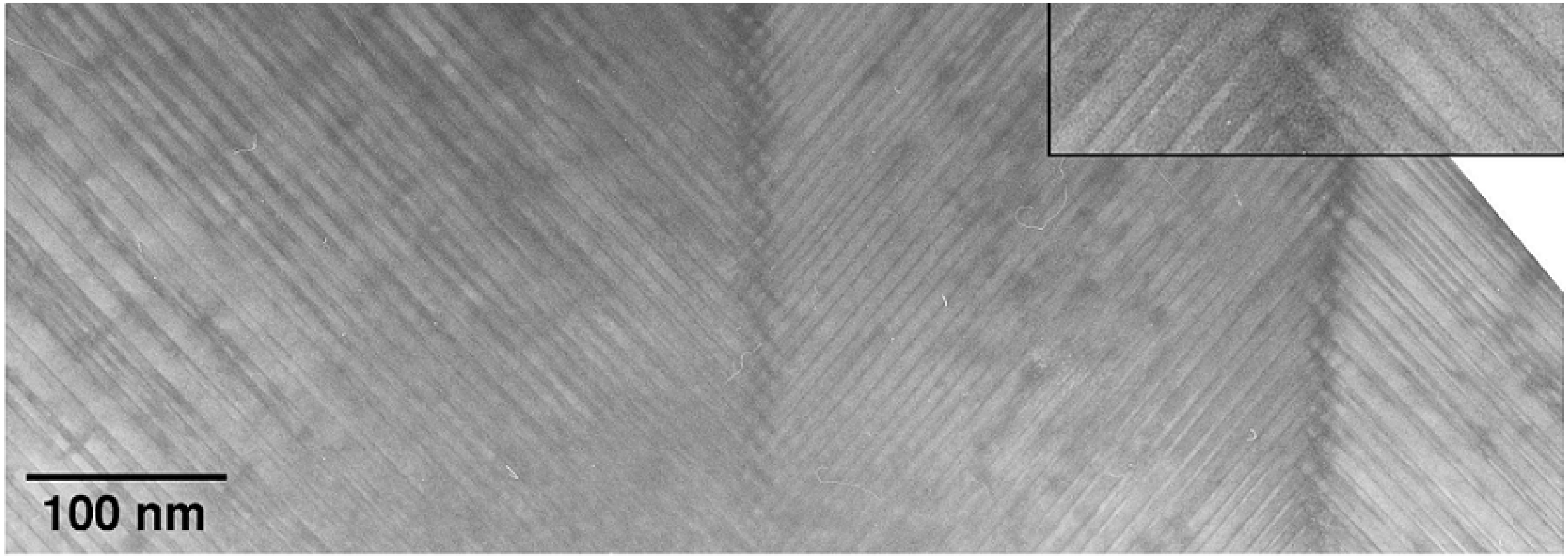
Troisième école de mécanique théorique:
Analyse Variationnelle et microstructuration
Quiberon, 22-27 September, 2014

Microstructure et interfaces dans les solides

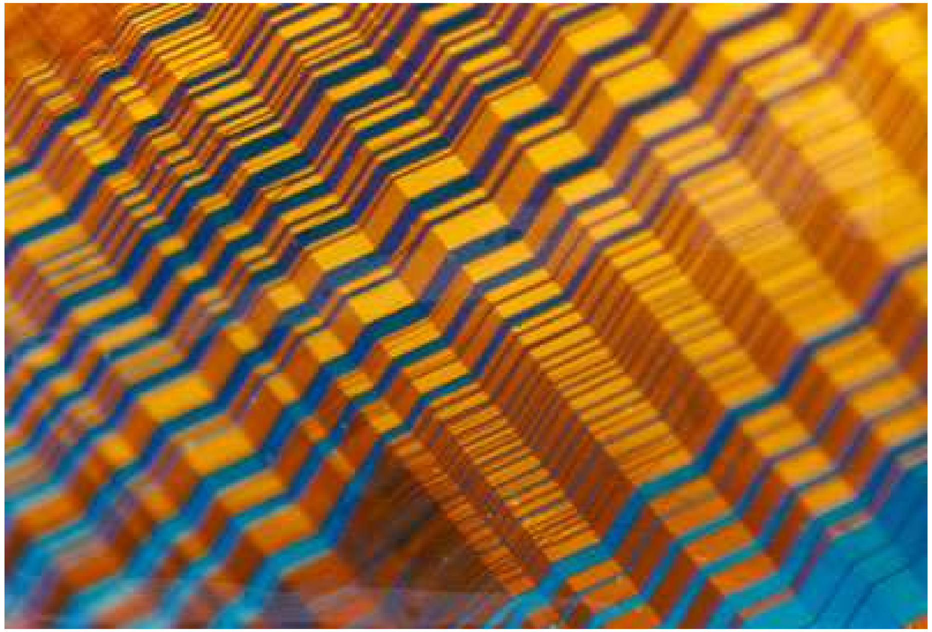
John Ball

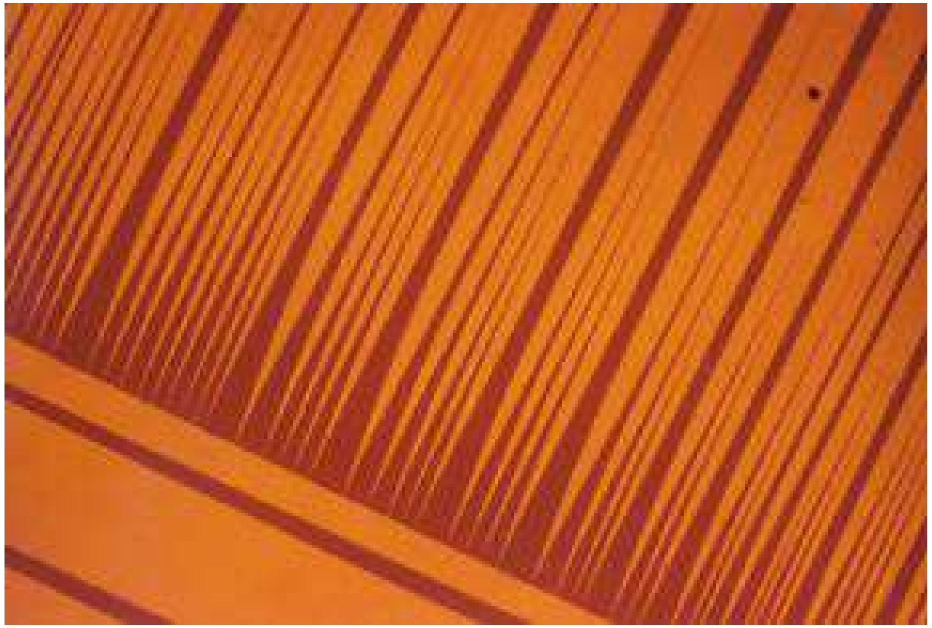
Notes à http://people.maths.ox.ac.uk/ball/teaching.shtml

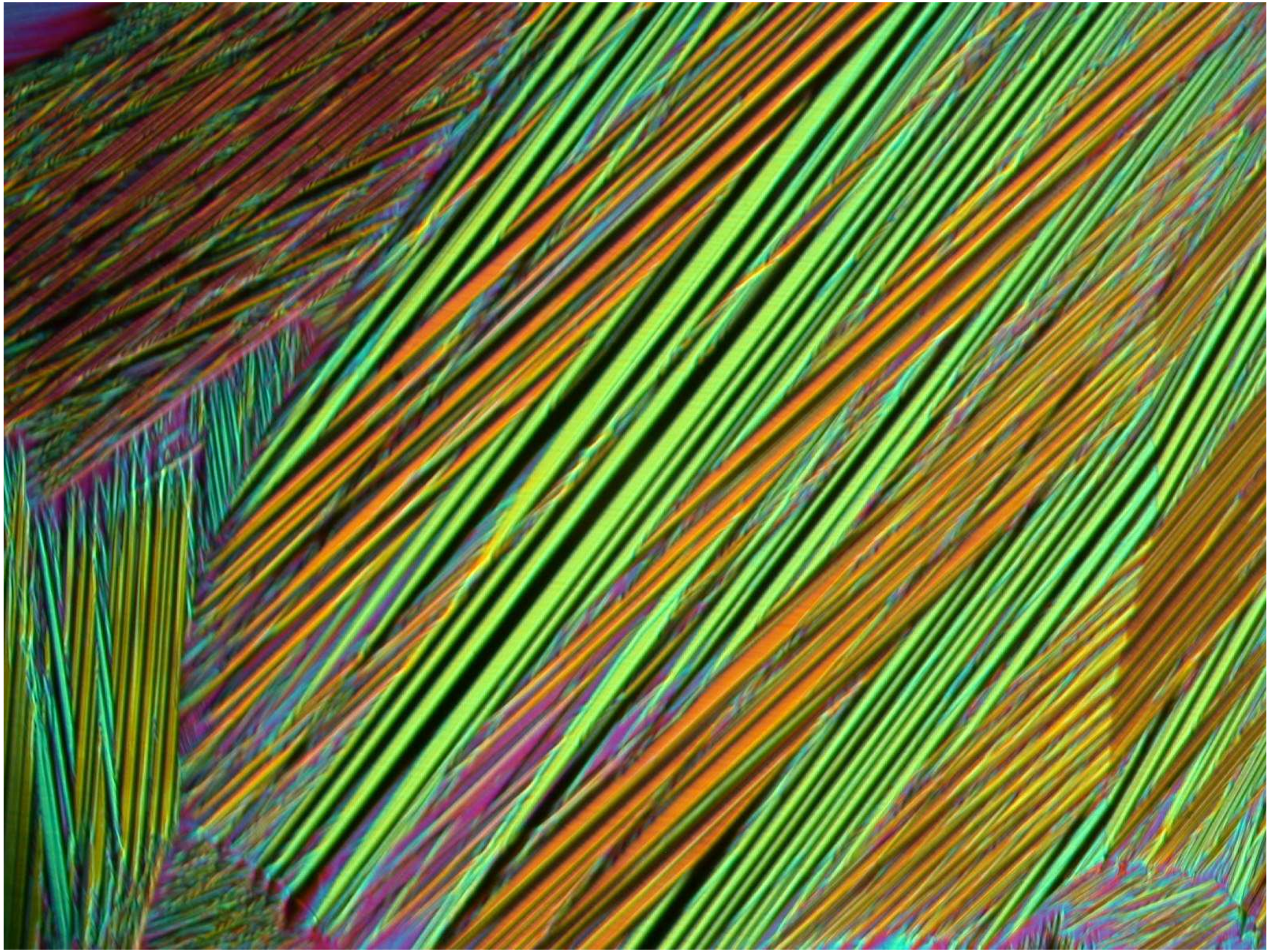
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



Martensitic microstructures in CuAlNi (Chu/James)







CuZnAl microstructure: Michel Morin (INSA de Lyon)

Plan of the course

Monday

1. Nonlinear elasticity.
2. Existence of minimizers and analysis tools.

Wednesday

3. Existence etc contd. and nonlinear elasticity model of crystals.
4. Microstructure.

Friday

5. Austenite-martensite interfaces.
6. Complex microstructures. Nucleation of austenite.

Saturday

7. Local minimizers with and without interfacial energy.

Nonlinear elasticity

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. 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. Wood and bone have a cellular structure …

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.

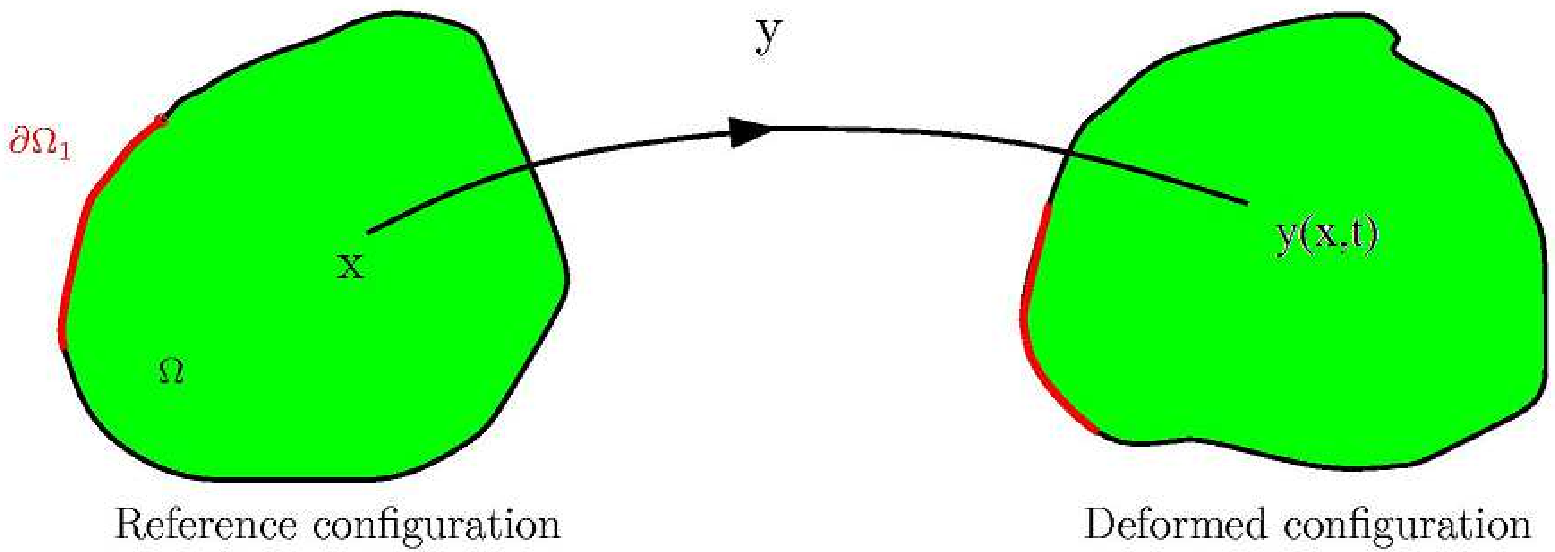
1927 A.E.H. Love, Treatise on linear elasticity

1950's R. Rivlin, Exact solutions in *incompressible* nonlinear elasticity (rubber)

1960 -- 80 Nonlinear theory clarified by J.L. Ericksen, C. Truesdell …

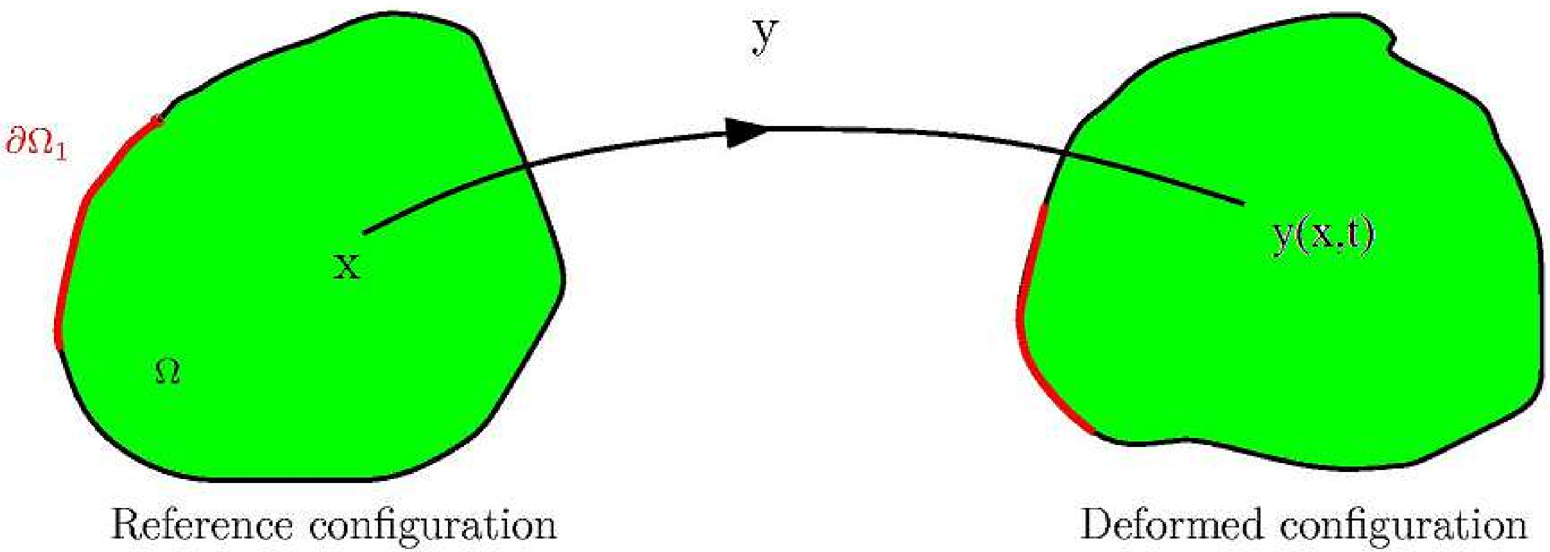
1980 -- Mathematical developments, applications to materials, biology …

Kinematics



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

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



Typical motion described by a sufficiently smooth map $y : \Omega \times [t_1, t_2] \to \mathbb{R}^3$, $y = y(x, t)$.

