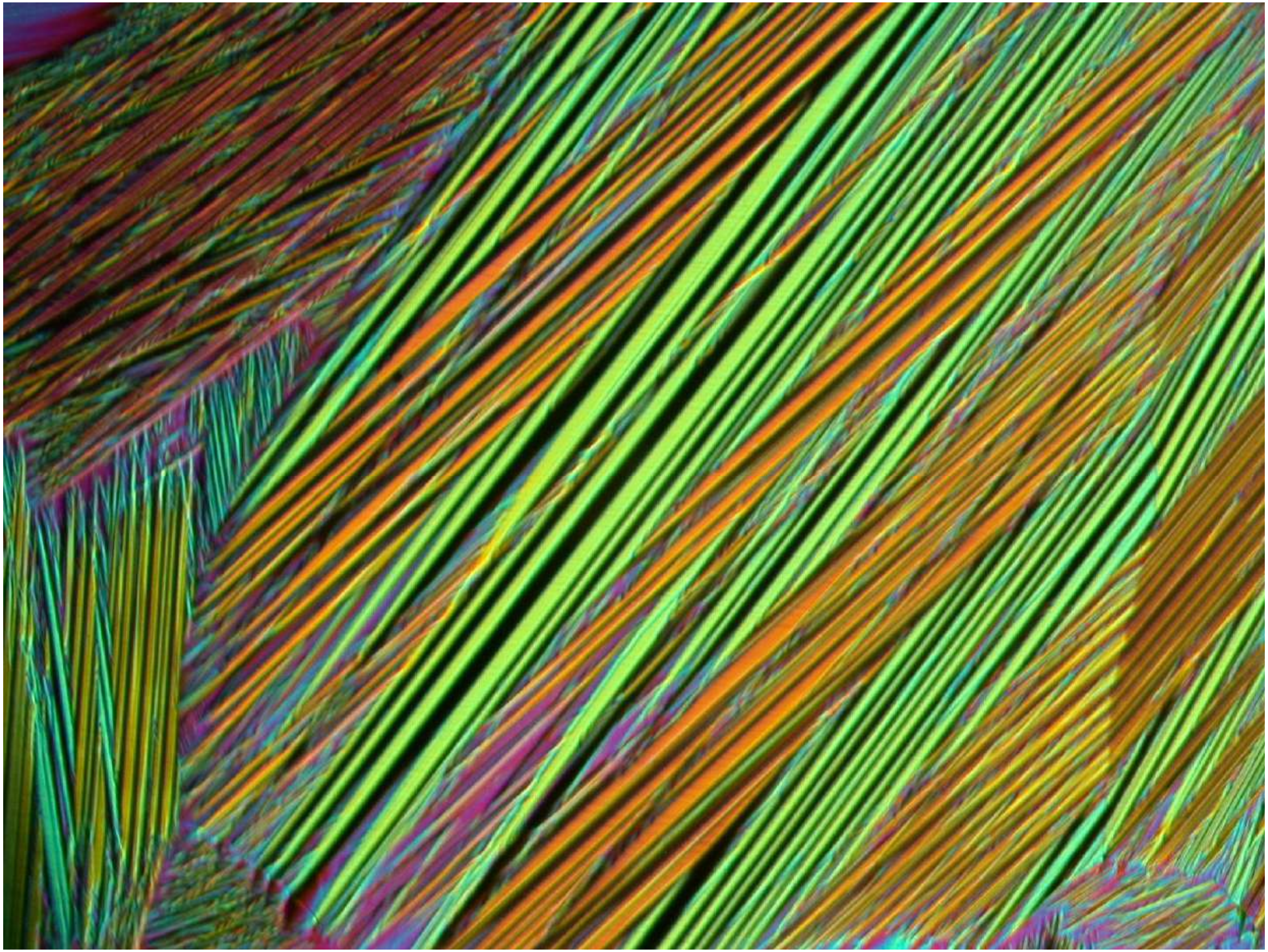
Possible nonclassical interface normals



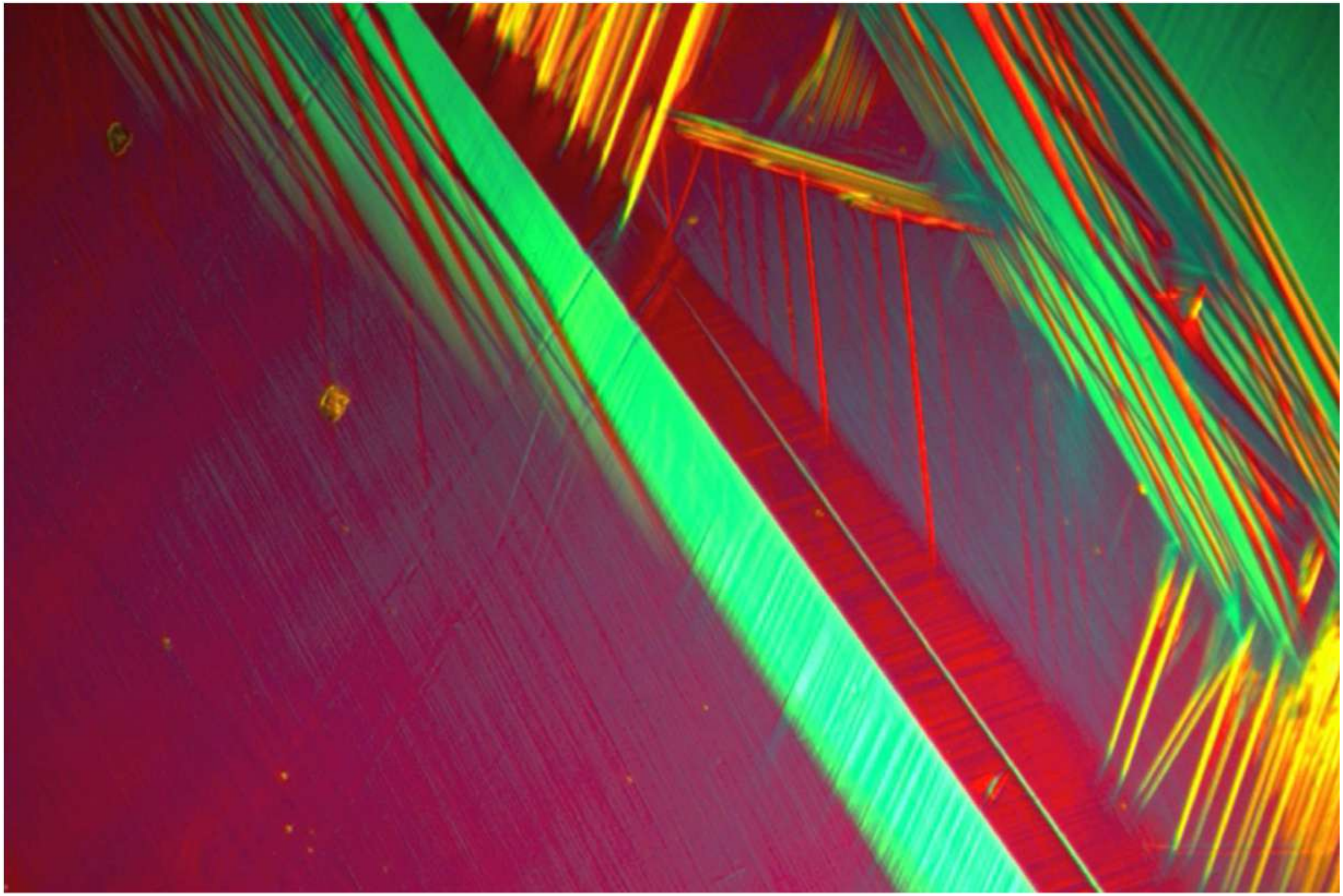


Curved interface between crossing twins and austenite resulting from the inhomogeneity of compound twinning. (Optical microscopy,H. Seiner): theory JB/Koumatos

6. Complex interfaces.



CuZnAl microstructure: Michel Morin (INSA de Lyon)