Deformation gradient

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

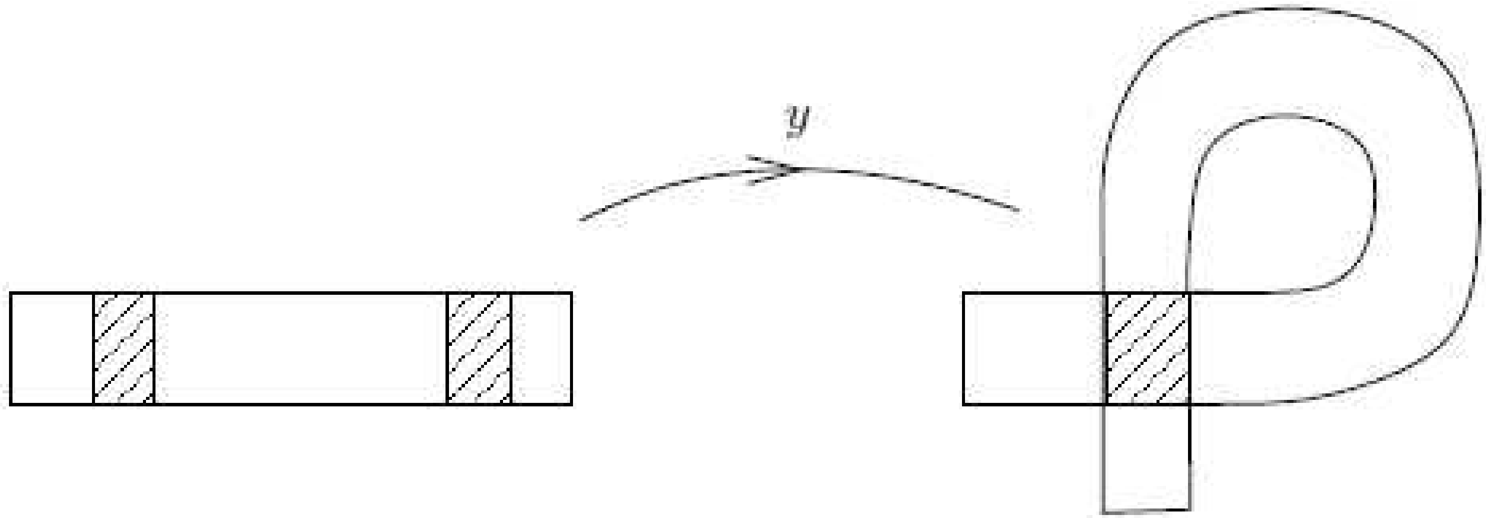
Invertibility

To avoid interpenetration of matter, we require that for each t, $y(\cdot, t)$ is invertible on Ω, with sufficiently smooth inverse $x(\cdot, t)$. We also suppose that $y(\cdot, t)$ is orientation preserving; hence

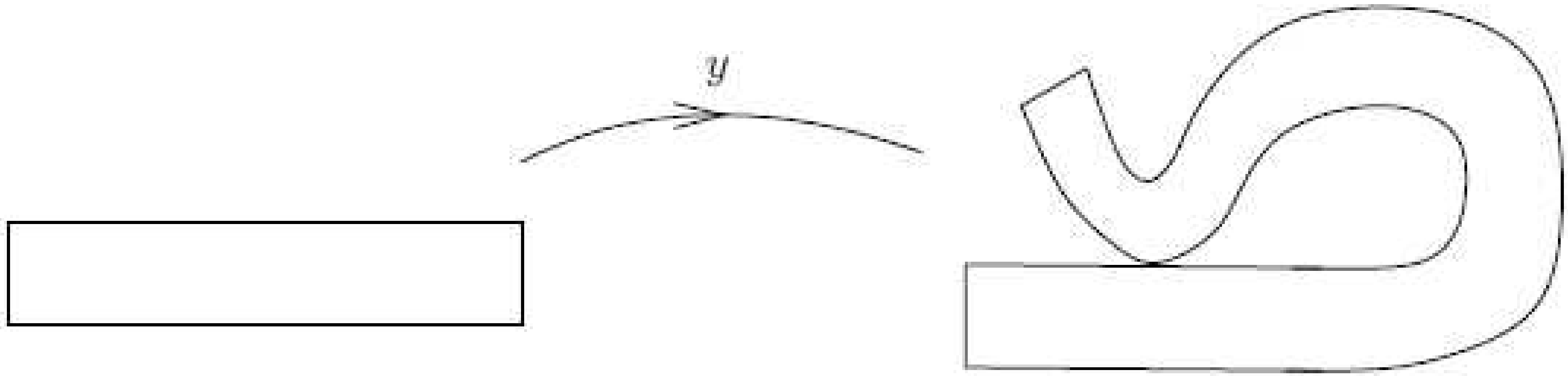
$$J = \det F(x, t) > 0 \qquad \text{for } x \in \Omega. \tag{1}$$

By the inverse function theorem, if $y(\cdot, t)$ is C^1, (1) implies that $y(\cdot, t)$ is locally invertible.

Examples.



locally invertible but not globally invertible



$y(\cdot, t)$ invertible on Ω
not on $\overline{\Omega}$

Global inverse function theorem for C^1 deformations

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

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

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

Proof uses degree theory. cf Meisters and Olech, Duke Math. J. 30 (1963) 63-80.

Notation

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

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 $c \in \mathbb{R}^3$.]

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

$$C = U^2$$

(we write $U = C^{1/2}$).

Formula for the square root

Since C is symmetric it has a spectral decomposition

$$C = \sum_{i=1}^{3} \lambda_i \widehat{e}_i \otimes \widehat{e}_i.$$

Since $C > 0$, it follows that $\lambda_i > 0$. Then

$$U = \sum_{i=1}^{3} \lambda_i^{1/2} \widehat{e}_i \otimes \widehat{e}_i$$

satisfies $U^2 = C$.

Polar decomposition theorem

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

$$F = RU = VR.$$

These representations (right and left respectively) are unique.

Proof. Suppose $F = RU$. Then $U^2 = F^T F :=$ C. Thus if the right representation exists U must be the square root of C. But if $a \in \mathbb{R}^3$ is nonzero, $Ca \cdot a = |Fa|^2 > 0$, since F is nonsingular. Hence $C > 0$. So by the square root theorem, $U = C^{1/2}$ exists and is unique.
Let $R = FU^{-1}$. Then

$$R^T R = U^{-1} F^T F U^{-1} = 1$$

and $\det R = \det F (\det U)^{-1} = +1$.
The representation $F = VR_1$ is obtained similarly using $B := FF^T$, and it remains to prove $R = R_1$. But this follows from $F = R_1 \left(R_1^T V R_1 \right)$, and the uniqueness of the right representation.

Strain tensors and singular values

For $F = Dy$, U and V are the *right* and *left stretch tensors*; $C = U^2 = F^T F$ and $B = V^2 = FF^T$ are the *right and left Cauchy–Green strain (tensors)* respectively.

The strictly positive eigenvalues v_1, v_2, v_3 of U (or V) are the *principal stretches* (= singular values of F).

Invariants

The characteristic polynomial of C is given by

$$\begin{aligned} \det(C - \lambda 1) &= -\lambda^3 + I_C\lambda^2 - II_C\lambda + III_C. \\ &= (v_1^2 - \lambda)(v_2^2 - \lambda)(v_3^2 - \lambda) \end{aligned}$$

Hence

$$\begin{aligned} I_C &= v_1^2 + v_2^2 + v_3^2 = \operatorname{tr} C \\ II_C &= v_1^2 v_2^2 + v_2^2 v_3^2 + v_3^2 v_1^2 \\ III_C &= (v_1 v_2 v_3)^2 = \det C. \end{aligned}$$

Note that the invariants of B are the same as those of C.

State of strain

Fix x, t. Then

$$y(x+z,t) = y(x,t) + F(x,t)z + o(|z|).$$

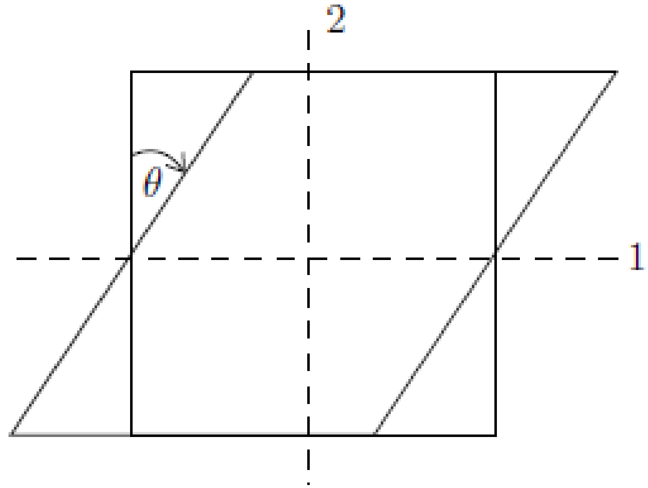
Thus to first order in z the deformation is given by a rotation followed by a stretching of amounts v_i along mutually orthogonal axes, or vice versa. Equivalently, since

$$F = RU = RQDQ^T = \tilde{R}DQ^T,$$

where $D = \mathrm{diag}\,(v_1, v_2, v_3)$, it is given by a rotation, followed by stretching along the coordinate axes, then another rotation.

Example: simple shear

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



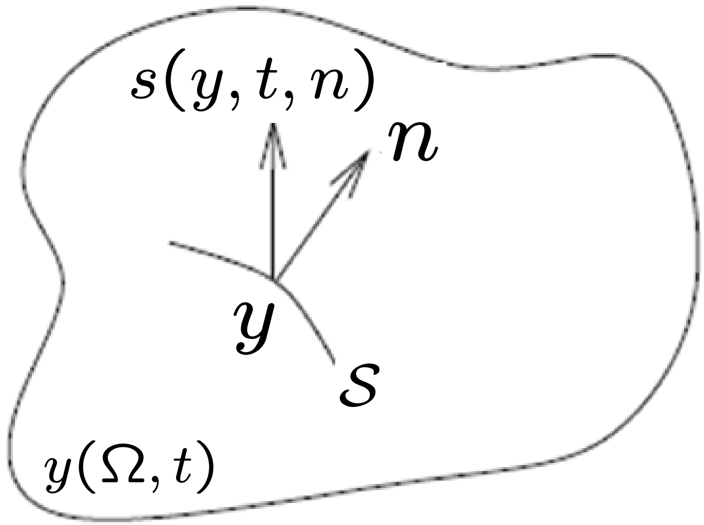
$\gamma = \tan\theta$

$\theta =$ angle of shear

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

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

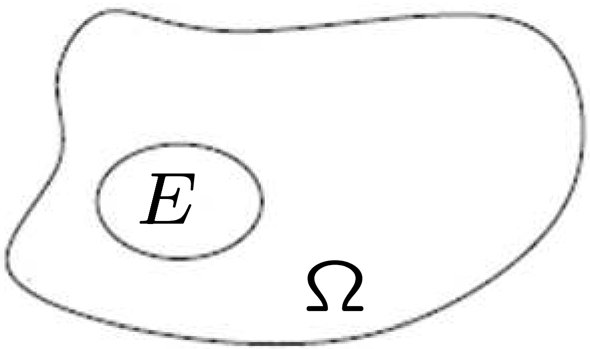
Cauchy's stress hypothesis

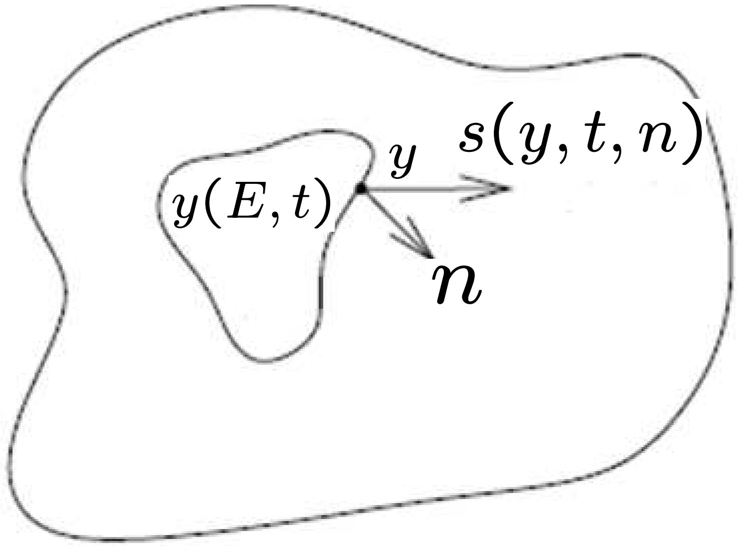


There is a vector field $s(y,t,n)$ (the *Cauchy stress vector*) that gives the force per unit area exerted across a smooth oriented surface $\mathcal{S}$ on the material on the negative side of $\mathcal{S}$ by the material on the positive side.

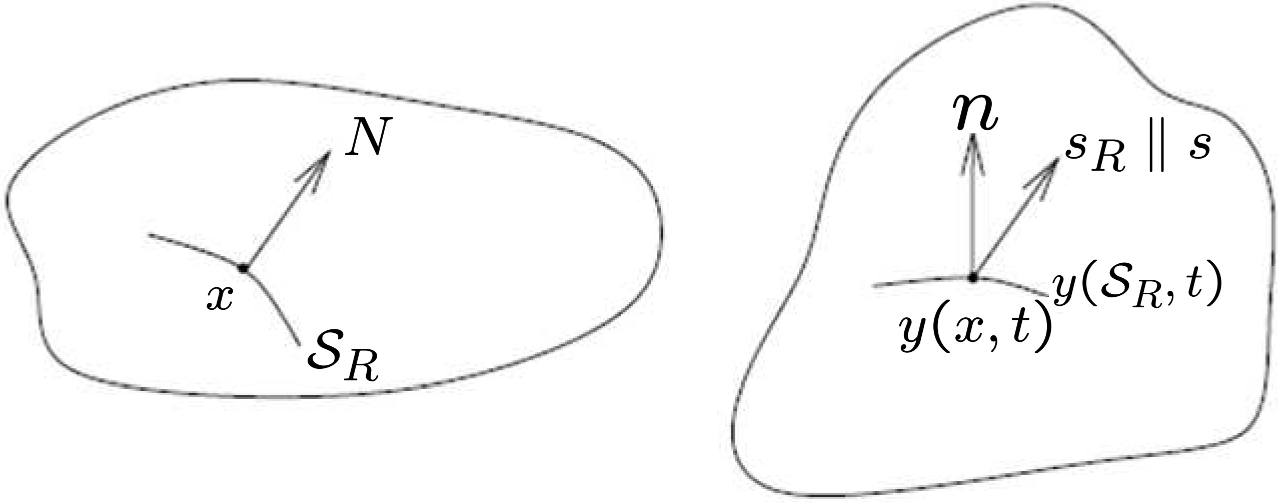
Resultant surface force on $y(E,t)$ is given by

$$\int_{\partial y(E,t)} s(y,t,n)\,da.$$





Piola-Kirchhoff stress vector



The *Piola–Kirchhoff stress vector* $s_R(x, t, N)$ is parallel to the Cauchy stress vector s, but measures the surface force per unit area *in the reference configuration*, acting across the (deformed) surface $y(\mathcal{S}_R, t)$ having normal N in the reference configuration.

So the resultant surface force on $y(E,t)$ can also be expressed as

$$\int_{\partial E} s_R(x,t,N)\,dA.$$

The change of variables formula

$$n\,da = (\mathrm{cof}\,F)N\,dA.$$

relates the normal n and area element da in the deformed configuration to the normal N and area element dA in the reference configuration.

Balance law of linear momentum

$$\frac{d}{dt}\int_E \rho_R v\, dx = \int_{\partial E} s_R(x,t,N)\, dA + \int_E \rho_R b\, dx,$$

for all E, where $v(x,t) = \dot{y}(x,t)$ is the velocity and $b = b(y,t)$ is the body force density.

Cauchy showed that this implies that s_R is *linear* in N, i.e.

$$s_R(x,t,N) = T_R(x,t)N$$

where the second order tensor (matrix) T_R is called the *Piola-Kirchhoff stress tensor*.

The Cauchy stress tensor

$$\begin{aligned} s_R\,dA &= T_R N\,dA \\ &= T_R(\mathrm{cof}\,F)^{-1}n\,da \\ &= T_R J^{-1}F^T n\,da \\ &= s\,da \end{aligned}$$

Hence $s(y,t) = T(y,t)n$, where the *Cauchy stress tensor* T is given by

$$T = J^{-1}T_R F^T.$$

T symmetric if and only balance of angular momentum holds.

Balance of Energy

$$\frac{d}{dt}\int_E \left(\frac{1}{2}\rho_R|y_t|^2 + \varepsilon\right)\,dx \;=\; \int_E b\cdot y_t\,dx + \int_{\partial E} t_R\cdot y_t\,dA \;+\; \int_E r\,dx - \int_{\partial E} q_R\cdot N\,dA, \quad (1)$$

for all $E \subset \Omega$, where $\rho_R = \rho_R(x)$ is the density in the reference configuration, ε is the internal energy density, b is the body force, t_R is the Piola-Kirchhoff stress vector, q_R the reference heat flux vector and r the heat supply.

Second Law of Thermodynamics

We assume this holds in the form of the *Clausius-Duhem inequality*

$$\frac{d}{dt}\int_E \eta\,dx \geq -\int_{\partial E}\frac{q_R\cdot N}{\theta}\,dS + \int_E \frac{r}{\theta}\,dx \quad (2)$$

for all E, where η is the entropy and θ the temperature.

Thermoelasticity

For a *homogeneous* *thermoelastic material* we assume that $T_R, q_R, \varepsilon, \eta$ are functions of $F, \theta, \nabla\theta$.

Define the *Helmholtz free energy* by $\psi = \varepsilon - \theta\eta$. Then a classical procedure due to Coleman and Noll shows that in order for such constitutive equations to be consistent with the Second Law, we must have

$$\psi = \psi(F, \theta), \quad \eta = -D_\theta\psi, \; T_R = D_F\psi.$$

The Ballistic Free Energy

Suppose that the the mechanical boundary conditions are that $y = y(x,t)$ satisfies $y(\cdot,t)|_{\partial\Omega_1} = \bar{y}(\cdot)$ and the condition that the applied traction on $\partial\Omega_2 = \partial\Omega \setminus \partial\Omega_1$ is zero, and that the thermal boundary condition is

$$\theta(\cdot,t)|_{\partial\Omega_3} = \theta_0,\ q_R \cdot N|_{\partial\Omega\setminus\partial\Omega_3} = 0,$$

where $\theta_0 > 0$ is a *constant*. Assume that the heat supply r is zero, and that the body force is given by $b = -\mathrm{grad}_y h(x,y)$, Thus from (1), (2) with $E = \Omega$ and the boundary conditions

$$\frac{d}{dt}\int_\Omega \left[\frac{1}{2}\rho_R|y_t|^2 + \varepsilon - \theta_0\eta + h\right] dx \;\; \leq$$

$$\int_{\partial\Omega} t_R \cdot y_t \, dS - \int_{\partial\Omega}\left(1 - \frac{\theta_0}{\theta}\right) q_R \cdot N \, dS \;\; = \;\; 0.$$

So $\mathcal{E} = \int_\Omega \left[\frac{1}{2}\rho_R|y_t|^2 + \varepsilon - \theta_0\eta + h\right] dx$ is a Lyapunov function. (Note that it is not the Helmholtz free energy $\psi(F,\theta) = \varepsilon(F,\theta) - \theta\eta(F,\theta)$ that appears in the expression for $\mathcal{E}$ but $\varepsilon(F,\theta) - \theta_0\eta(F,\theta)$, where θ_0 is the boundary temperature.)

Thus it is reasonable to suppose that typically (y_t, y, θ) tends as $t \to \infty$ to a (local) minimizer of $\mathcal{E}$. If the dynamics and boundary conditions are such that as $t \to \infty$ we have $y_t \to 0$ and $\theta \to \theta_0$, then this is close to saying that y tends to a local minimizer of

$$I_{\theta_0}(y) = \int_\Omega [\psi(Dy, \theta_0) + h(x, y)]\, dx.$$

(The calculation given follows work of Duhem, Ericksen and Coleman & Dill.)

Of course a lot of work would be needed to justify this (we would need well-posedness of suitable dynamic equations plus information on asymptotic compactness of solutions and more; this is currently out of reach). And what if the minimum of the energy is not attained?

For some remarks on the case when θ_0 depends on x see J.M. Ball and G. Knowles, *Lyapunov functions for thermoelasticity with spatially varying boundary temperatures*. Arch. Rat. Mech. Anal., 92:193–204, 1986.

Variational formulation of nonlinear elastostatics

The preceding calculation motivates seeking a deformation $y = y(x)$ minimizing the total free energy at temperature θ given by

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

subject to suitable boundary conditions, where we have assumed for simplicity that the body-force potential is zero.

We regard θ as a constant parameter (no heat conduction etc).

Properties of ψ

Assume

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

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

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

Hence $\psi(F,\theta) = \psi(RU,\theta) = \psi(U,\theta) = \tilde{\psi}(C,\theta)$.

Frame-indifference implies T symmetric

Hence balance of angular momentum is automatically satisfied.

Proof. Let K be skew. Then

$$\begin{aligned} 0 &= \frac{d}{dt}\psi(e^{Kt}F,\theta)|_{t=0} \\ &= D_F\psi(e^{Kt}F,\theta)\cdot Ke^{Kt}F|_{t=0} \\ &= J\mathrm{tr}\,(TK^T) \\ &= JT_{ij}K_{ij}, \end{aligned}$$

where we used that $T = J^{-1}T_RF^T$.

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 $H \in M_+^{3\times3}$ do not change ψ? That is, for which H do we have

$$\psi(F,\theta) = \psi(FH,\theta) \qquad \text{for all } F \in M_+^{3\times3}?$$

These H form a subgroup $\mathcal{S}$ of $M_+^{3\times3}$, 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

The following conditions are equivalent:

(i) ψ is isotropic;

(ii) $\psi(F,\theta) = h(I_B, II_B, III_B, \theta)$ for some h;

(iii) $\psi(F,\theta) = \Phi(v_1, v_2, v_3, \theta)$ for some Φ that is symmetric with respect to permutations of v_1, v_2, v_3;

(iv) $T(F,\theta) = a_0 1 + a_1 B + a_2 B^2$, where a_0, a_1, a_2 are scalar functions of I_B, II_B, III_B and θ (Rivlin–Ericksen representation)

Linear elasticity

This is not a special case of nonlinear elasticity but a linearization of it about a stress free state, taken to be the reference configuration, so that $T_R(1,\theta) = D_F\psi(1,\theta) = 0$.

We write $y(x,t) = x + u(x,t)$ where $u(x,t)$ is the *displacement*. Then

$$F(x,t) = 1 + \nabla u(x,t),$$

and we seek a theory that applies when ∇u is small.

The elasticity tensor

Writing $F = 1 + H$ and assuming $\psi(\cdot, \theta)$ is C^2 near 1 we have that

$$\begin{aligned}\psi(1+H,\theta) &= \psi(1,\theta) + \frac{1}{2}D_F^2\psi(1,\theta)(H,H) + o(|H|^2)\\ T_R(1+H,\theta) &= D_F T_R(1,\theta)\cdot H + o(|H|).\end{aligned}$$

Set $C(\theta) = D_F T_R(1,\theta) = D_F^2\psi(1,\theta)$ (*elasticity tensor*). Thus $C : M^{3\times 3} \to M^{3\times 3}$, with

$$(C(\theta)H)_{ij} = c_{ijkl}(\theta)H_{kl}$$

where the *elasticities*

$$c(\theta)_{ijkl} = \frac{\partial^2\psi}{\partial F_{ij}\partial F_{kl}}(1,\theta).$$

Symmetries of the elasticity tensor

Major symmetries $c_{ijkl} = c_{klij}$

Minor symmetries (frame indifference)

$c_{ijkl} = c_{jikl} = c_{ijlk}$

Isotropy: linearized stress given by

$Ce = 2\mu e + \lambda(\mathrm{tr}\, e)\, 1$, where $e = \frac{1}{2}(Du + (Du)^T)$,

and λ, μ are the Lamé constants.

Exercise

A homogeneous isotropic elastic body in a stress-free state in the reference configuration is rigidly rotated through an angle θ, so that the deformation is $y(x) = R(\theta)x$, where

$$R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Show that according to nonlinear elasticity the body remains stress-free ...

... but that according to linear elasticity the Cauchy stress has the form

$$T = -2(1-\cos\theta)\begin{pmatrix} \lambda+\mu & 0 & 0 \\ & \lambda+\mu & 0 \\ 0 & 0 & \lambda \end{pmatrix}.$$

For a certain mild steel, $\lambda = 102.9$GPa, $\mu = 80.86$GPa. Calculate the value of θ for which the maximum 'phantom' stress $(=|T_{11}|)$ reaches the value 465×10^{-3}GPa (which would in tension cause fracture of the material).

Lecture 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

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

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

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

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

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

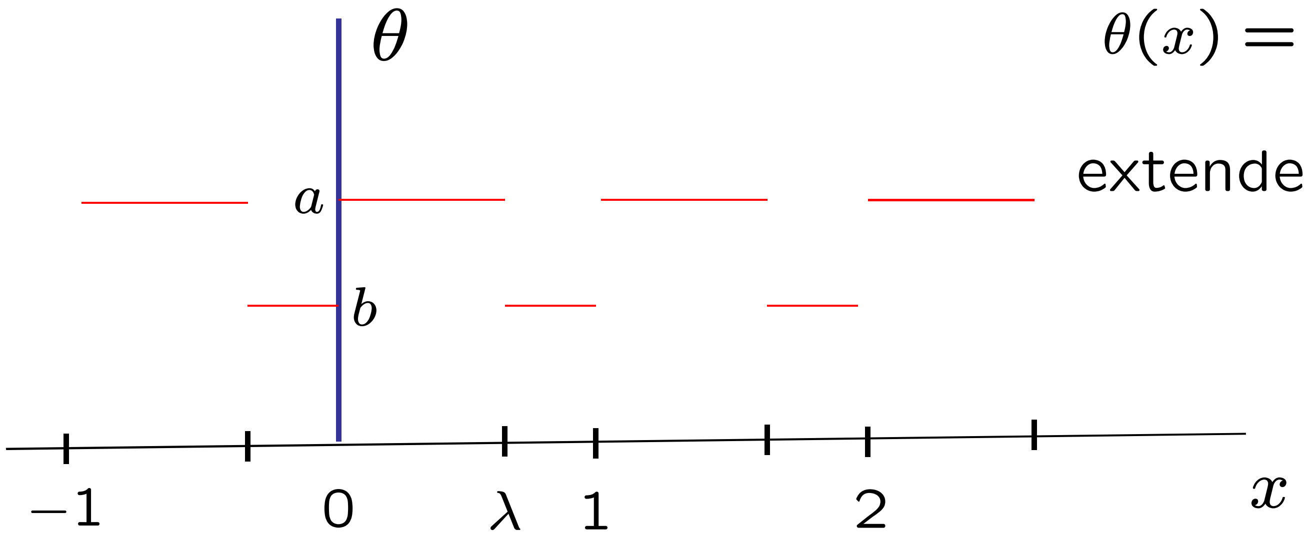
where $\frac{1}{p} + \frac{1}{p'} = 1$.

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 $\mathbb{R}$.

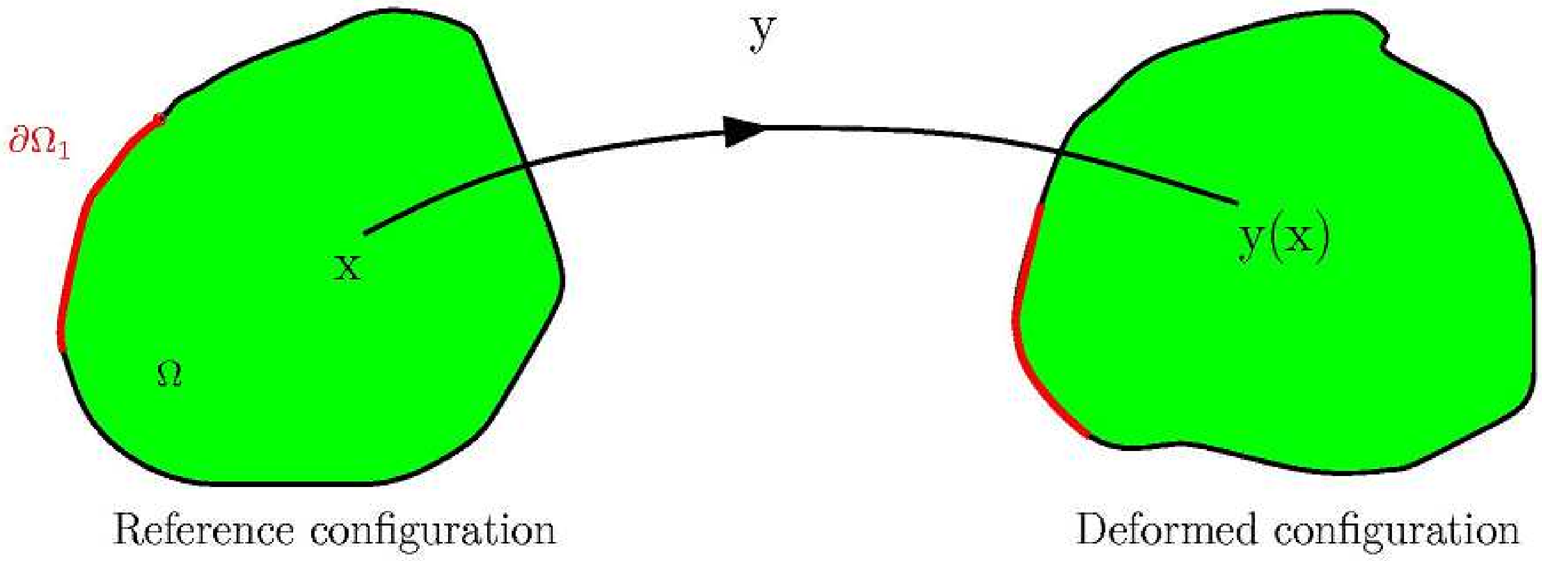
Exercise. Define $\theta^{(j)}(x) = \theta(jx)$.

(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 $\stackrel{*}{\rightharpoonup}$ if $p = \infty$).