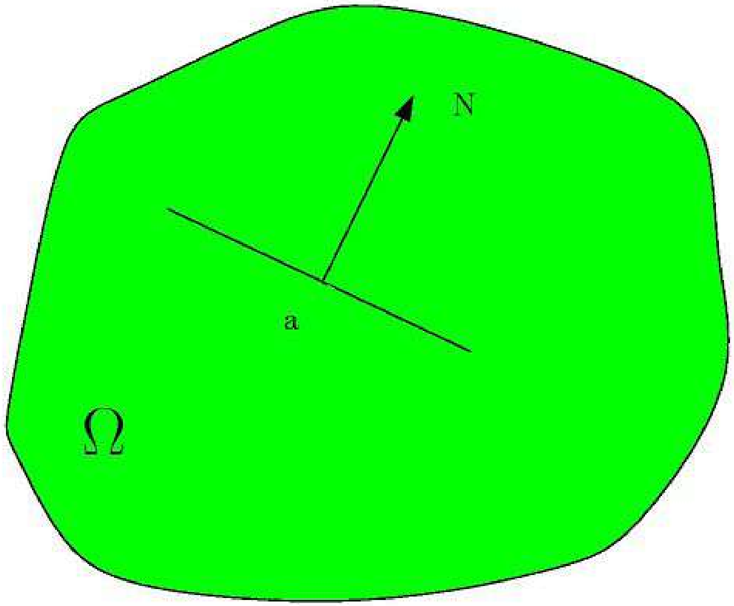


$Zn_{45}Au_{30}Cu_2$ ultra low hysteresis alloy

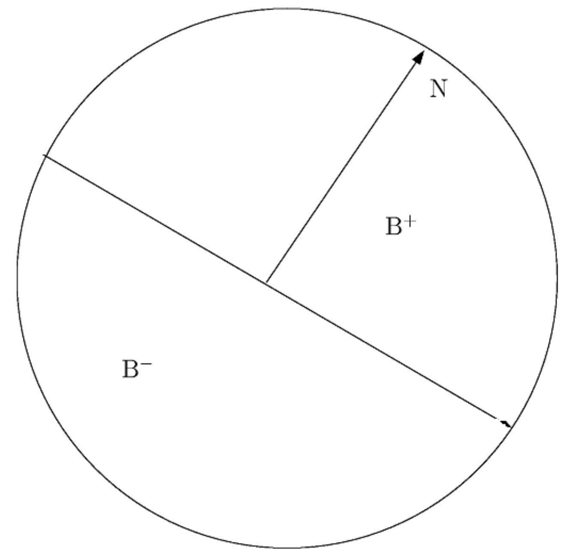
Yintao Song, Xian Chen, Vivekanand Dabade,
Thomas W. Shield, Richard D James, Nature, 502, 85–88 (03 October 2013)

Question: in general, how are the gradients or gradient Young measures on either side of an interface related?

Knowledge of this could help in understanding microstructure morphology.



Suppose $y \in W^{1,\infty}(\Omega; \mathbf{R}^m)$,
i.e y Lipschitz.
Can we define $Dy^+(a), Dy^-(a)$,
and if so how are they related?



Blow up. For $x \in B(0,1)$ let
$z_\delta(x) = \delta^{-1} y(a + \delta x)$.
Then $Dz_\delta(x) = Dy(a + \delta x)$.

Let $\delta_j \to 0$ to get gradient
Young measure ν_x, $x \in B(0,1)$.

Let $G(a,y)$ be the set of such $\nu = (\nu_x)_{x \in B(0,1)}$.

$$Dy^{\pm}(a) = \bigcup_{\nu \in G(a,y)} \bigcap \{E \text{ closed } : \operatorname{supp} \nu_x \subset E \text{ a.e. } x \in B^{\pm}\}$$

Theorem 1 (JB/Carstensen) At every point a in an open set $\Omega \subset \mathbb{R}^n$, for any direction $N \in S^{n-1}$, and for any locally Lipschitz $y : \Omega \to \mathbb{R}^m$, we have

$$0 \in [Dy^{+N}(a)(\mathbf{1}-N\otimes N)]^{\text{qc}} - [Dy^{-N}(a)(\mathbf{1}-N\otimes N)]^{\text{qc}}.$$

Corollary *There exists* $b \in \mathbf{R}^n$ *with*

$$b \otimes N \in Dy^{+}(a)^c - Dy^{-}(a)^c.$$

Proof. By the theorem

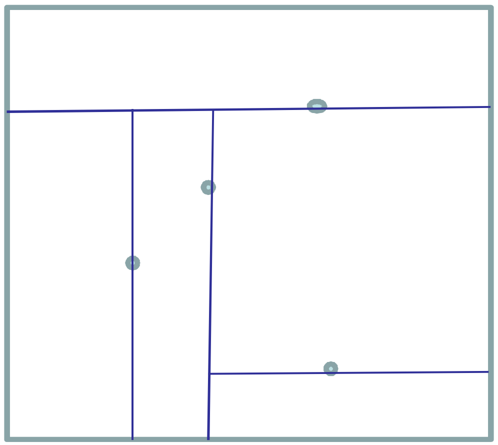
$$\begin{aligned} 0 &\in [Dy^{+N}(a)(\mathbf{1}-N\otimes N)]^c - [Dy^{-N}(a)(\mathbf{1}-N\otimes N)]^c \\ &= [Dy^{+N}(a)^c - Dy^{-N}(a)^c](\mathbf{1}-N\otimes N). \end{aligned}$$

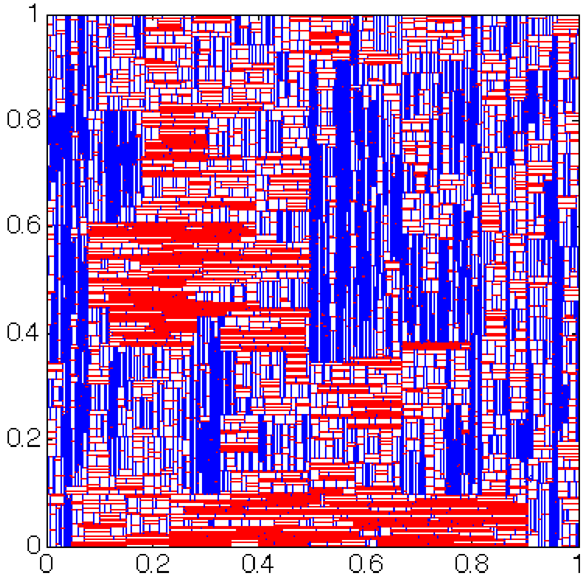
Theorem 2 (JB/Carstensen).
Let $m = n = 2$. *Then there exists* $b \in \mathbf{R}^2$ *with* $b \otimes N \in Dy^+(a)^{pc} - Dy^-(a)^{pc}$.

Proof of Theorem 2 uses quasiregular maps, which are useful also in constructing nonpolyconvex quasiconvex functions. False in higher dimensions (Iwaniec, Verhota, Vogel 2002)

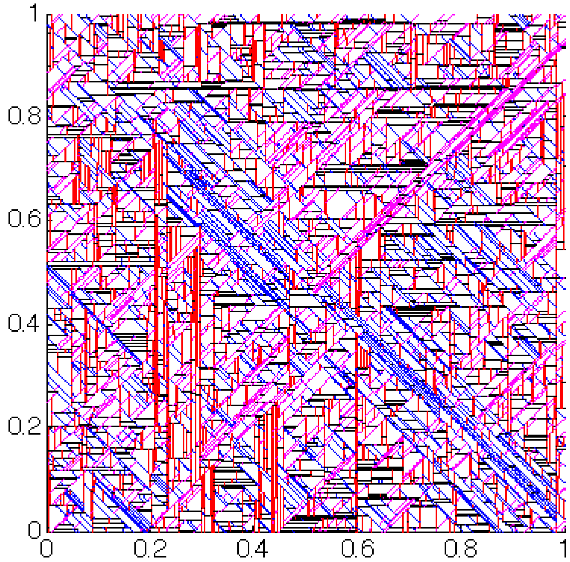
A probabilistic model for martensitic avalanches.

JB/P. Cesana/B. Hambly 2015





2 directions



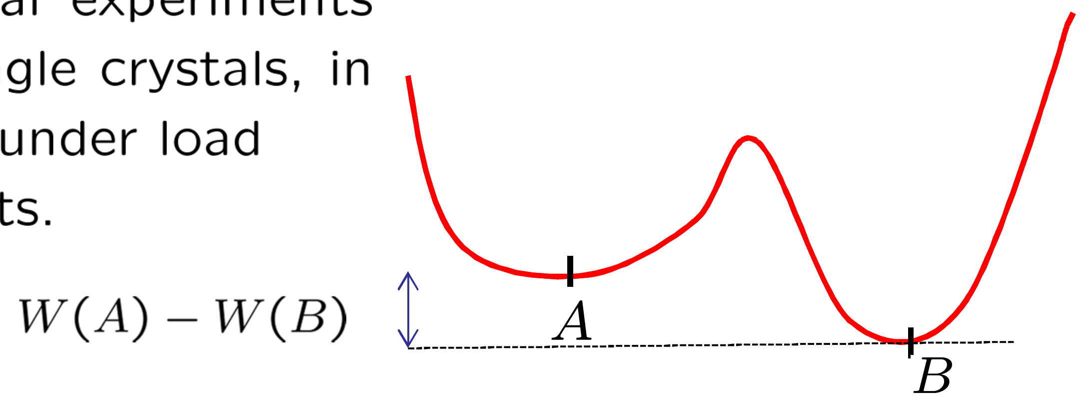
4 directions

General branching random walk analysis (Cesana/Hambly) predicts approximate power laws for plate lengths, as observed for acoustic emissions.

7. Incompatibility induced metastability and nucleation of austenite

Two examples of incompatibility-induced metastability

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.