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



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

Writing $W(F) = \psi(F, \theta)$ we want to minimize

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

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 for the time being 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) $\quad W : M_+^{3\times 3} \to [0,\infty)$ is C^1,

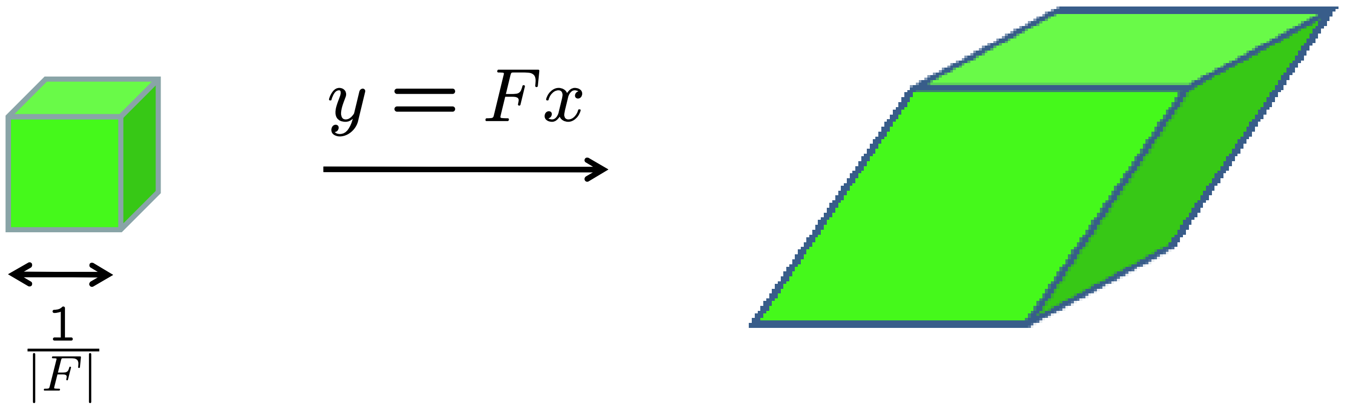
(H2) $\quad W(F) \to \infty$ as $\det F \to 0+$,

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

(H3) $\quad W(RF) = W(F)$ 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



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

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

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

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

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

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 W is never convex

(Recall that W is convex if

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

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

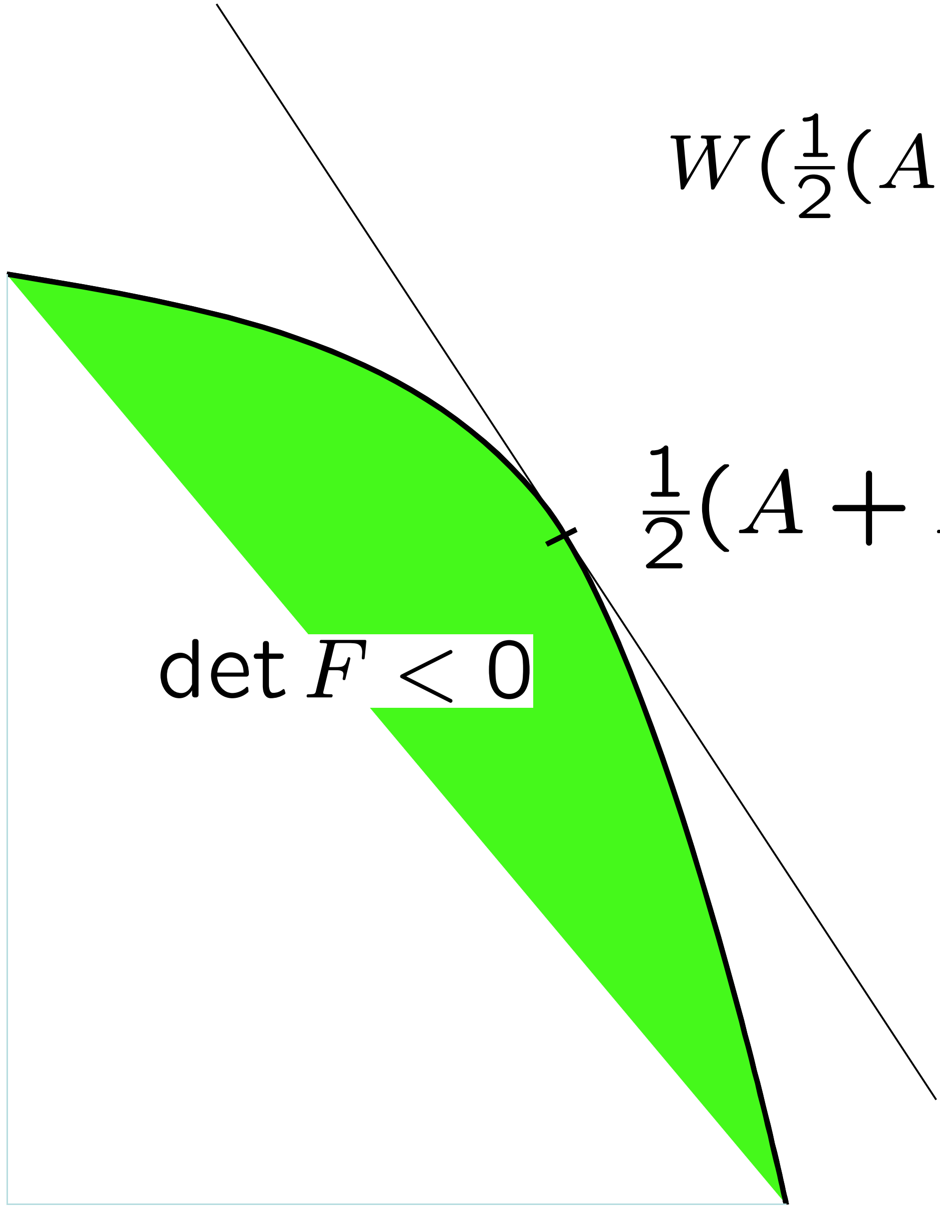
Reasons

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

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

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

$W(\frac{1}{2}(A+B)) = \infty$
$> \frac{1}{2}W(A) + \frac{1}{2}W(B)$



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

$\det F > 0$

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

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

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

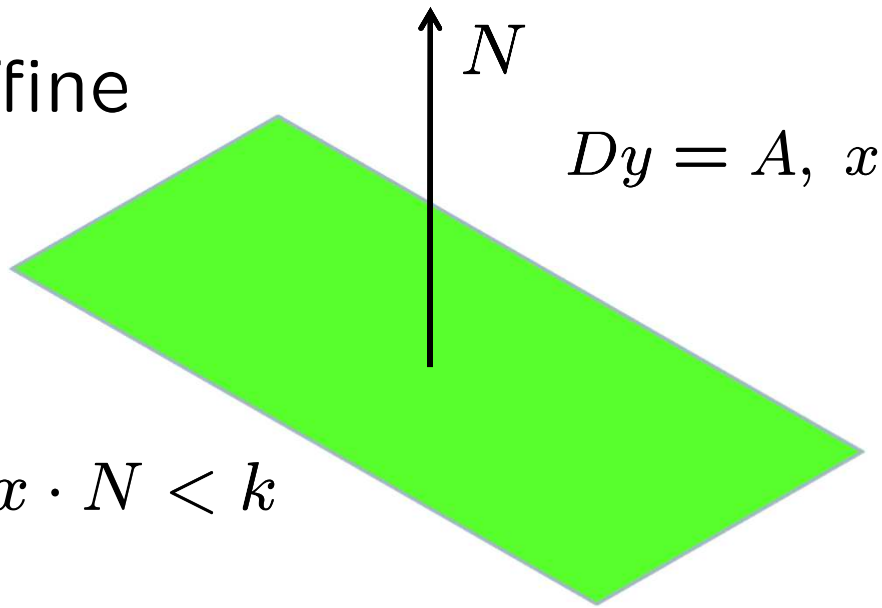
Proof.

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

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

Rank-one matrices and the Hadamard jump condition

y piecewise affine

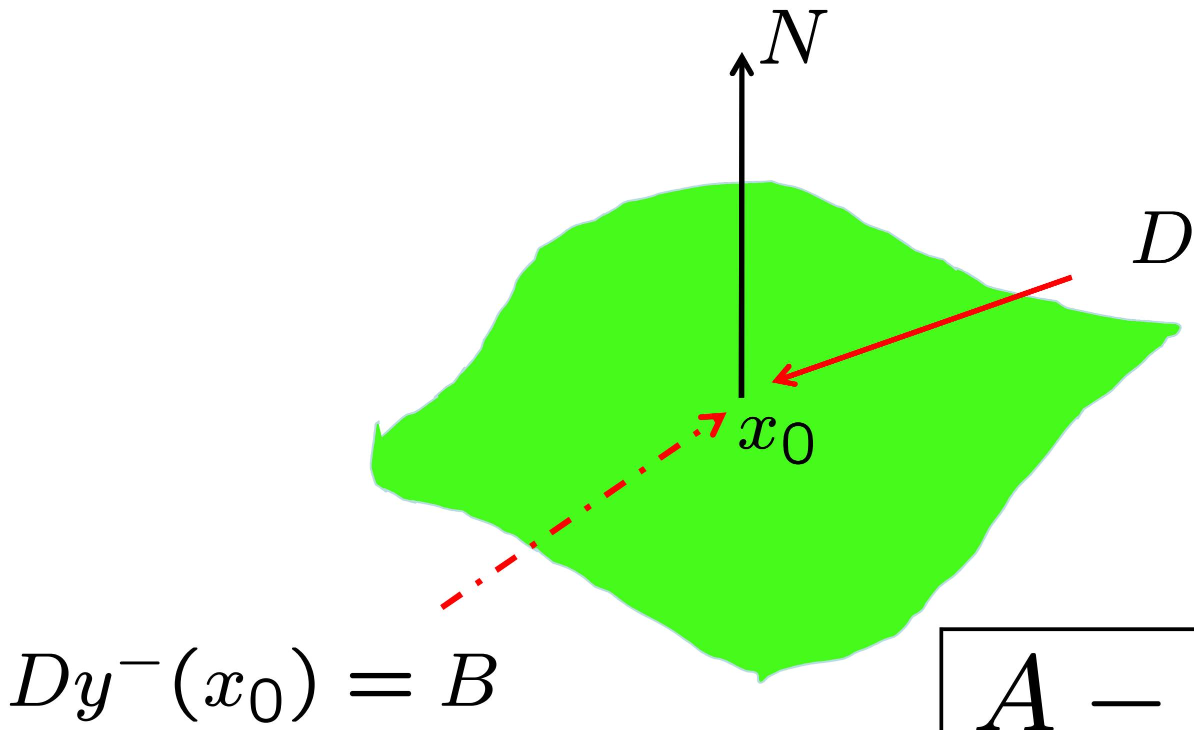


Let $C = A - B$. Then $Cx = 0$ if $x \cdot N = 0$. Thus $C(z - (z \cdot N)N) = 0$ for all z, and so $Cz = (CN \otimes N)z$. Hence

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

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

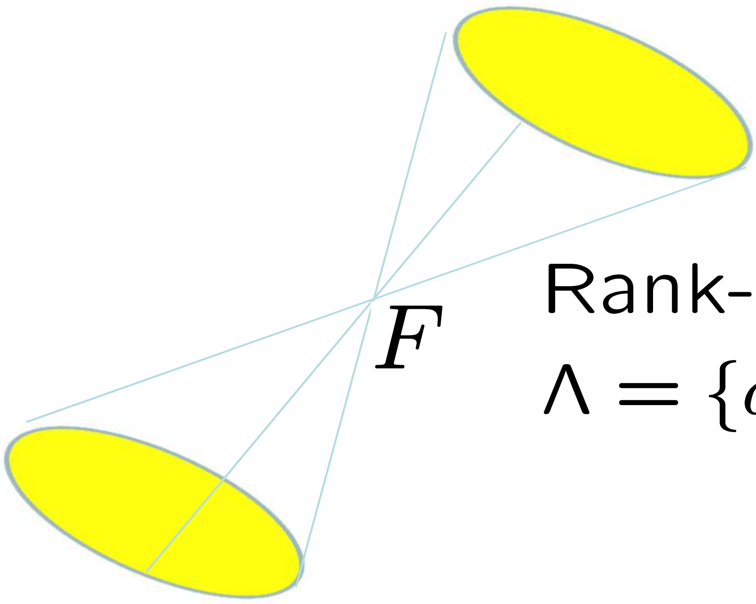
W is *rank-one convex* if the map $t \mapsto W(F + ta \otimes N)$ is convex for each $F \in M^{3\times 3}$ and $a \in \mathbb{R}^3, N \in \mathbb{R}^3$.

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

Equivalently,

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

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

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

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

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

(Legendre-Hadamard condition).

Quasiconvexity (C.B. Morrey,1952)

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

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

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 W is quasiconvex if for any $F \in M^{3\times 3}$ the pure displacement problem to minimize

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

subject to the linear boundary condition

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

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

Another form of the definition that is equivalent for finite continuous W is that

$$\int_Q W(Dy)\,dx \geq (\mathrm{meas}\,Q)W(F)$$

for any $y \in W^{1,\infty}$ such that Dy is the restriction to a cube Q (e.g. $Q = (0,1)^n$) of a Q-periodic map on $\mathbb{R}^n$ with $\frac{1}{\mathrm{meas}\,Q}\int_Q Dy\,dx = F$.

One can even replace periodicity with almost periodicity (see J.M. Ball, J.C. Currie, and P.J. Olver, J. Functional Anal., 41:135–174, 1981).

Theorem
If W is continuous and quasiconvex then W is rank-one convex.

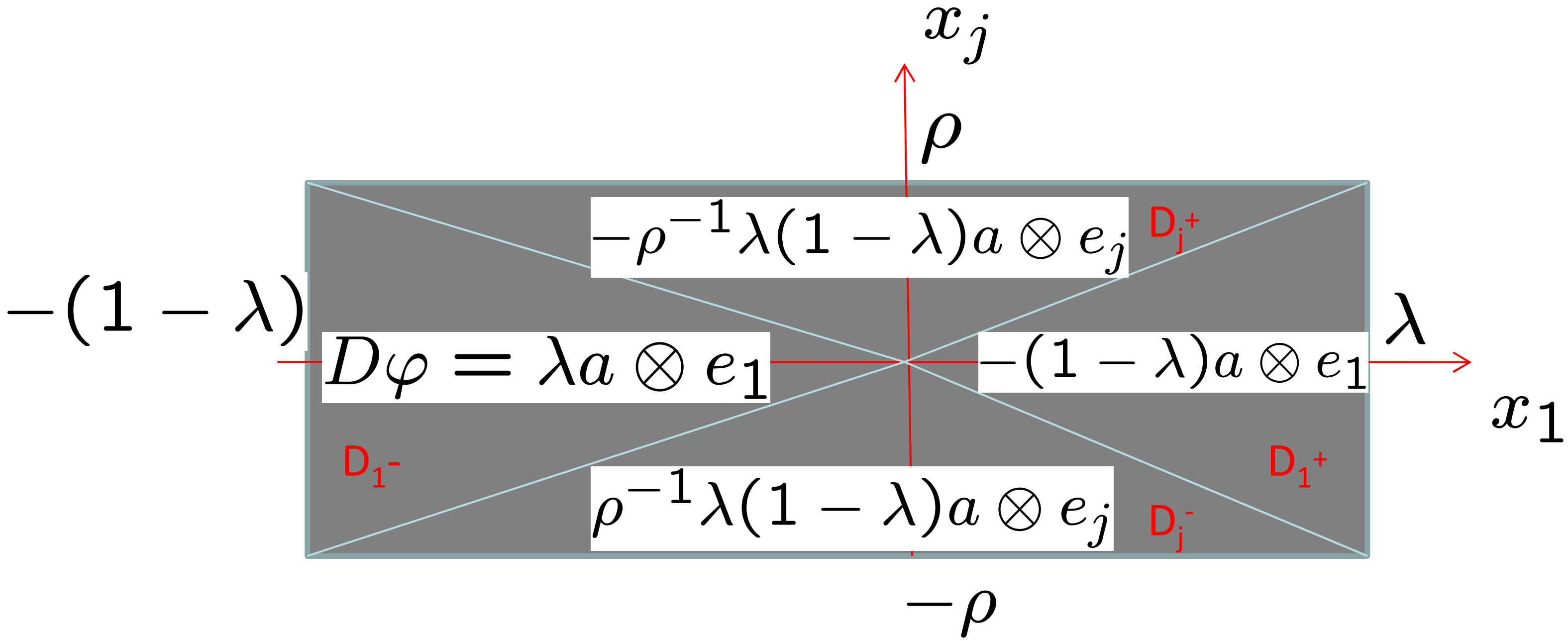
Proof
We prove that

$$W(F) \leq \lambda W(F-(1-\lambda)a\otimes N)+(1-\lambda)W(F+\lambda a\otimes N)$$

for any $F \in M^{m\times n}, a \in \mathbb{R}^m, N \in \mathbb{R}^n, \lambda \in (0,1)$.

Without loss of generality we suppose that $N = e_1$. We follow an argument of Morrey.

Let $D = (-(1-\lambda), \lambda) \times (-\rho, \rho)^{n-1}$ and let $D_j^{\pm}$ be the pyramid that is the convex hull of the origin and the face of D with normal $\pm e_j$.



Let $\varphi \in W_0^{1,\infty}(D; \mathbb{R}^m)$ be affine in each $D_j^{\pm}$ with $\varphi(0) = \lambda(1-\lambda)a$.

The values of $D\varphi$ are shown.