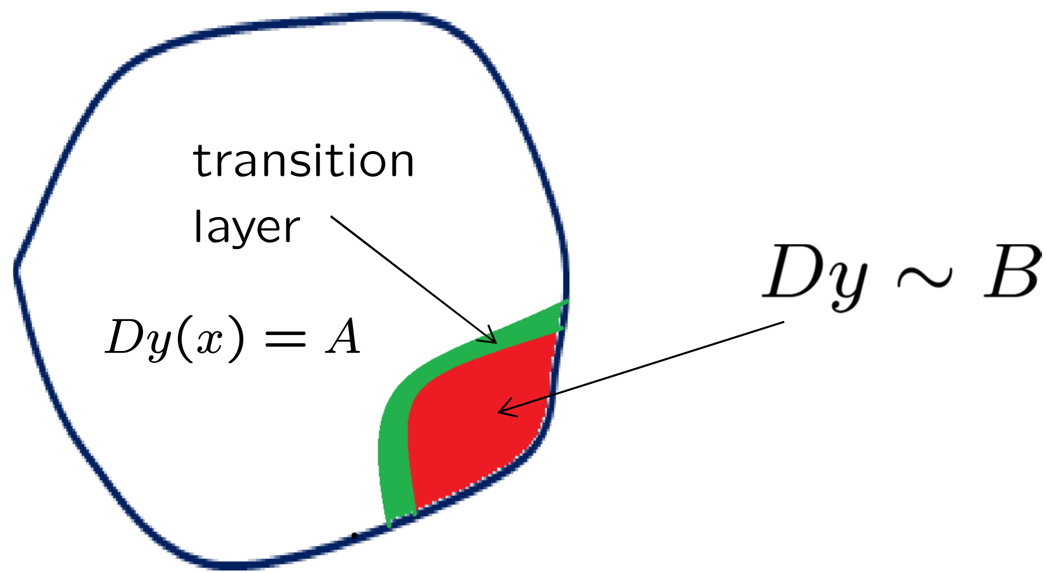
Consider the integral

$$I(y) = \int_\Omega W(Dy)\,dx, \qquad W(A) = \psi(A,\theta) - T\cdot A$$

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

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

Idea: since A and B are incompatible, if we nucleate a region in which $Dy(x) \sim B$ 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

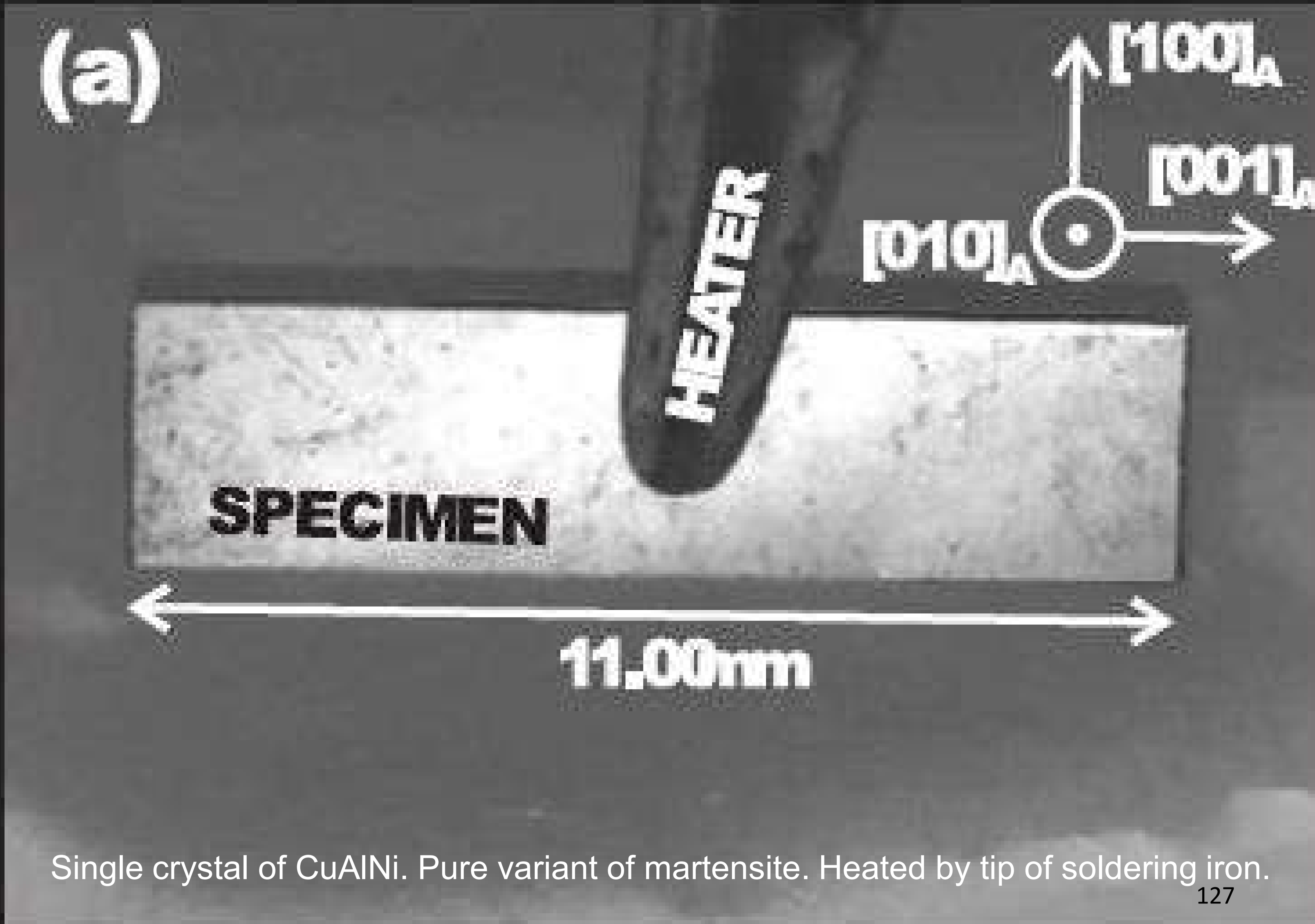
Nucleation of austenite in martensite

JB, Konstantinos Koumatos, Hanus Seiner 2012, 2013

Localized heating experiment:

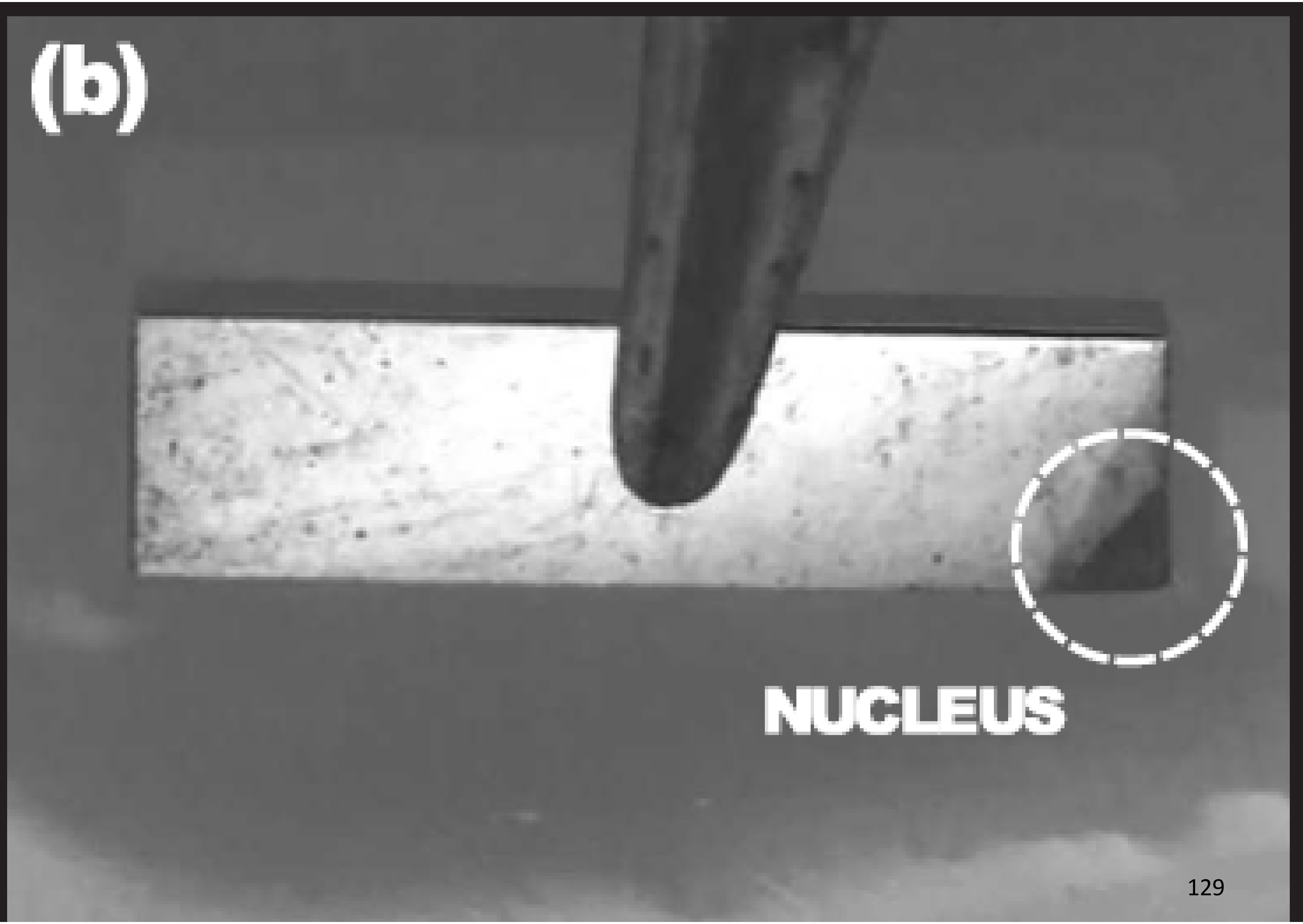
Specimen: single crystal of CuAlNi prepared by the Bridgeman method in the form of a prismatic bar of dimensions $12\times3\times3\text{mm}^3$ in the austenite with edges approximately along the principal cubic directions.

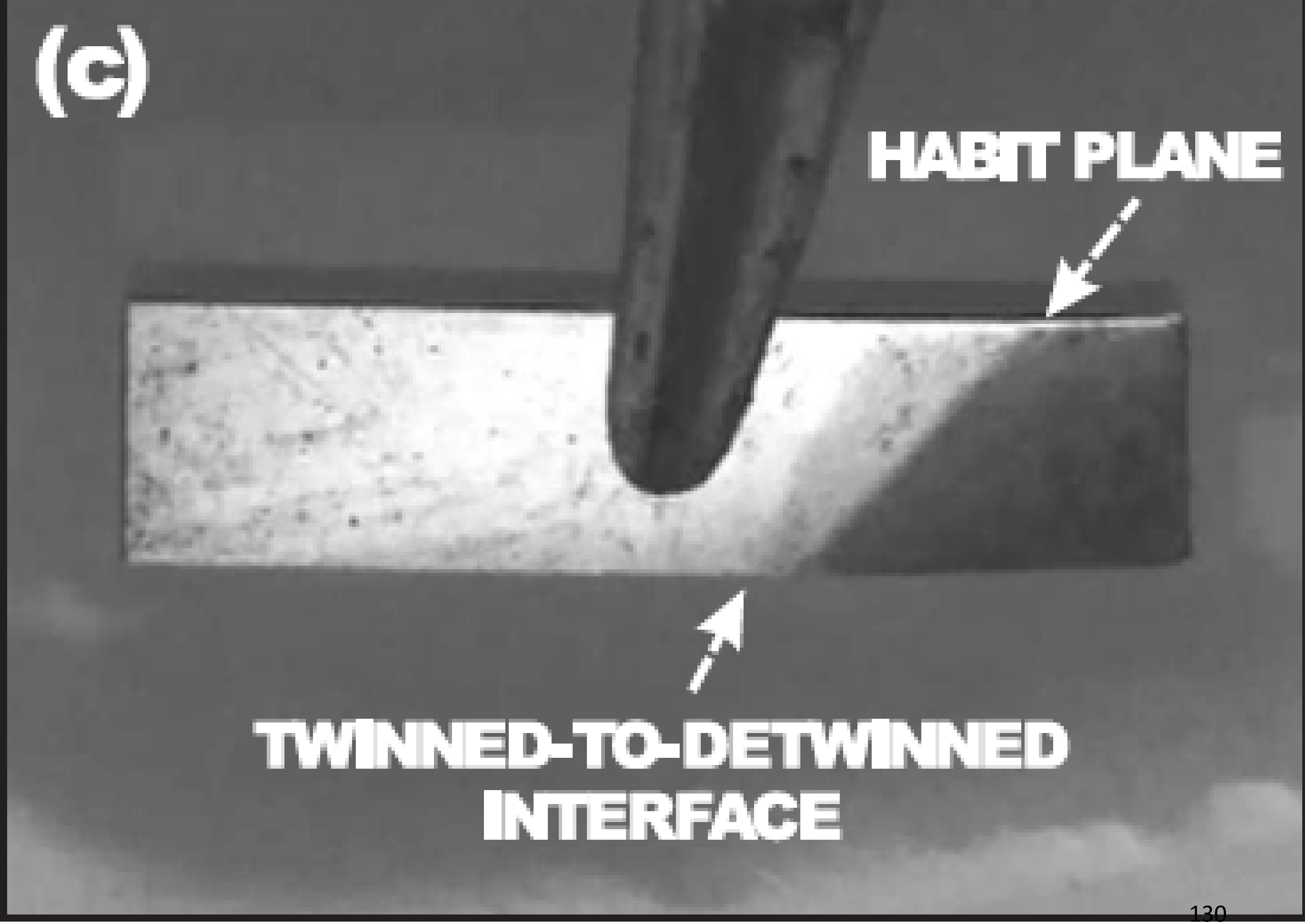
By unidirectional compression along its longest edge, the specimen was transformed into a single variant of mechanically stabilized martensite. Due to the mechanical stabilization effect the reverse transition did not occur during unloading.



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

When touched at a corner, nucleation of austenite occured there immediately. When touched at an edge or face, nucleation did not occur at the site of the localized heating, but at some corner, after a time delay (sufficient for heat conduction to make the temperature there large enough).


(b)
NUCLEUS


(c)
HABIT PLANE
TWINNED-TO-DETWINNED
INTERFACE

Proposed explanation. Nucleation is geometrically impossible in the interior, on faces and at edges, but not at a corner. We express this by proving in a simplified model that if U_s denotes the initial pure variant of martensite then at U_s the free-energy function is quasiconvex (in the interior), quasiconvex at the boundary faces, and quasiconvex at the edges, but not at a corner.

To make the problem more tractable we assume that $\psi(A, \theta) := W(A)$ is infinite outside the austenite and martensite energy wells.

Idealized model

$$I(\nu) = \int_\Omega \langle \nu_x, W \rangle \, dx = \int_\Omega \int_{M^{3\times 3}} W(A) \, d\nu_x(A) \, dx,$$

where

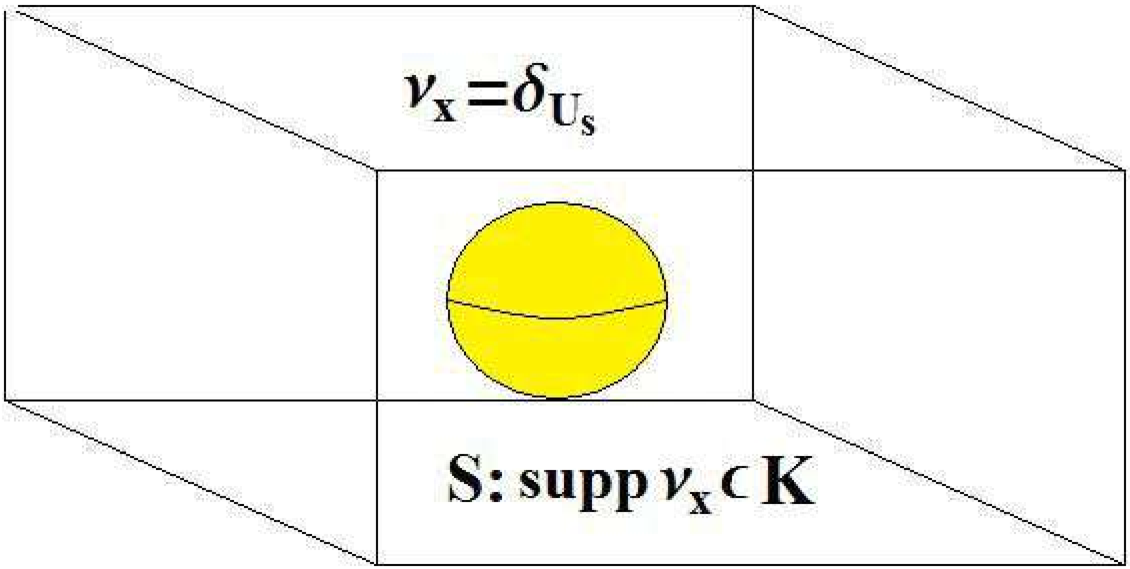
$$W(A) = \begin{cases} -\delta & A \in SO(3) \\ 0 & A \in \bigcup_{i=1}^{6} SO(3)U_i \\ +\infty & \text{otherwise} \end{cases},$$

and $\delta > 0$.