By quasiconvexity

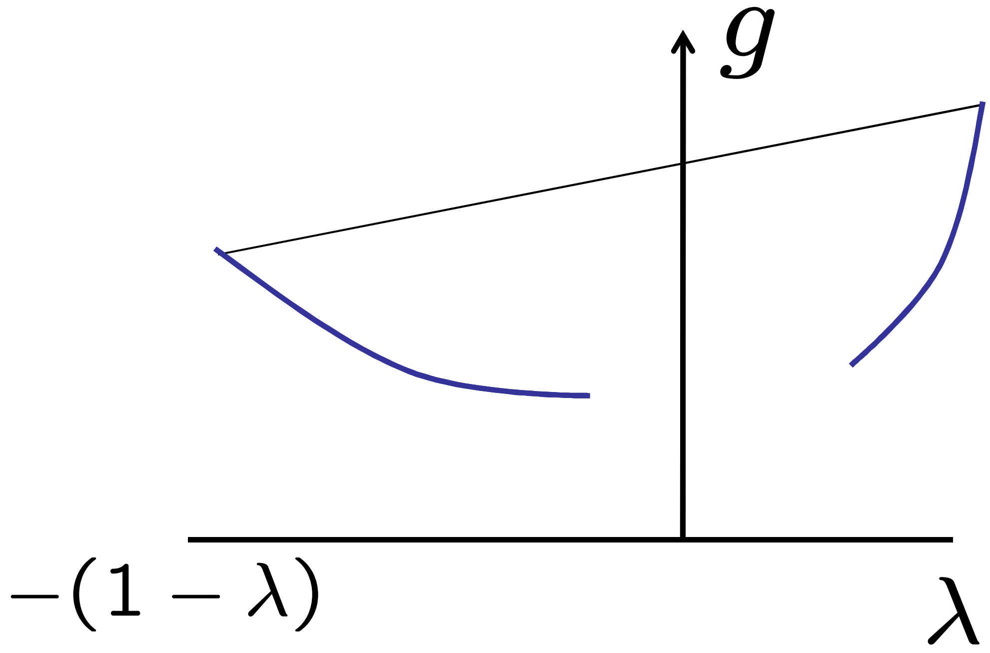
$$
\begin{aligned}
(2\rho)^{n-1}W(F) \leq \frac{(2\rho)^{n-1}\lambda}{n}&W(F-(1-\lambda)a\otimes e_1) \\
+\frac{(2\rho)^{n-1}(1-\lambda)}{n}&W(F+\lambda a\otimes e_1) \\
+\sum_{j=2}^{n}\frac{(2\rho)^{n-1}}{2n}&[W(F+\rho^{-1}\lambda(1-\lambda)a\otimes e_j) \\
&+W(F-\rho^{-1}\lambda(1-\lambda)a\otimes e_j)]
\end{aligned}
$$

Suppose $W(F)<\infty$. Then dividing by $(2\rho)^{n-1}$, letting $\rho\to\infty$ and using the continuity of W, we obtain

$$
W(F)\leq\lambda W(F-(1-\lambda)a\otimes e_1)+(1-\lambda)W(F+\lambda a\otimes e_1)
$$

as required.

Now suppose that $W(F-(1-\lambda)a\otimes e_1)$ and $W(F+\lambda a\otimes e_1)$ are finite. Then $g(\tau)=W(F+\tau a\otimes e_1)$ lies below the chord joining the points $(-(1-\lambda), g(-(1-\lambda))), (\lambda, g(\lambda))$ whenever $g(\tau)<\infty$, and since g is continuous it follows that $g(0)=W(F)<\infty$.



Corollary

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

Proof.

If $m = 1$ or $n = 1$ then rank-one convexity is the same as convexity. If W is convex (for any dimensions) then W is quasiconvex by Jensen's inequality:

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

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

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

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

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

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

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 $\operatorname{Div} D_F L(Du) = 0$ 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).

Polyconvexity

Definition

W 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

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

Lecture 3

Existence etc contd. and nonlinear elasticity model of crystals

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

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

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

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

Remark

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

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

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

$$W \text{ convex} \underset{}{\overset{\not\Leftarrow\ W=\det}{\Rightarrow}} W \text{ polyconvex} \overset{\not\Leftarrow\ \text{Zhang}}{\Rightarrow} W \text{ quasiconvex}$$

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

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 W 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
W quasiconvex $\Leftrightarrow$ W 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 W).

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 W is everywhere finite, whereas this is contradicted by (H2).

Existence based on polyconvexity

We will show that it is possible to prove the existence of minimizers for mixed boundary value problems if we assume W 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.

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

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

where $\alpha_i, \beta_i, p_i, q_i$ are constants and h 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

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

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),

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

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.

Invertibility

We cheated and replaced the physical requirement that y be invertible (non-interpenetration of matter) with the local condition $\det Dy(x) > 0$.

For pure displacement boundary-value problems, i.e. $y|_{\partial\Omega} = \bar{y}|_{\partial\Omega}$, there are extensions of the global inverse function theorem for C^1 maps to mapping belonging to Sobolev spaces (JB 1981, Šverák 1988)

For mixed boundary-value problems P.G. Ciarlet and J. Nečas (1985) proposed minimizing

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

subject to the boundary condition $y|_{\partial\Omega_1} = \bar{y}$ and the global constraint

$$\int_\Omega \det Dy(x)\, dx \leq \text{volume}\,(y(\Omega)),$$

They showed that IF a minimizer y^* is sufficiently smooth then this constraint corresponds to smooth self-contact.

They then proved the existence of minimizers satisfying the constraint for mixed boundary conditions under the growth condition

$$W(F) \geq c_0(|F|^p + |\mathrm{cof}\, F|^q + (\det F)^{-s}) - c_1,$$

with $p > 3, q \geq \frac{p}{p-1}, s > 0$. (The point is to show that the constraint is weakly closed.)

Martensitic phase transformations

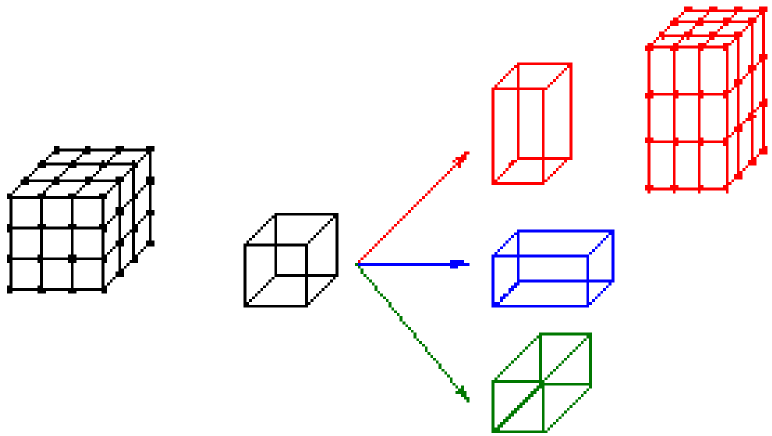
These involve a change of shape of the crystal lattice of some alloy at a critical temperature.

e.g. cubic to tetragonal

$\theta > \theta_c$

cubic

austenite

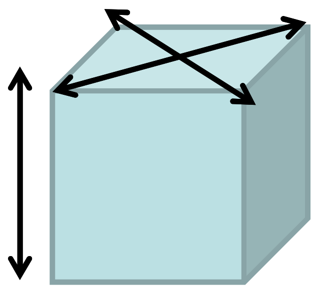


$\theta < \theta_c$

three tetragonal variants

of martensite

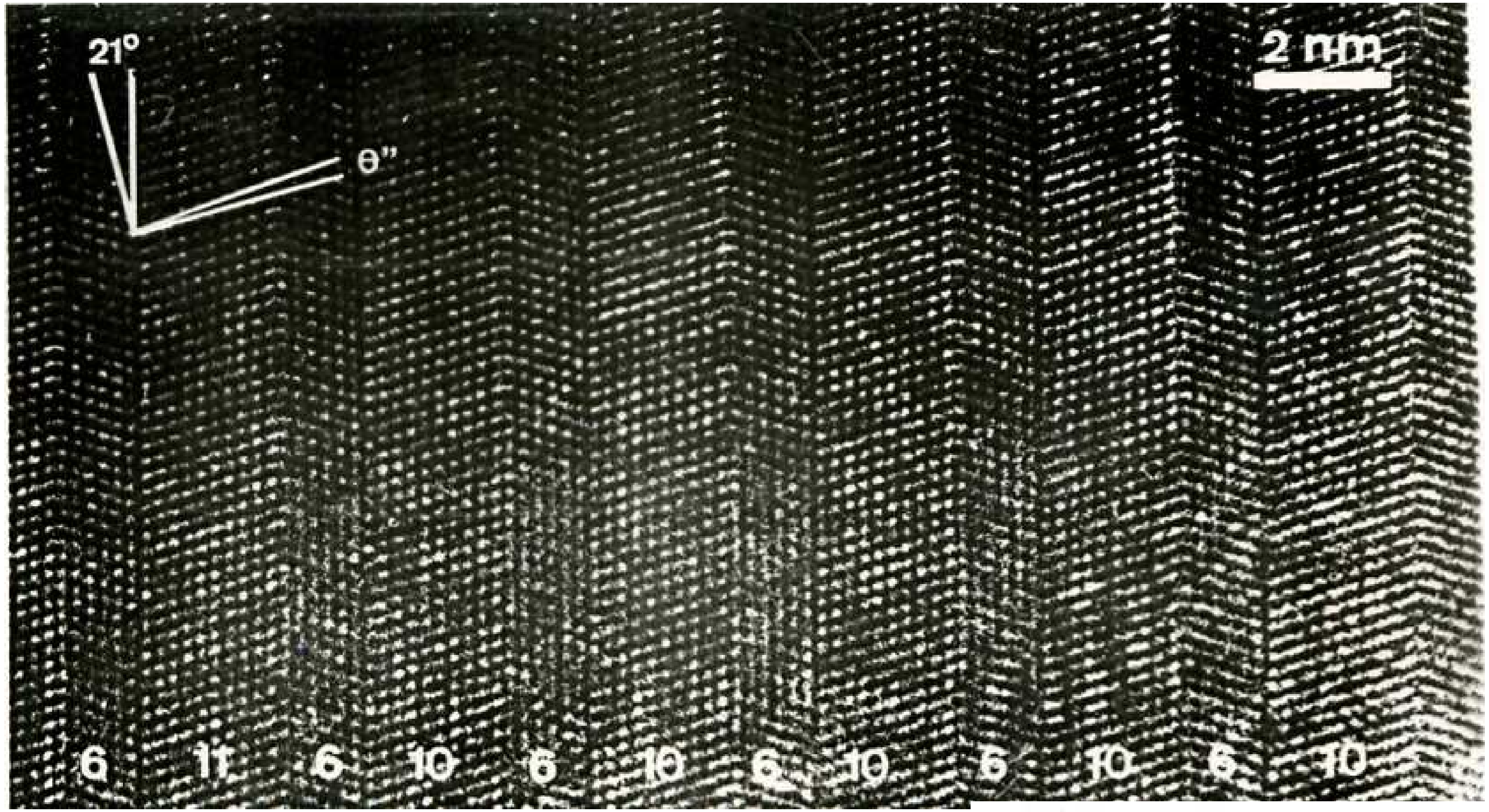
cubic to
orthorhombic
(e.g. CuAlNi)



$\theta < \theta_c$

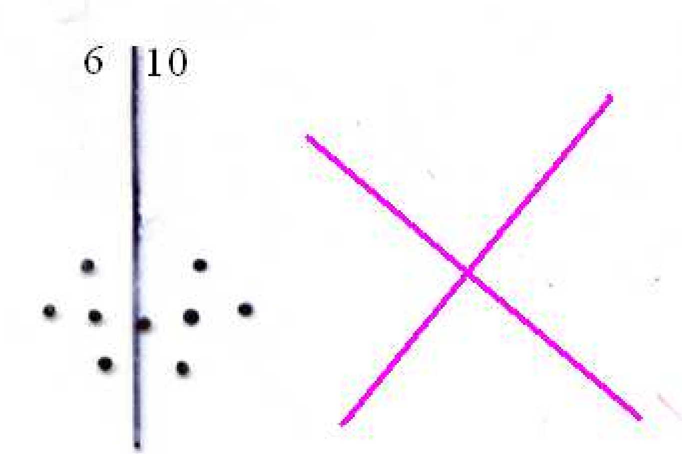
six orthorhombic variants

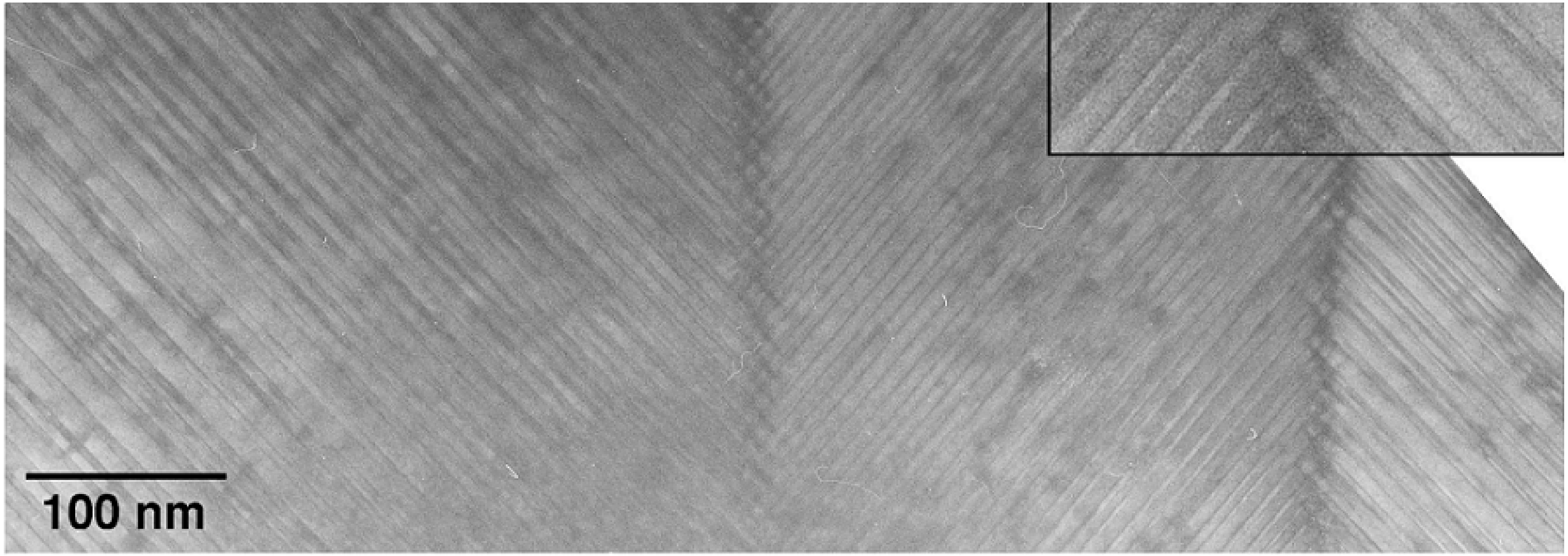
of martensite



Atomistically sharp interfaces for
cubic to tetragonal transformation
in NiMn

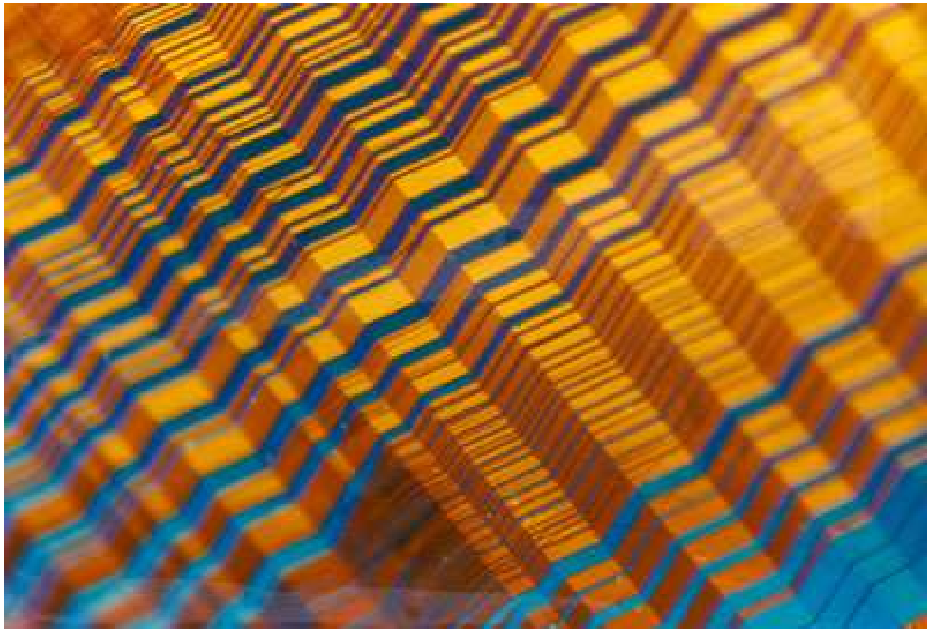
Baele, van Tenderloo, Amelinckx

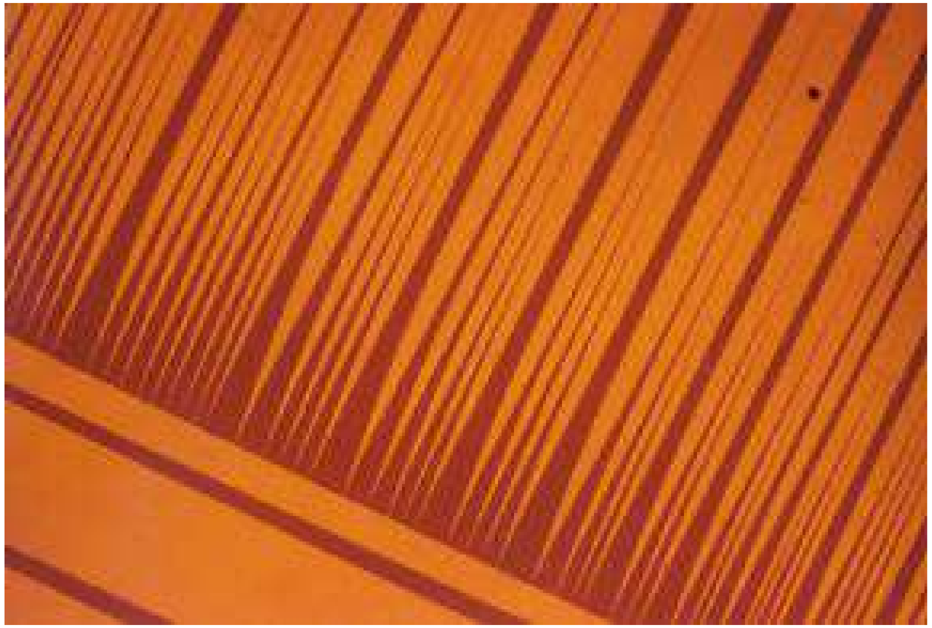




Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)