So $W(A) < \infty$ on

$$K = SO(3) \cup \bigcup_{i=1}^{6} SO(3)U_i$$

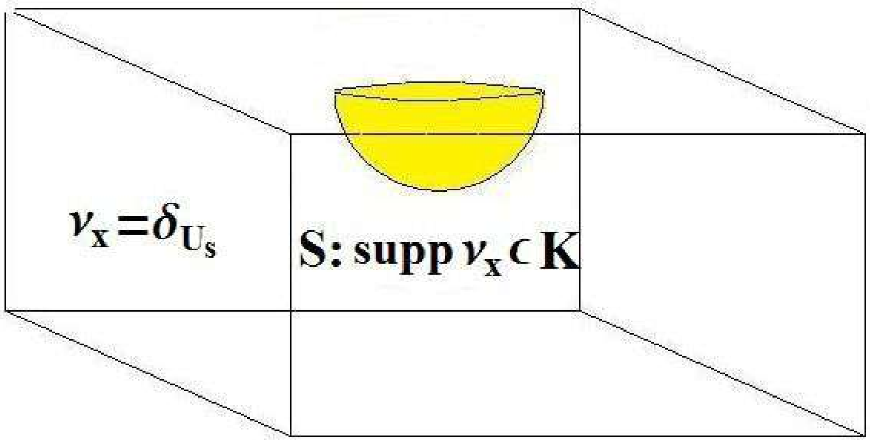
Nucleation impossible in the interior

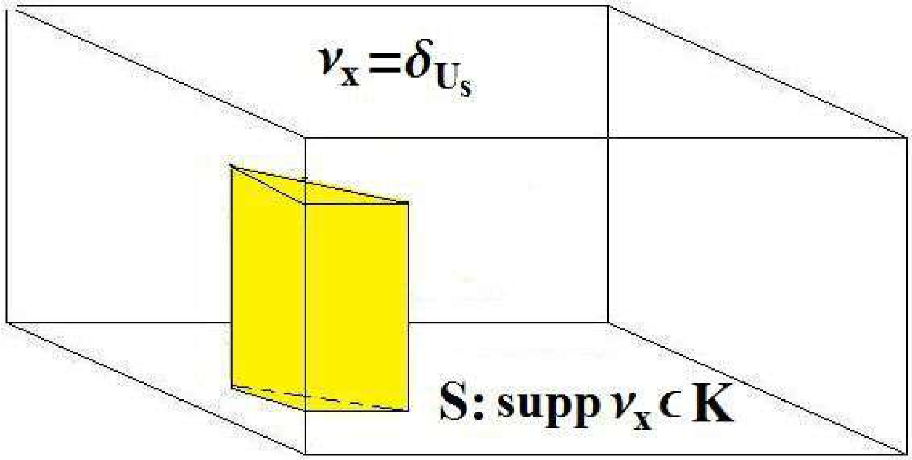


$$\text{Theorem} \quad I(\nu) \geq I(\delta_{U_s})$$

(quasiconvexity at U_s)

Nucleation impossible at faces or edges

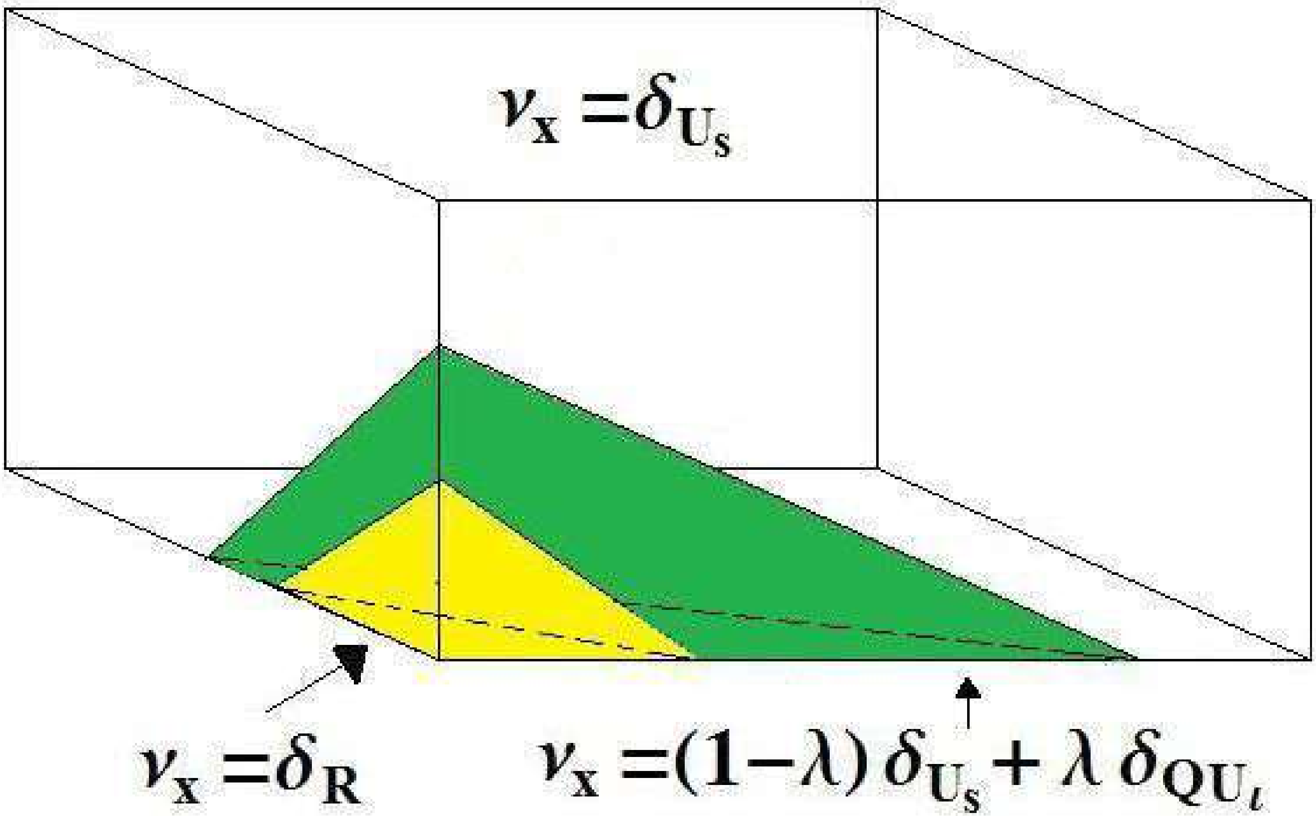




Similarly in these cases we have

Theorem $I(\nu) \geq I(\delta_{U_s})$
(quasiconvexity at the boundary and edges at U_s)

Nucleation possible at a corner



$$I(\nu) < I(\delta_{U_s})$$

I *not* quasiconvex at such a corner.

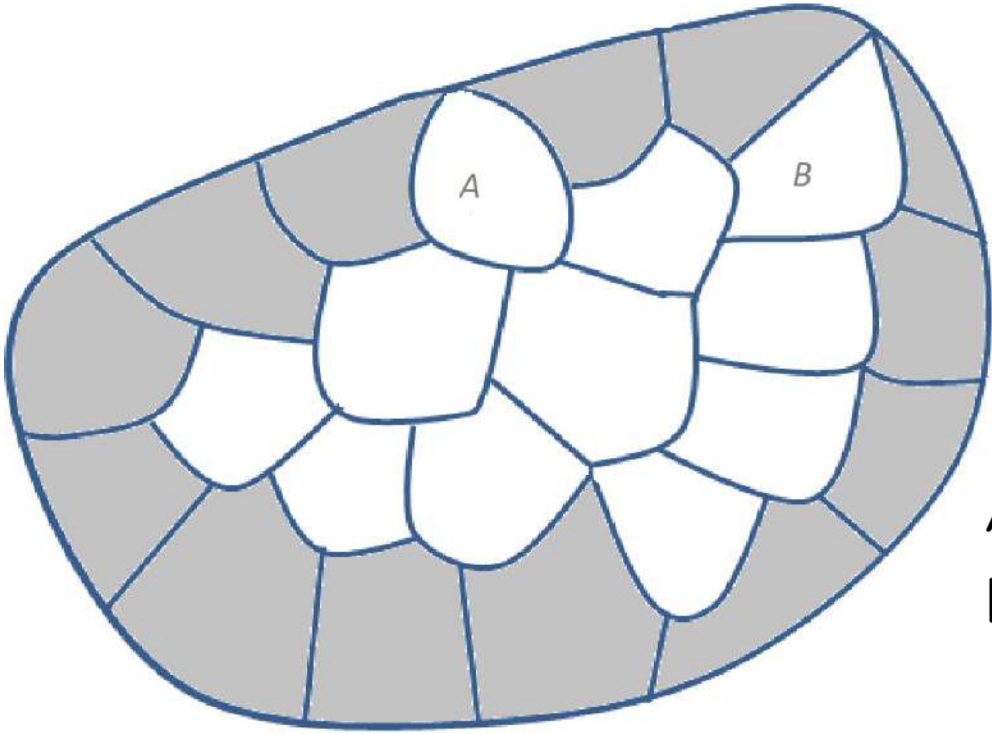
8. Remarks on polycrystals

Description of polycrystals

Consider a polycrystal occupying in a reference configuration a bounded domain $\Omega \subset \mathbb{R}^n$, composed of a finite number of disjoint grains $\Omega_j, j = 1, \ldots, N$, where each Ω_j is a bounded domain, so that

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

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



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

The set of *triple points* is

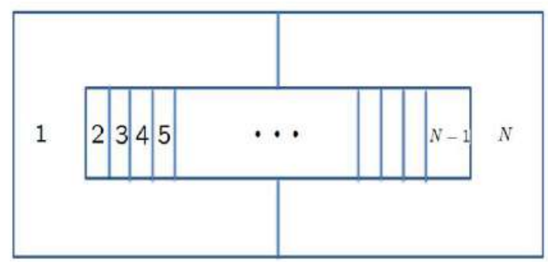
$$T = \bigcup_{1 \le i_1 < i_2 \le i_3} \partial\Omega_{i_1} \cap \partial\Omega_{i_2} \cap \partial\Omega_{i_3}.$$

The union of grain boundaries is $D = \bigcup_{i=1}^{N} \partial\Omega_i$.

Theorem (JB/Carstensen). Suppose each grain Ω_j is convex. Then every interior grain is a convex polyhedron (i.e. an intersection of a finite number of open half-spaces).