Martensitic microstructures in CuAlNi (Chu/James)





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 $A \in M_+^{3\times 3}$, where

$$M_+^{3\times 3} = \{A \in M^{3\times 3} : \det A > 0\}.$$

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

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

For cubic to orthorhombic $N = 6$ and

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

Lecture 4

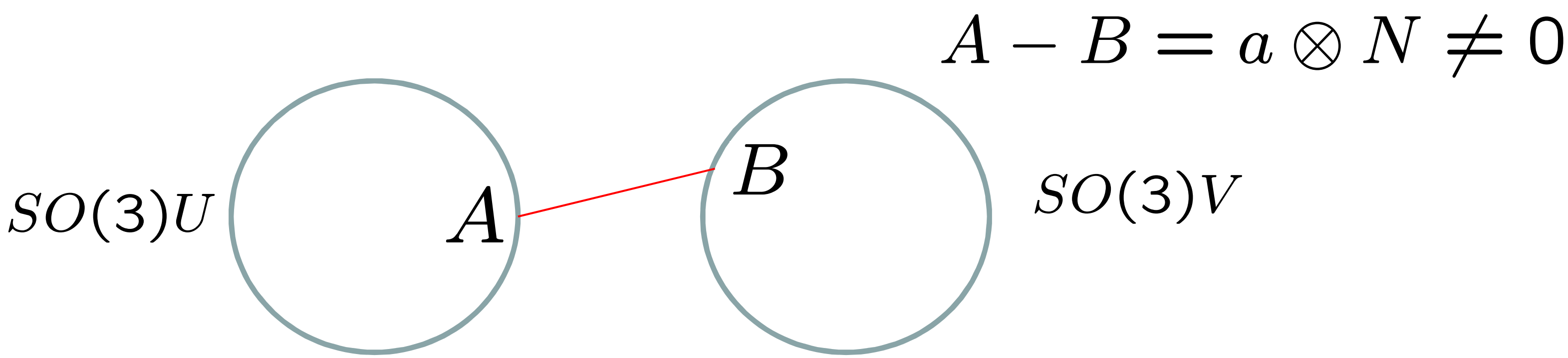
Microstructure

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 $SO(3)U$, $SO(3)V$.



Theorem
Let $U = U^T > 0$, $V = V^T > 0$. Then SO(3) U, 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 SO(3) U given by

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

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

Proof. Note first that

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

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

$$\begin{aligned}U^2 &= (V + N \otimes a)(V + a \otimes N) \\ &= V^2 + Va \otimes N + N \otimes Va + |a|^2 N \otimes N \\ &= V^2 + (Va + \frac{1}{2}|a|^2 N) \otimes N + N \otimes (Va + \frac{1}{2}|a|^2 N).\end{aligned}$$

If $a \neq 0$ then $Va + \frac{1}{2}|a|^2 N \neq 0$, since otherwise

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

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

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

$$a = cr + ts$$

where $|cr+ts|^2+2t = 0$ and $1+(cr+ts)\cdot s > 0$, where we have written $r = V^{-1}M$, $s = V^{-1}N$. The quadratic for t has the form

$$t^2|s|^2 + 2t(1 + cr \cdot s) + c^2|r|^2 = 0$$

which has roots

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

Since $\det U^2 = \det V^2 \det(1 + c(r \otimes s + s \otimes r))$, $\det(1+c(r\otimes s+s\otimes r)) = (1+cr\cdot s)^2 - c^2|r|^2|s|^2$ is positive and the roots are real. In order to satisfy $1 + cr \cdot s + t|s|^2 > 0$ we must take the $+$ sign, giving a unique a, and thus unique R such that $RU = V + a \otimes N$.

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

To complete the proof it suffices to check the following

Lemma

If $c(M \otimes N + N \otimes M) = c'(P \otimes Q + Q \otimes P)$ for unit vectors P, Q and some constant c', then either $P \otimes Q = \pm M \otimes N$ or $P \otimes Q = \pm N \otimes M$.

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

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

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

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

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 no rank-one connection between pairs of matrices $A \in SO(3)$ and $B \in SO(3)U_i$ *unless U_i has middle eigenvalue* 1.

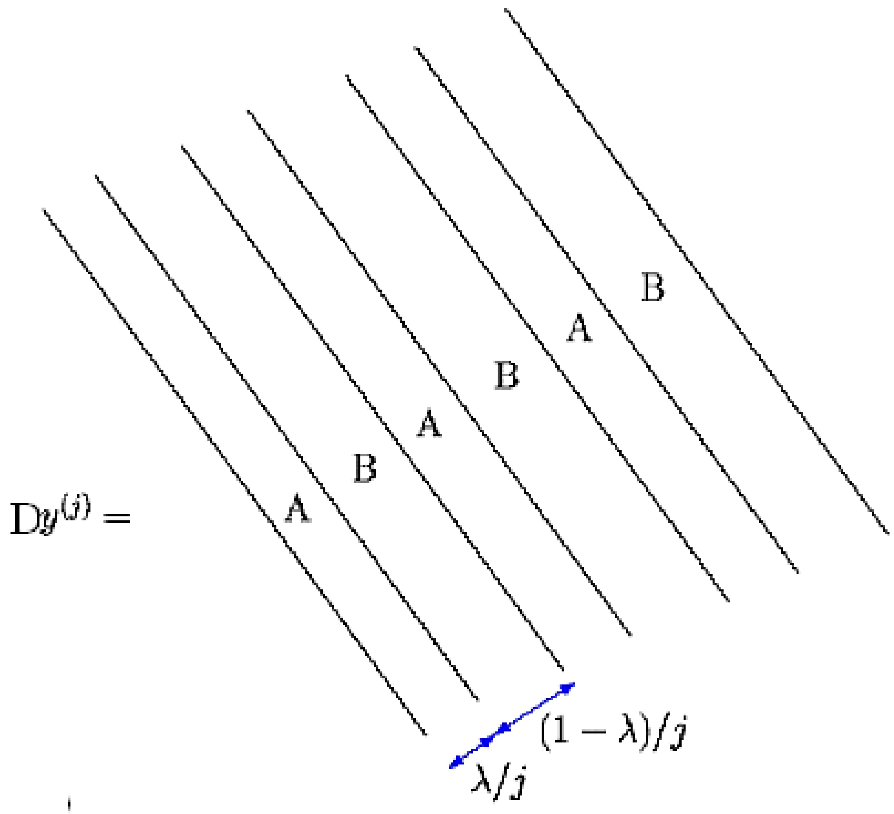
Proof. If there is a rank-one connection then 1 is an eigenvalue since $\det(U_i^2 - 1) = 0$.

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

$$U_i^2 - 1 = \frac{\lambda_3^2 - \lambda_1^2}{2}\left((\alpha e_1 + \beta e_3) \otimes (-\alpha e_1 + \beta e_3)\right.$$
$$\left. + (-\alpha e_1 + \beta e_3) \otimes (\alpha e_1 + \beta e_3)\right),$$

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

Layering twins



Simple laminate

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

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

Some general considerations

The microstructures arising from martensitic transformations are driven by compatibility of gradients. The product phases have to fit together geometrically, generating a microgeometry that is partly captured by gradient Young measures (see below).

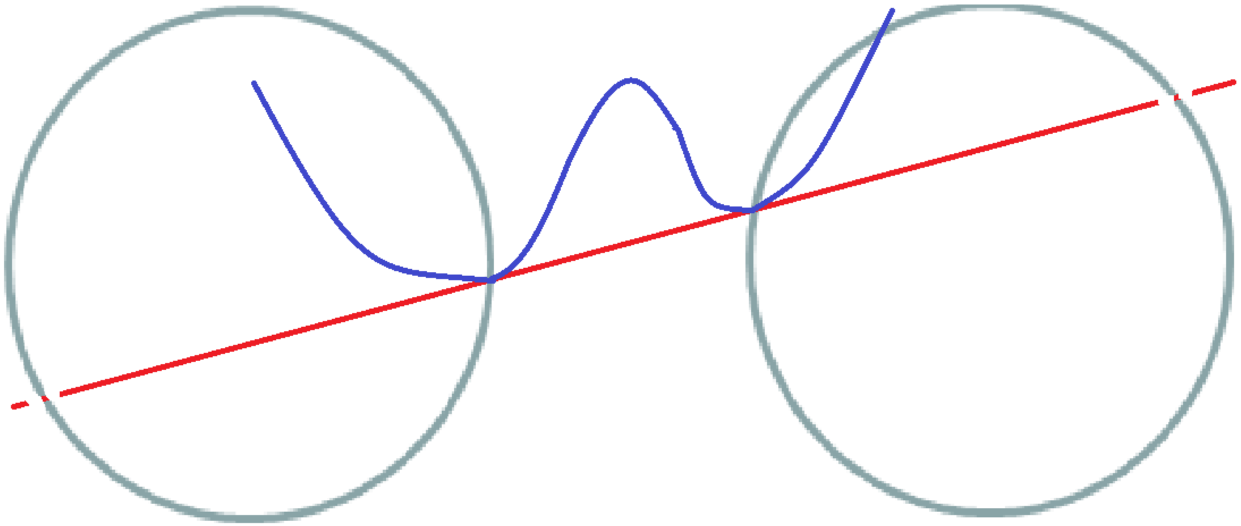
In trying to understand why we see some microstructures and not others, we will use methods based on energy minimization. However, the formation of microstructure is obviously a pattern formation problem, which really should be treated using an appropriate dynamical model.

Such a model should tell us which morphological features are predictable (e.g. via invariant manifolds, attractors) in a given experiment, and predict them.

However it is not clear what are appropriate dynamical equations, and both theoretical and numerical analysis currently intractable for any such model.

Unfortunately static theories are not truly predictive:
(i) Large redundancy in energy minimizers.
(ii) The microstructure geometry is typically assumed a priori, and shown to be consistent with the theory (although interesting details may be predicted).

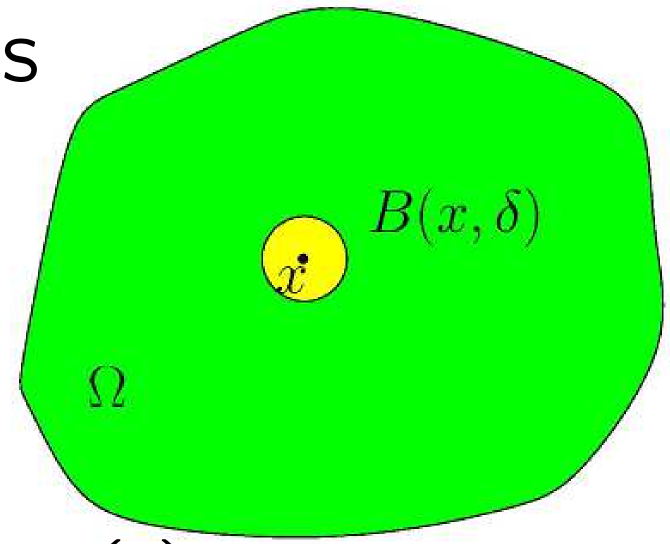
The free-energy function $\psi(\cdot,\theta)$ is not quasi-convex. This is because the existence of twins implies that $\psi(\cdot,\theta)$ is not rank-one convex.



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.



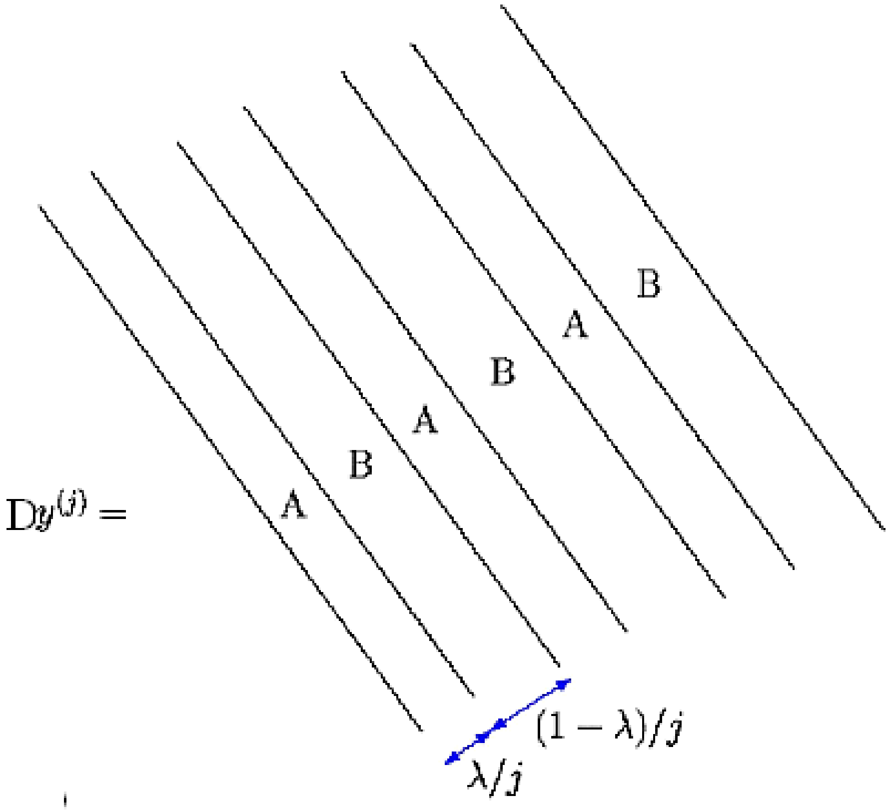
Let $E \subset M^{3\times3}$, where $M^{3\times3} = \{3 \times 3 \text{ matrices}\}$

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

$$\nu_x(E) = \lim_{\delta\to0} \lim_{j\to\infty} \nu_{x,j,\delta}(E)$$

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* $(\nu_x)_{x\in\Omega}$ *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:

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

Of sets:

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

Let $K \subset M^{3\times 3}$ be compact,
e.g. $K = \bigcup_{i=1}^{N} SO(3)U_i(\theta)$.

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

$\psi^{\mathrm{qc}}(F,\theta)$ 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.

Lecture 5

Austenite-martensite interfaces

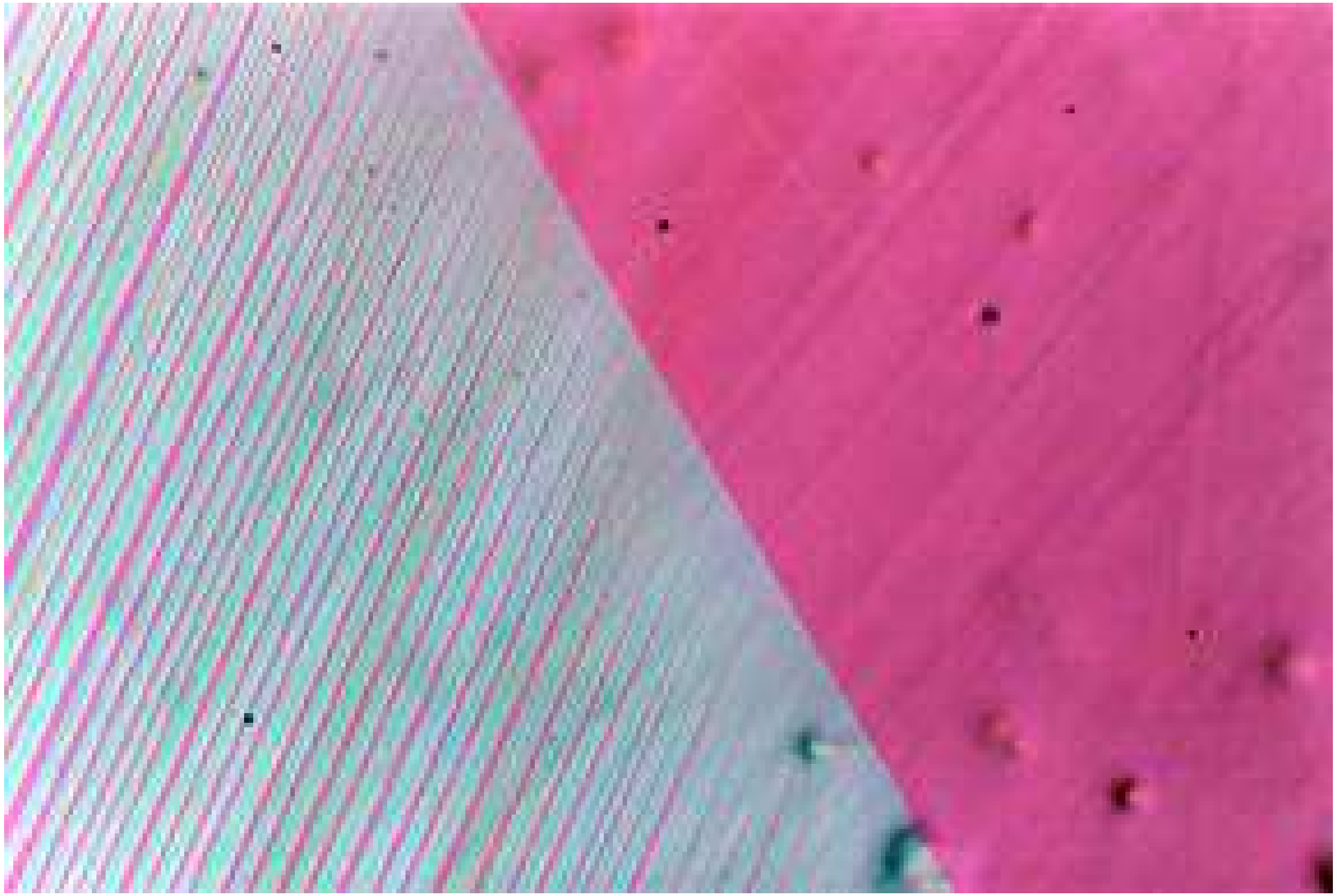
How does austenite transform to martensite as θ passes through θ_c?

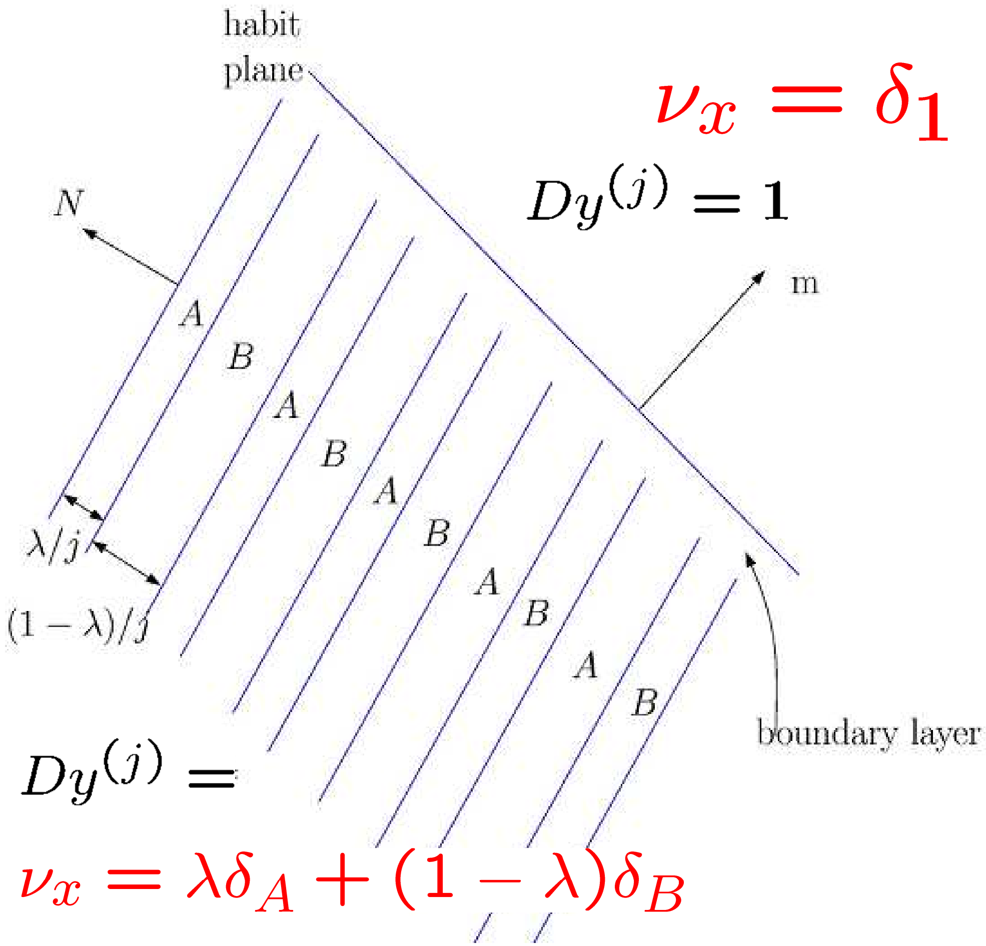
It cannot do this by means of an exact interface between austenite and martensite, because this requires the middle eigenvalue of U_i to be one, which in general is not the case (but see studies of James et al on low hysteresis alloys).

So what does it do?

(Classical) austenite-martensite interface in CuAlNi

(courtesy C-H Chu and R.D. James)





$$\nu_x = \delta_1$$

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

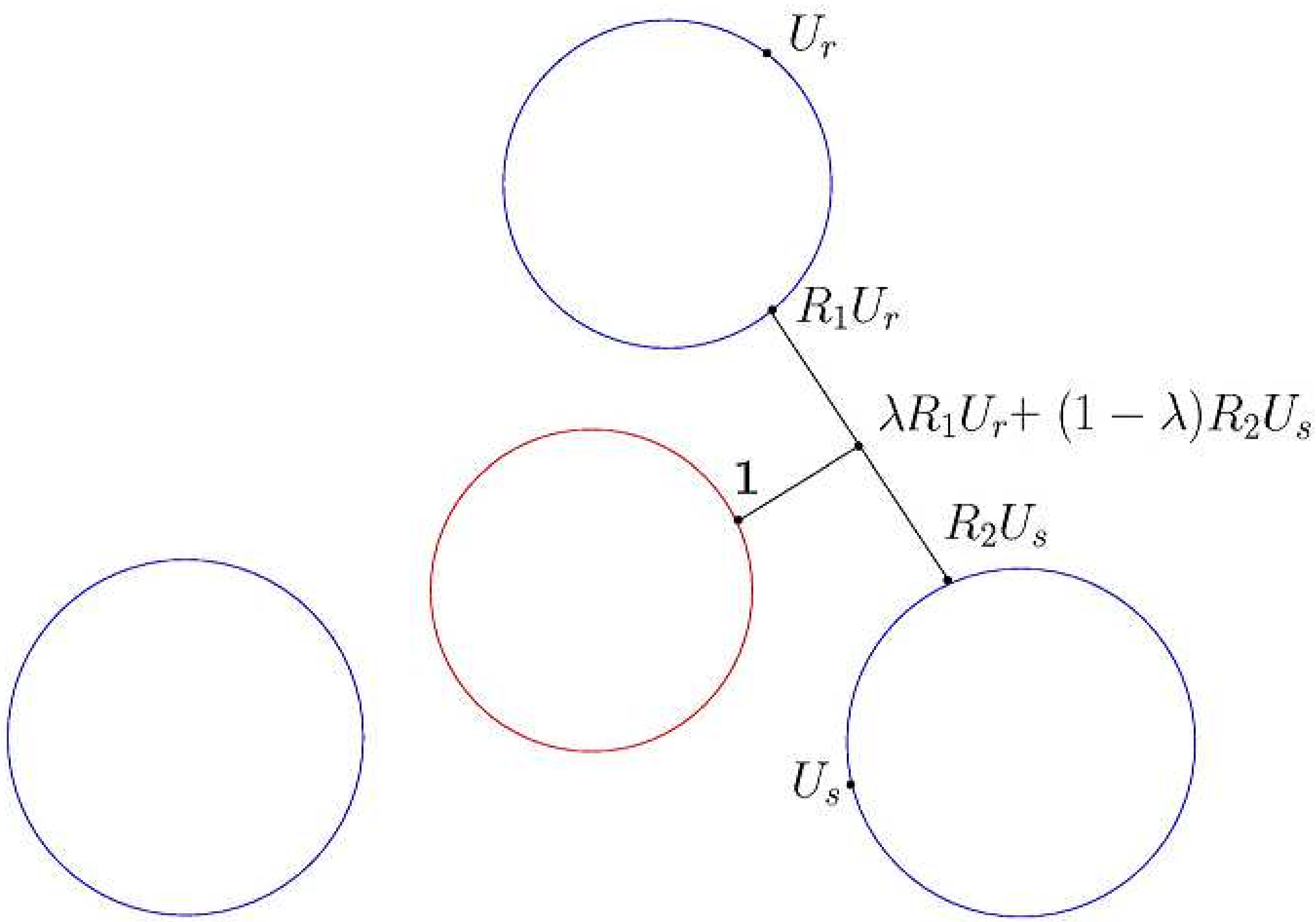
$$Dy^{(j)} =$$

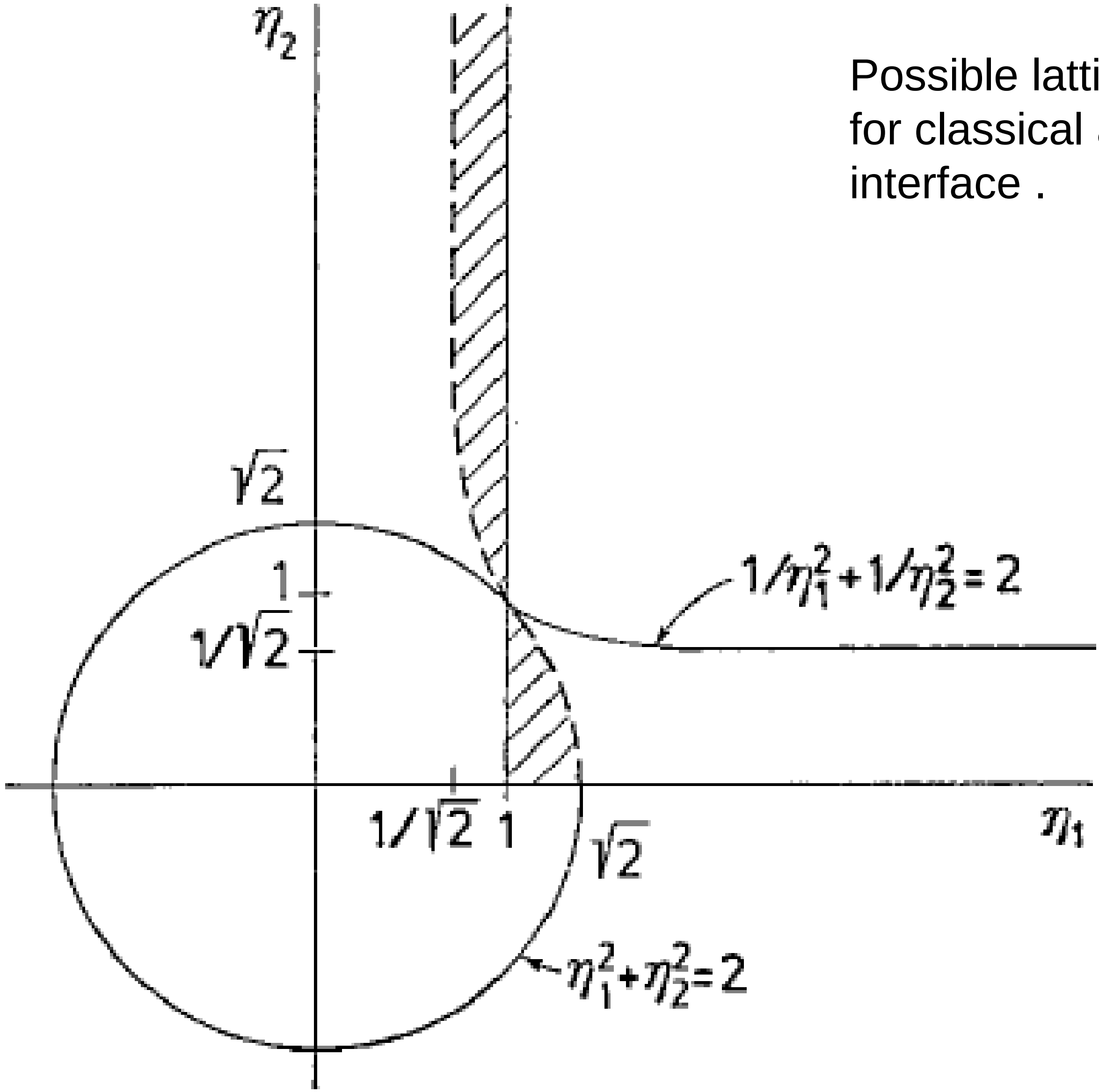
$$\nu_x = \lambda\delta_A + (1-\lambda)\delta_B$$