Theorem. (JB/Carstensen) If $n = 2$ and each grain is the interior of a closed Jordan curve, then there are at most $2(N-2)$ triple points.

The bound is sharp.



Theorem.(JB/Carstensen). For $n \geq 2$, if each $\overline{\Omega}_j$ is a topological manifold with boundary then T is nowhere dense in D.

Two results using the nonlinear elasticity model without interfacial energy.

In this model, at a constant temperature the total free energy of the polycrystal in a deformation $y : \Omega \to \mathbb{R}^3$ is given by

$$I(y) = \int_\Omega W(x, Dy(x))\, dx,$$

where $W(x, A) = \psi(AR_j)$ for $x \in \Omega_j$, $\psi = \psi(A)$ is the free-energy density corresponding to a single crystal, and $R_j \in SO(3)$.

Suppose we are at a temperature for which the free-energy of the martensite (taken to be zero) is less than that for the austenite. Then $\psi \geq 0$ and

$$K = \{A : \psi(A) = 0\} = \bigcup_{i=1}^{M} SO(3)U_i.$$

Microstructures are described by gradient Young measures $\nu = (\nu_x)_{x\in\Omega}$, with corresponding energy

$$\begin{aligned} \widehat{I}(\nu) &= \int_\Omega \int_{M^{3\times 3}} W(x,A)\, d\nu_x(A)\, dx \\ &= \sum_{j=1}^{M} \int_{\Omega_j} \int_{M^{3\times 3}} \psi(AR_j)\, d\nu_x(A)\, dx. \end{aligned}$$

(Here we assume that the grains have sufficiently regular, e.g. Lipschitz, boundaries.)

Zero-energy microstructures thus correspond to ν such that $\operatorname{supp}\nu_x \subset KR_j^T$ for $x \in \Omega_j$.

For cubic-to-tetragonal (more generally for cubic austenite) a result of Bhattacharya on self-accommodation implies that in the absence of boundary conditions on $\partial\Omega$ there is always a zero-energy microstructure with uniform macroscopic deformation gradient

$$\bar{\nu}_x = \int_{M^{3\times 3}} A\, d\nu_x(A) = \nabla y(x) = (\det U_1)^{\frac{1}{3}}\mathbf{1}.$$

How complicated does ν_x have to be?

Cubic to tetragonal: $K = \bigcup_{i=1}^{3} SO(3)U_i$, where

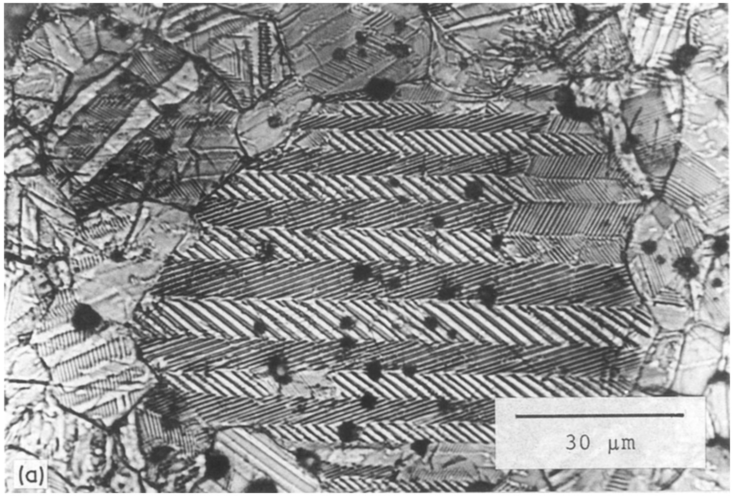
$$U_1 = \text{diag}\,(\eta_2, \eta_1, \eta_1),\ U_2 = \text{diag}\,(\eta_1, \eta_2, \eta_1),$$
$$U_3 = \text{diag}\,(\eta_1, \eta_1, \eta_2).$$

Theorem There is no homogeneous gradient Young measure

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

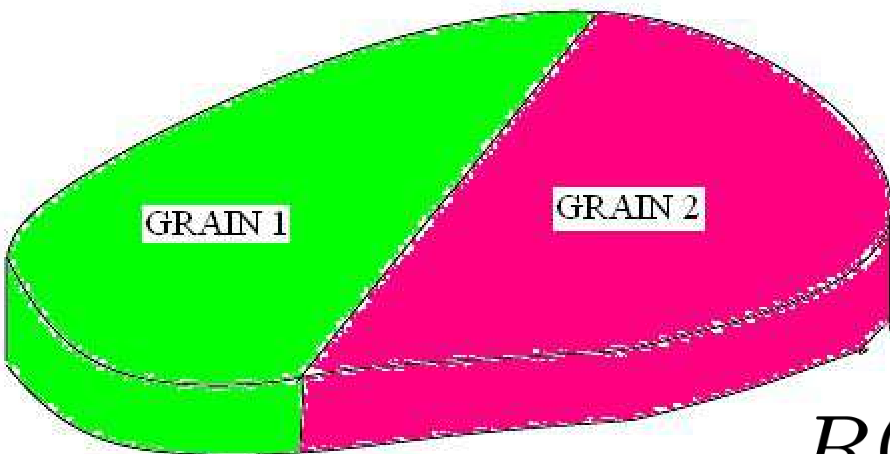
with $A_i \in K$ and $\bar{\nu} = (\eta_1^2 \eta_2)^{1/3}\mathbf{1}$.

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



Zero-energy microstructures for a bicrystal

$$K = \mathrm{SO}(3)U_1 \cup \mathrm{SO}(3)U_2$$



Grain 1

$\mathrm{supp}\, \nu_x \subset K$

Grain 2

$\mathrm{supp}\, \nu_x \subset K R(\alpha)$

$R(\alpha)e_3 = e_3$

$\alpha =$ angle of rotation.

Always possible to have zero-energy microstructure with $\nabla y = \bar{\nu}_x = (\eta_1^2 \eta_2)^{1/3} \mathbf{1}$

Question: Is it true that whatever the orientation of the planar interface between the two grains there must be a nontrivial microstructure in both grains?

Result 1. Whatever the orientation there always exists a zero-energy microstructure which has a pure phase (i.e. $\nu_x = \delta_A$) in one of the grains.

Now consider the case when the boundary between the two grains has the form $S \times (0, d)$, where S is a smooth curve in the plane, so that the normal at any point is of the form $(\cos\theta, \sin\theta, 0)$.

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 $\theta' \in D_2$, where

$$D_1 = (\frac{\pi}{8}, \frac{3\pi}{8}) \cup (\frac{5\pi}{8}, \frac{7\pi}{8}) \cup (\frac{9\pi}{8}, \frac{11\pi}{8}) \cup (\frac{13\pi}{8}, \frac{15\pi}{8})$$

$$D_2 = (\frac{-\pi}{8}, \frac{\pi}{8}) \cup (\frac{3\pi}{8}, \frac{5\pi}{8}) \cup (\frac{7\pi}{8}, \frac{9\pi}{8}) \cup (\frac{11\pi}{8}, \frac{13\pi}{8})$$

Proofs use:

1. A reduction to the case $m = n = 2$ using the plane strain result for the two-well problem (JB/James).

2. The characterization of the quasiconvex hull of two wells (JB/James), which equals their polyconvex hull.

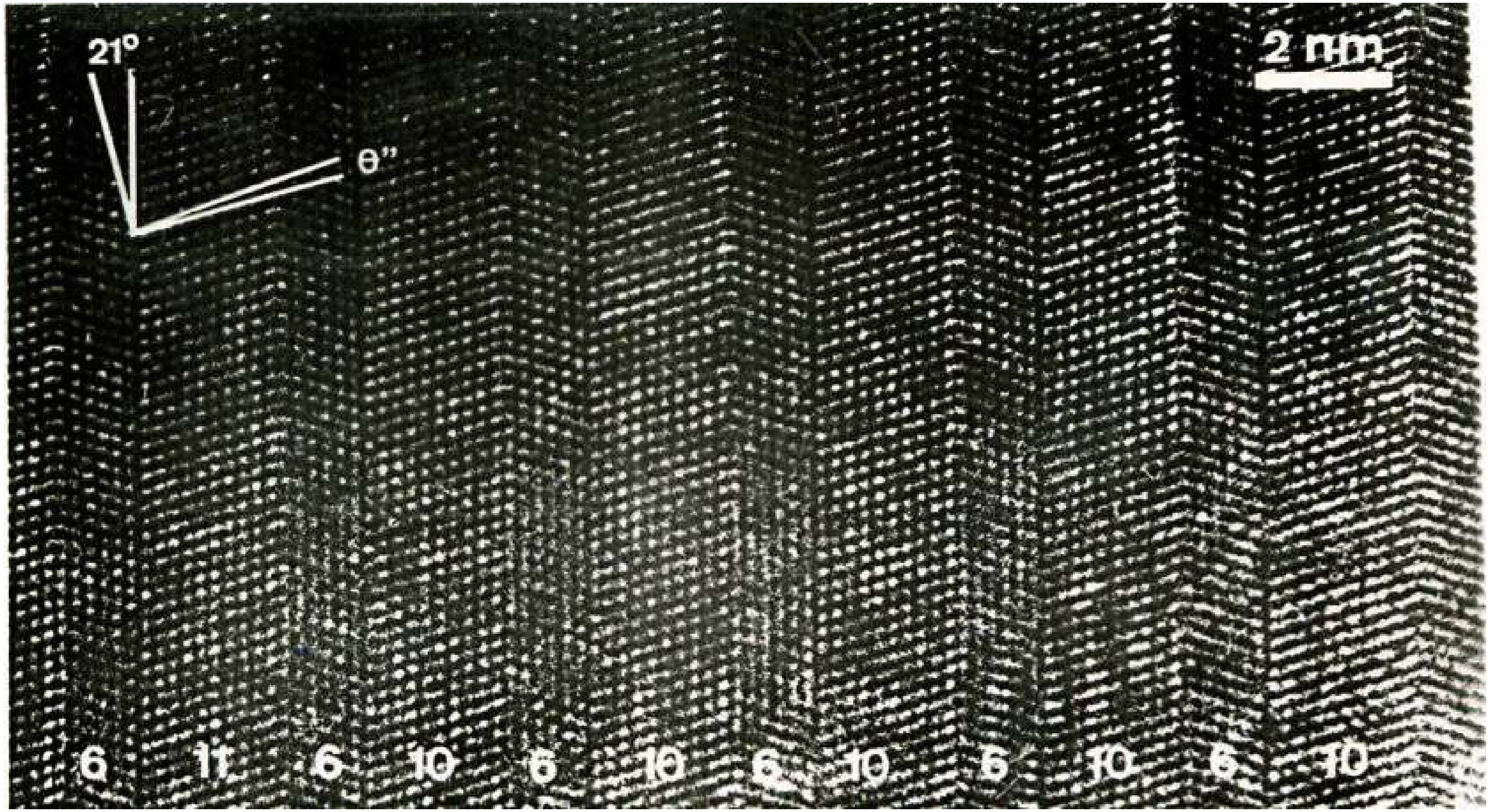
3. Use of a generalized Hadamard jump condition to show that there has to be a rank-one connection $b \otimes N$ between the polyconvex hulls for each grain.

4. Long and detailed calculations.

9. Local minimizers with and without interfacial energy

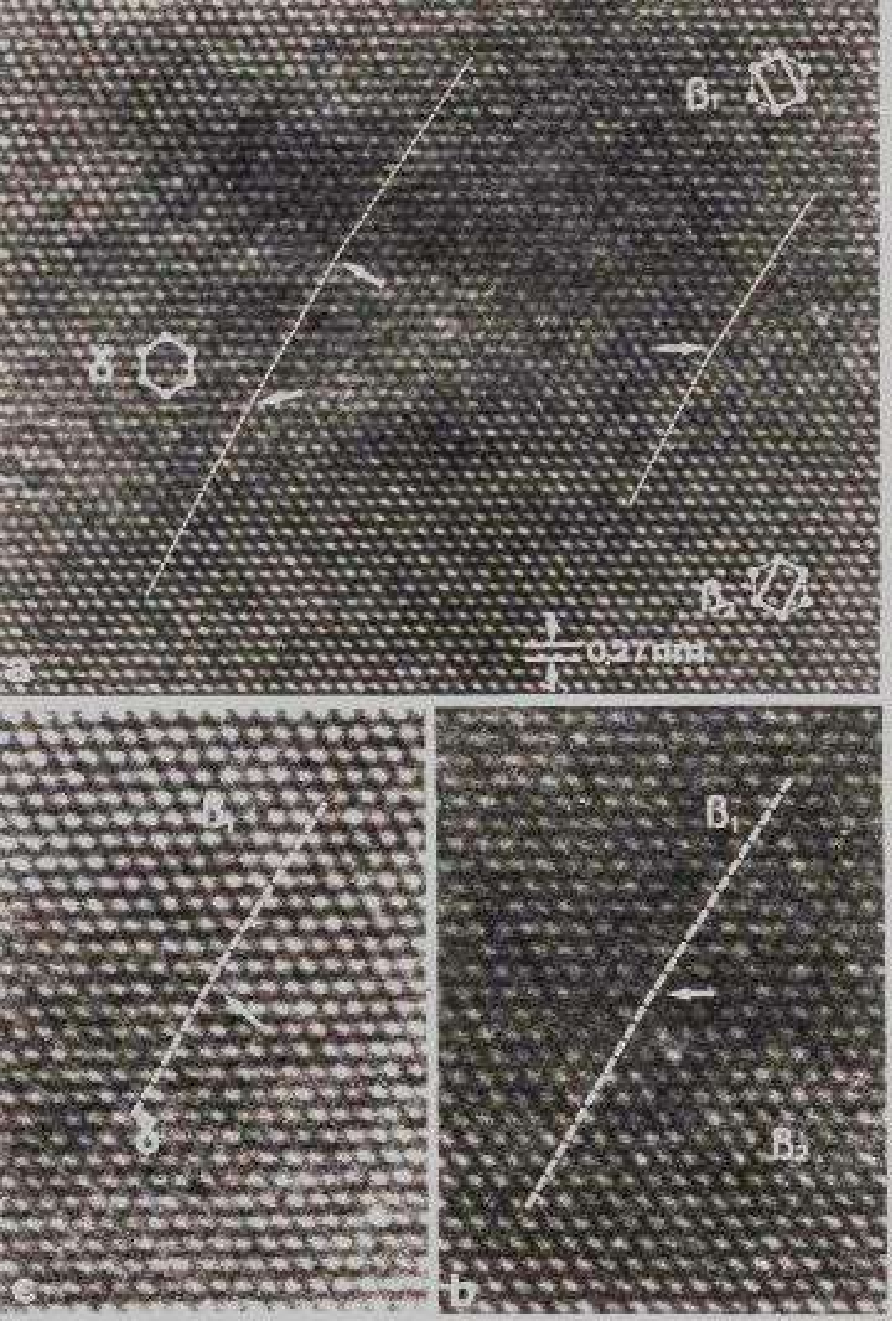
Interfacial energy

Some interfaces are atomistically sharp



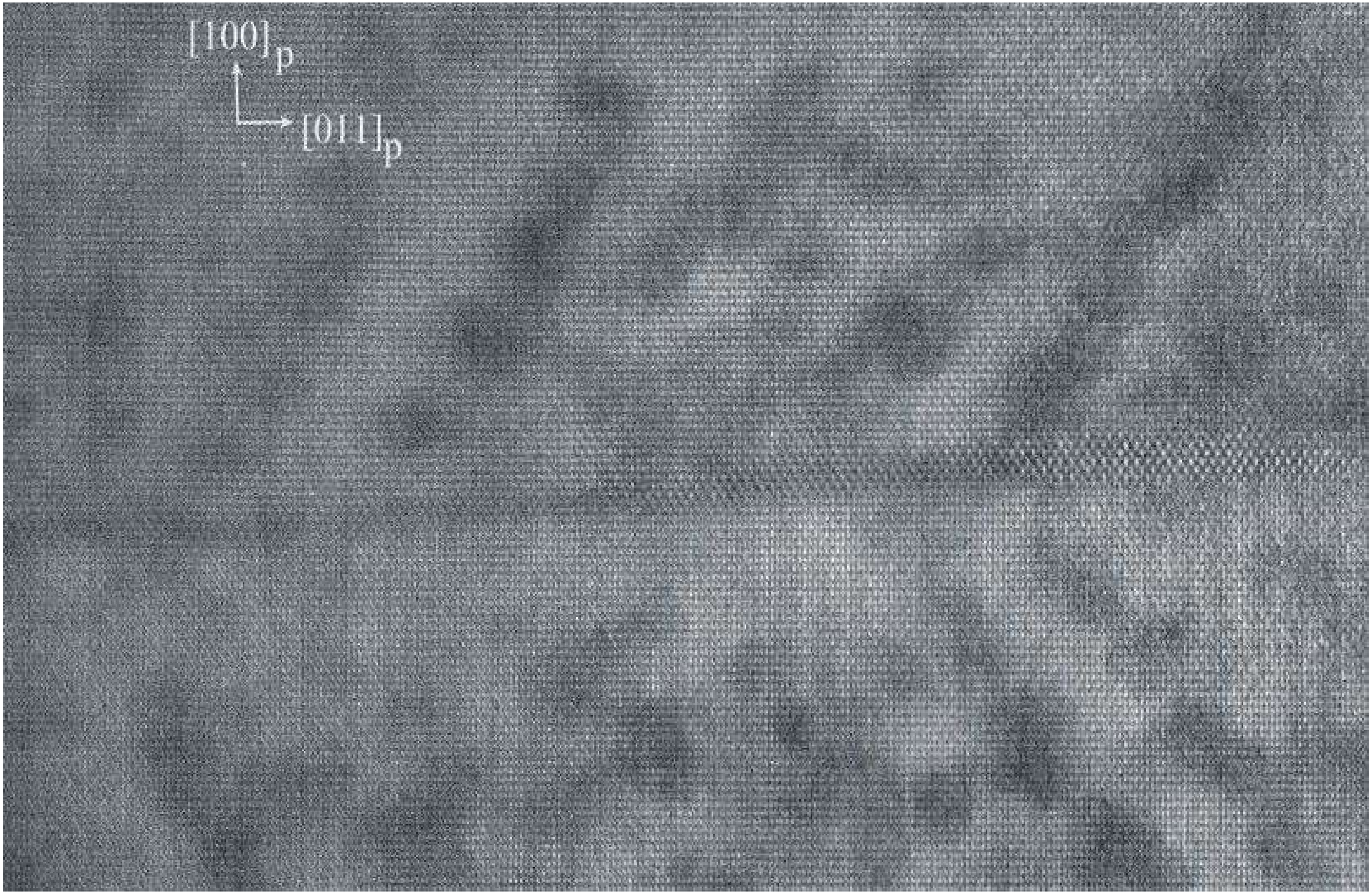
NiMn   Baele, van Tenderloo, Amelinckx

while others are diffuse …



Diffuse (smooth) interfaces in $Pb_3V_2O_8$

Manolikas, van Tendeloo, Amelinckx



Diffuse interface in perovskite (courtesy Ekhard Salje)

No interfacial energy

Suppose that

$$D\psi(\alpha(\theta)\mathbf{1},\theta)=0,$$

$$D^2\psi(\alpha(\theta)\mathbf{1},\theta)(G,G)\geq\mu|G|^2 \text{ for all } G=G^T,$$

some $\mu>0$. Then $\bar{y}(x)=\alpha(\theta)x+c$ is a local minimizer of

$$I_\theta(y)=\int_\Omega\psi(Dy,\theta)\,dx$$

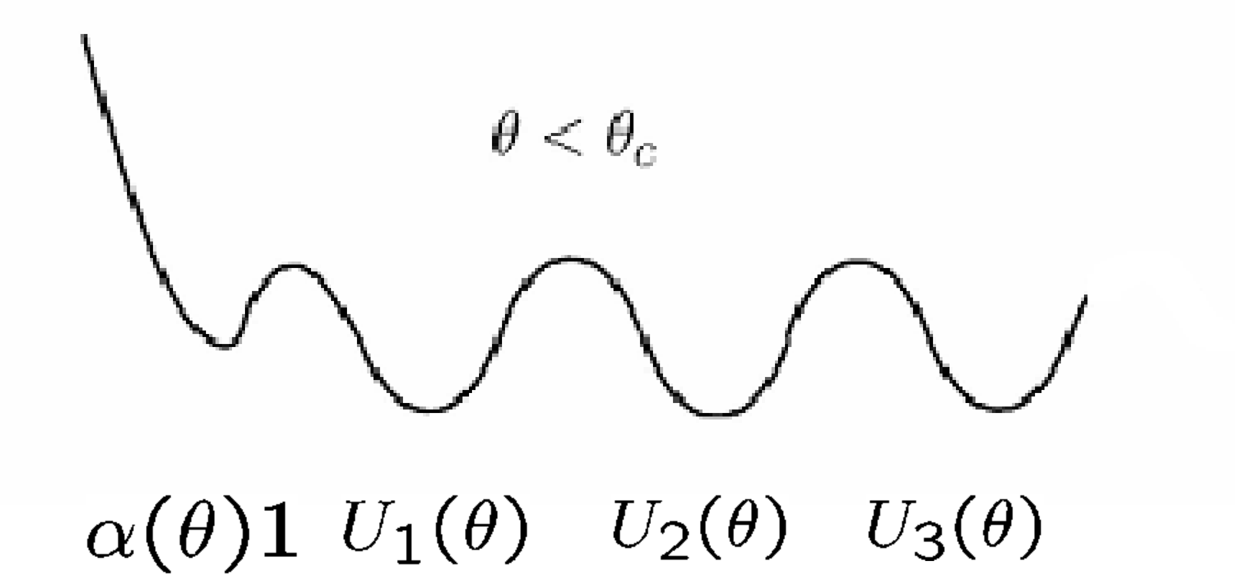
in $W^{1,\infty}(\Omega;\mathbf{R}^3)$.

But $\bar{y}(x)=\alpha(\theta)x+c$ is *not* a local minimizer of I_θ in $W^{1,p}(\Omega;\mathbf{R}^3)$ for $1\leq p<\infty$ because nucleating an austenite-martensite interface reduces the energy.

Second gradient model for diffuse interfaces

JB/Elaine Crooks (Swansea)

How does interfacial energy affect the predictions of the elasticity model of the austenite–martensite transition?



Use simple second gradient model of interfacial energy (cf Barsch & Krumhansl, Salje), for which energy minimum is always attained.

Fix $\theta < \theta_c$, write $\psi(A) = \psi(A, \theta)$, and define

$$I(y) = \int_\Omega \left(\psi(Dy) + \varepsilon^2 |D^2 y|^2\right)\, dx$$

where $|D^2 y|^2 = y_{i,\alpha\beta} y_{i,\alpha\beta}$, $\varepsilon > 0$,

It is not clear how to justify this model on the basis of atomistic considerations (the wrong sign problem – see, for example, Blanc, LeBris, Lions).

Hypotheses

No boundary conditions (i.e. boundary traction free), so result will apply to all boundary conditions.

Assume $\psi \in C^2(M_+^{3\times 3})$,
$\psi(A) = \infty$ for $\det A \leq 0$,
$\psi(A) \to \infty$ as $\det A \to 0+$,
$\psi(RA) = \psi(A)$ for all $R \in SO(3)$,
ψ bounded below, $\varepsilon > 0$.

$D\psi(\alpha \mathbf{1}) = 0$
$D^2\psi(\alpha \mathbf{1})(G, G) \geq \mu |G|^2$ for all $G = G^T$,
for some $\mu > 0$. Here $\alpha = \alpha(\theta)$.

Theorem. $\bar{y}(x) = \alpha R x + a$, $R \in \mathrm{SO}(3), a \in \mathbf{R}^3$, *is a local minimizer of* I *in* $L^1(\Omega; \mathbf{R}^3)$.
More precisely,

$$I(y) - I(\bar{y}) \geq \sigma \int_\Omega \left(|\sqrt{Dy^T Dy} - \alpha \mathbf{1}|^2 + |D^2 y|^2 \right) dx$$

for some $\sigma > 0$ *if* $\|y - \alpha R x - a\|_1$ *is sufficiently small.*

Remark.

$$\int_\Omega |\sqrt{Dy^T Dy} - \alpha \mathbf{1}|^2 \, dx$$

$$\geq c_0 \inf_{\bar{R} \in \mathrm{SO}(3), \bar{a} \in \mathbf{R}^3} \left(\|y - \alpha \bar{R} x - \bar{a}\|_2^2 + \|Dy - \bar{R}\|_2^2 \right).$$

by Friesecke, James, Müller Rigidity Theorem

Idea of proof

Reduce to problem of local minimizers for

$$I(U) = \int_\Omega (\psi(U) + m\rho^2\varepsilon^2|DU|^2)\,dx,$$

studied by Taheri (2002), using

$$|D_A U(A)| \leq \rho$$

for all A, where $U(A) = \sqrt{A^T A}$.

Smoothing of twin boundaries

Seek solution to equilibrium equations for

$$I(y) = \int_{\mathbf{R}^3} (W(Dy) + \varepsilon^2 |D^2 y|^2)\, dx$$

such that

$Dy \to A$ as $x \cdot N \to -\infty$

$Dy \to B$ as $x \cdot N \to +\infty$,

where $A, B = A + a \otimes N$ are twins.

Lemma

Let $Dy(x) = F(x{\cdot}N)$, where $F \in W^{1,1}_{\text{loc}}(\mathbf{R}; M^{3\times 3})$ and

$$F(x \cdot N) \to A, B$$

as $x \cdot N \to \pm\infty$. Then there exist a constant vector $a \in \mathbf{R}^3$ and a function $u : \mathbf{R} \to \mathbf{R}^3$ such that

$$u(s) \to 0, a \text{ as } s \to -\infty, \infty,$$

and for all $x \in \mathbf{R}^3$

$$F(x \cdot N) = A + u(x \cdot N) \otimes N.$$

In particular

$$B = A + a \otimes N.$$

The ansatz

$$Dy(x) = A + u(x \cdot N) \otimes N.$$

leads to the 1D integral

$$\begin{aligned} \mathcal{F}(u) &= \int_{\mathbf{R}} [W(A + u(s) \otimes N) + \varepsilon^2 |u'(s)|^2] \, ds \\ &:= \int_{\mathbf{R}} [\tilde{W}(u(s)) + \varepsilon^2 |u'(s)|^2] \, ds. \end{aligned}$$

For cubic $\rightarrow$ tetragonal or orthorhombic (under a nondegeneracy assumption) we have

$$\tilde{W}(0) = \tilde{W}(a) = 0, \ \tilde{W}(u) > 0 \text{ for } u \neq 0, a,$$

and so by energy minimization (Alikakos & Fusco 2008) we get a solution.

Remarks

1. The solution generates a solution to the full 3D equilibrium equations. However if we use instead the ansatz

$$Dy(x) = A + v(x \cdot N) a \otimes N$$

with v a scalar, then the corresponding solution does not in general generate a solution to the 3D equations.

2. The solution is not in general unique even within the class given by the ansatz, but more work needs to be done in this direction.