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

24 habit planes for cubic-to-tetragonal

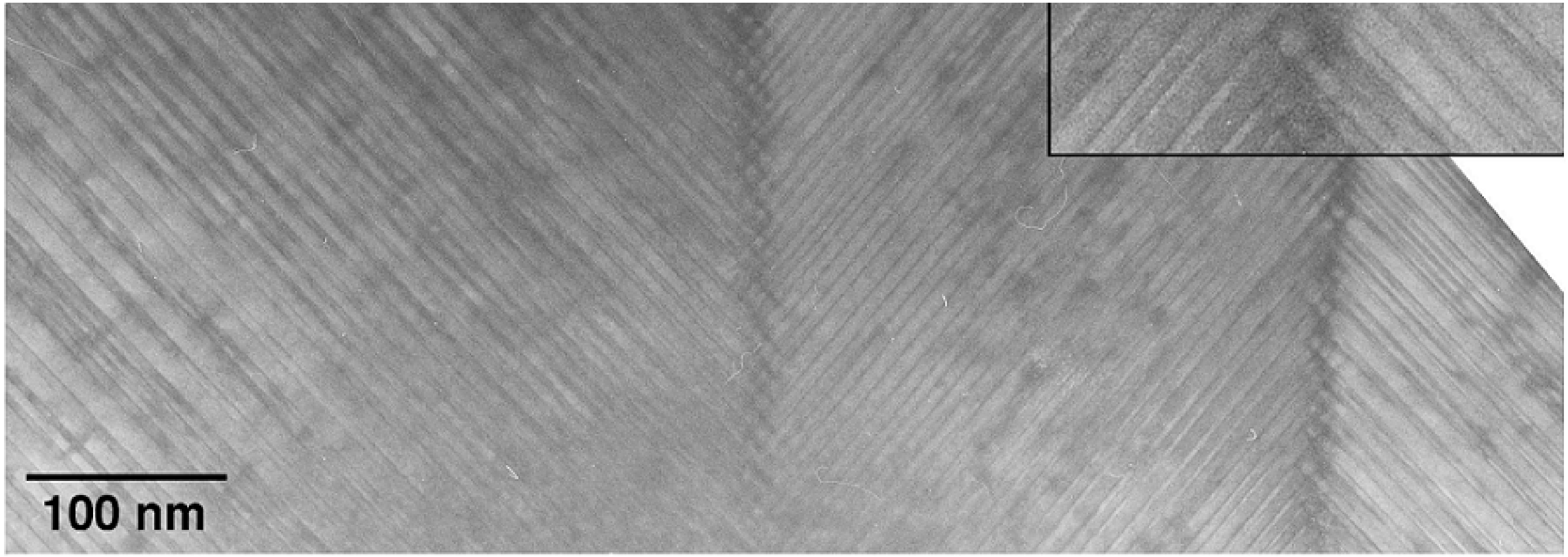
Rank-one connections for A/M interface



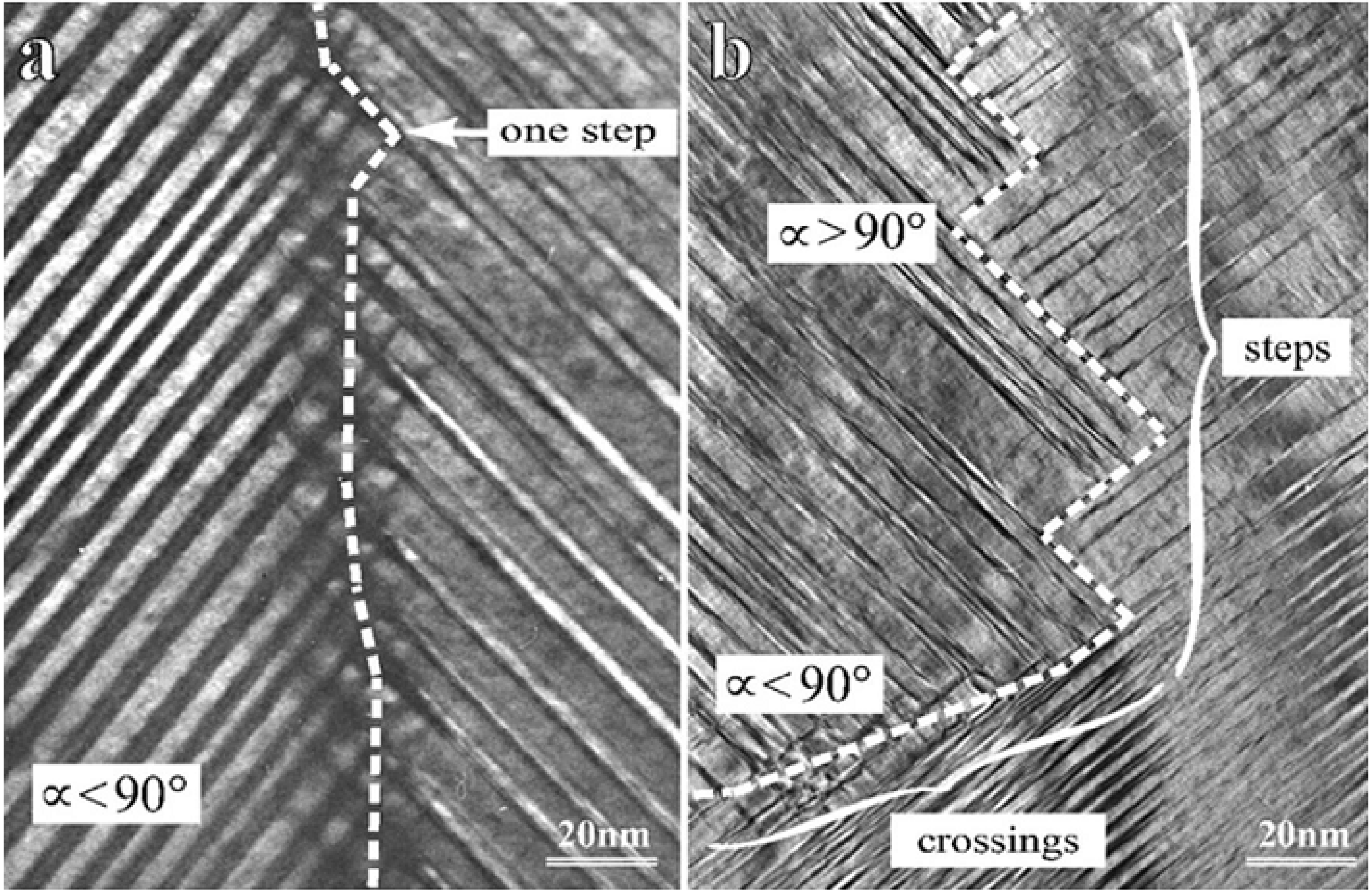


Possible lattice parameters
for classical austenite-martensite
interface .

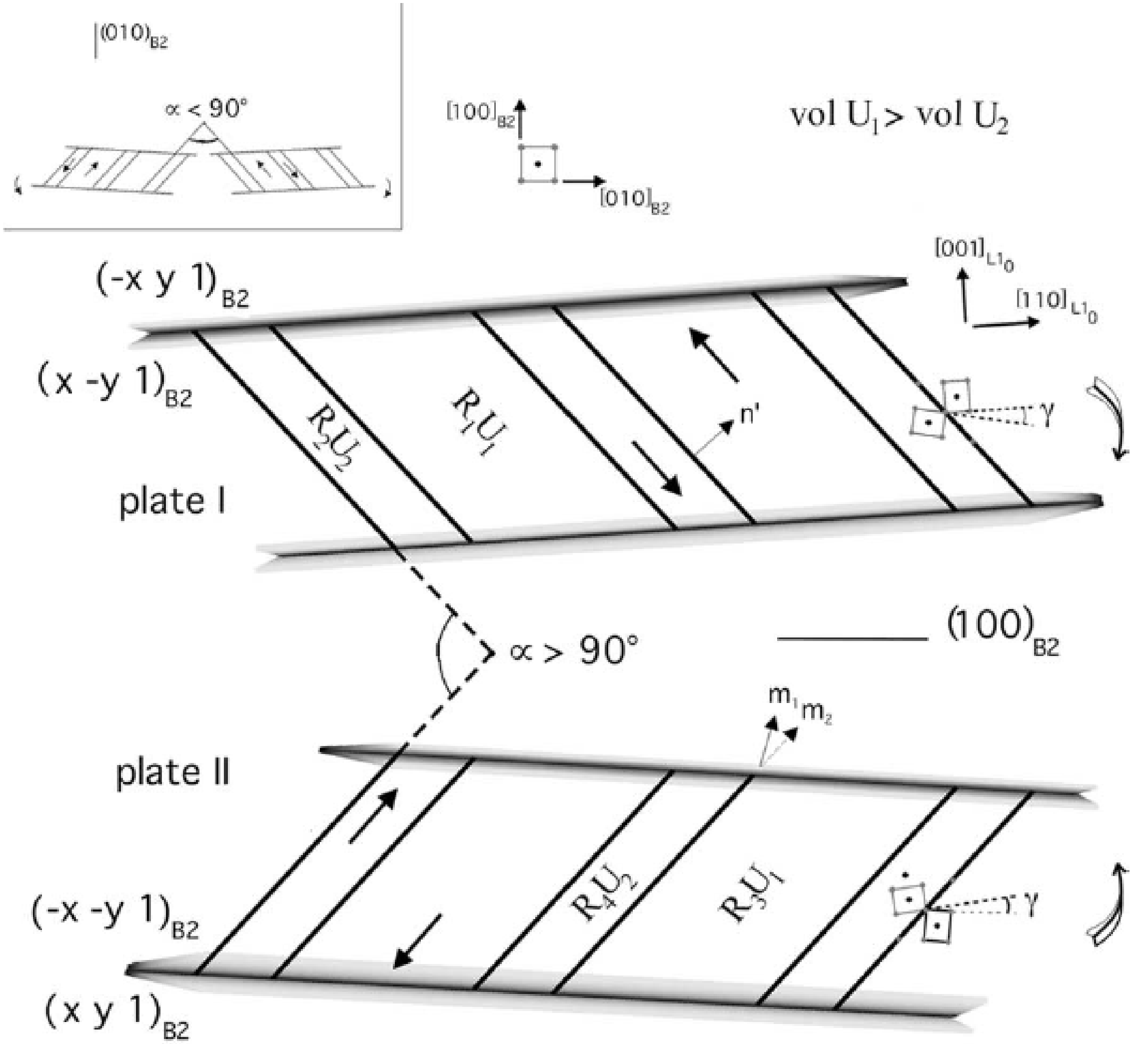
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)

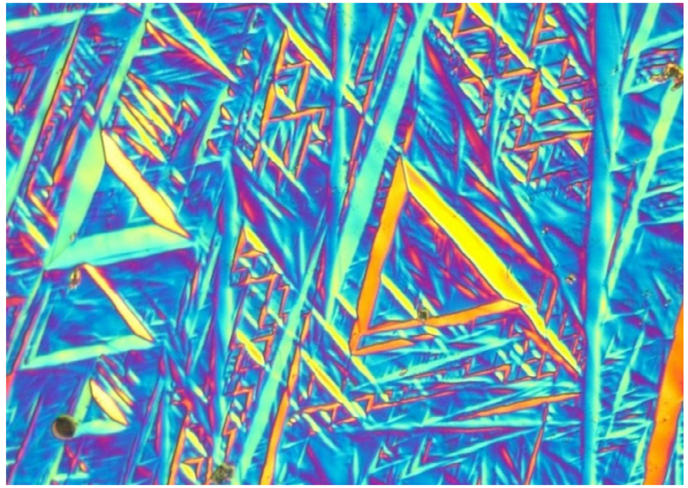


Crossings and steps



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

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

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

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

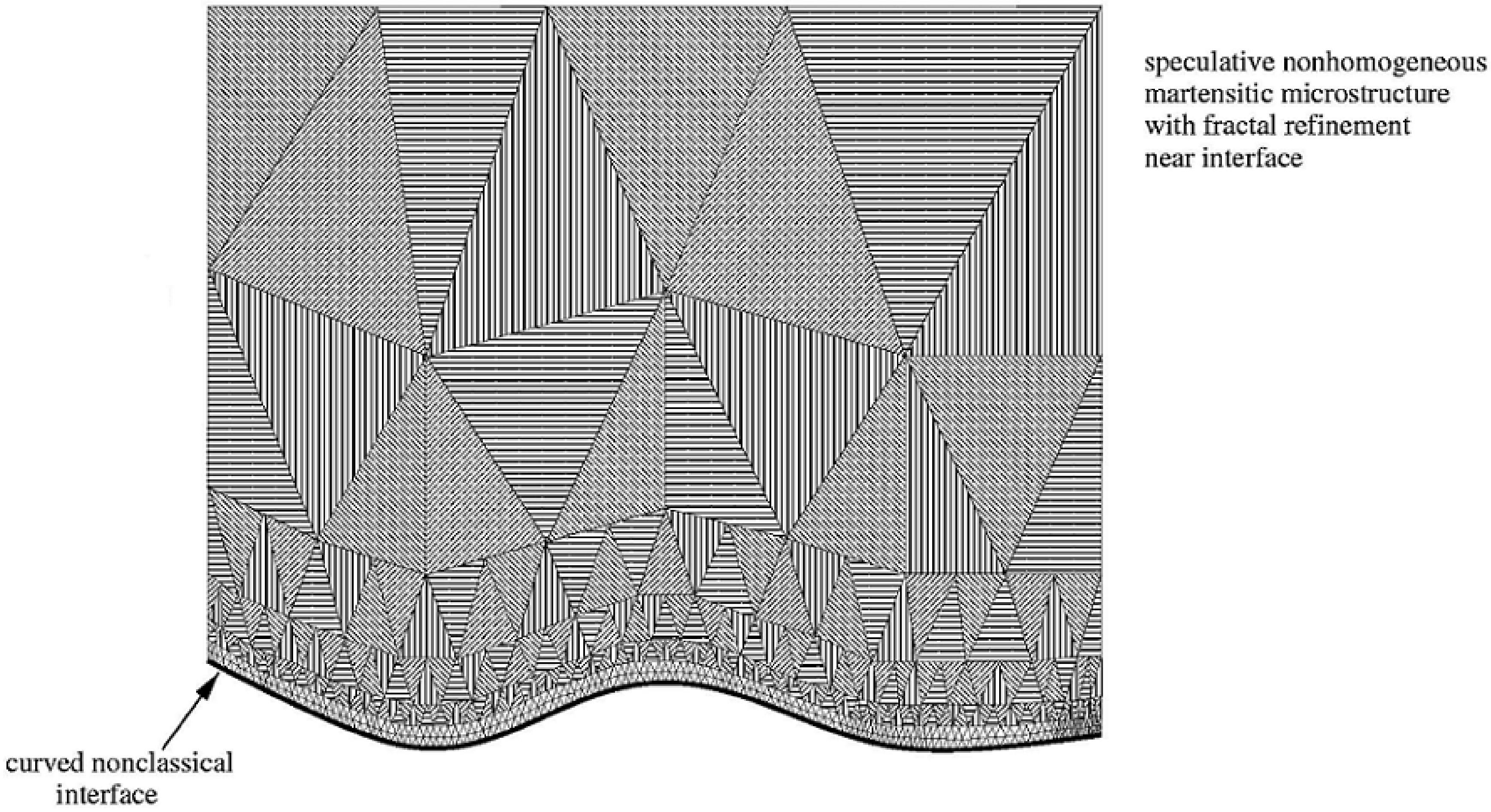
B/Schryvers 2003

Different martensitic plates never compatible (Bhattacharya)

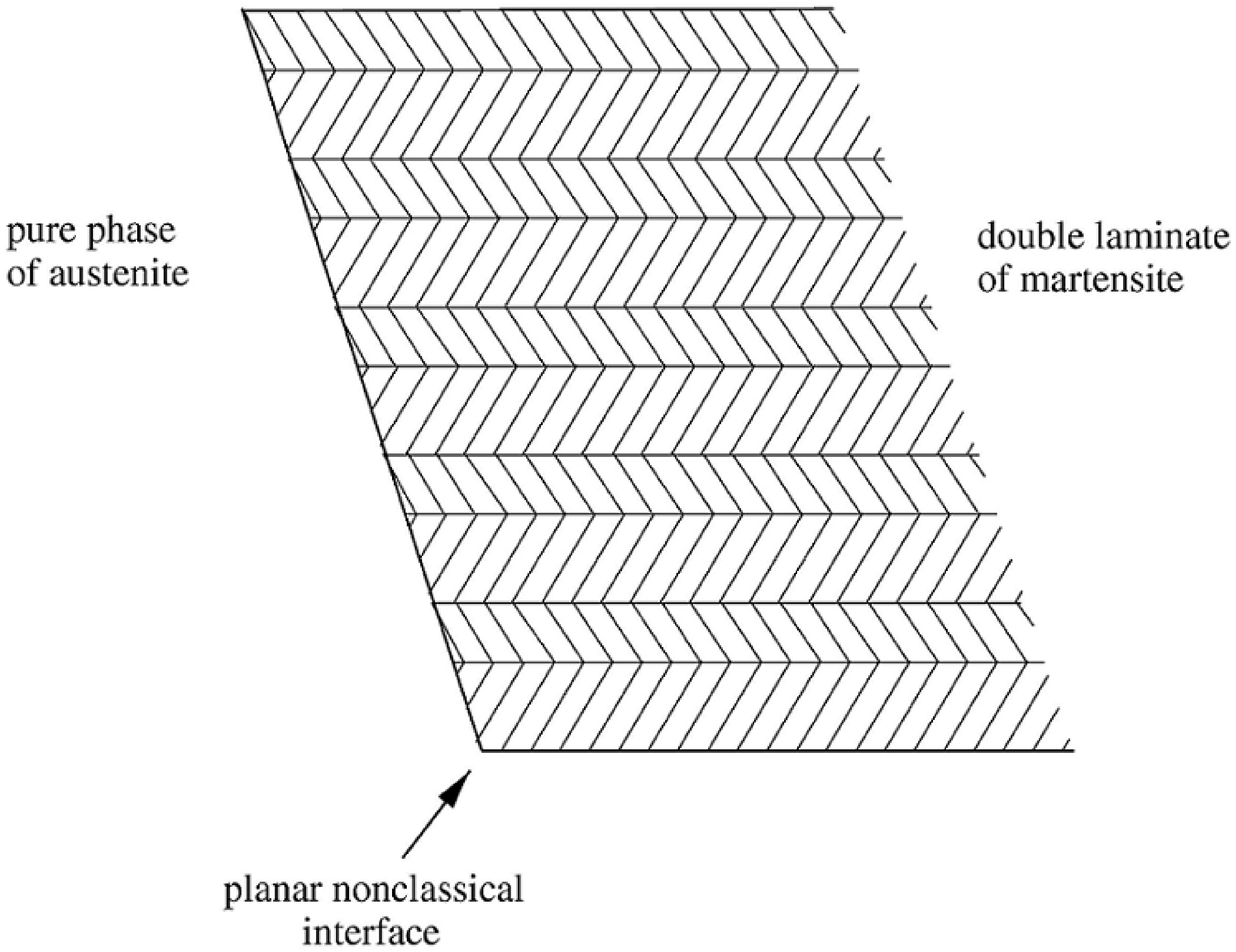
Table 1: Rotations Q_1 and Q_2 that bring Plate II into compatibility with Plate I ($\kappa_1 = \chi_1 = \nu_1 = 1$) and the corresponding macrotwin normals N_1 and N_2. The direction of rotation is that of a right-handed screw in the direction of the given axis. For the case $\kappa_2 = \nu_2 = 1, \chi_2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

$$Dy(x) = \mathbf{1}$$

m

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

$$Dy(x) = F = \bar{\nu}$$
$$F \in \left(\bigcup_{i=1}^{N} SO(3)U_i\right)^{\mathrm{qc}}$$

(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$)$ $0 < \eta_{\mathrm{min}} \leq \eta_{\mathrm{mid}} \leq \eta_{\mathrm{max}}$.

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

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

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

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

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

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

Combining these inequalities we get that

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

For cubic to tetragonal we have that

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

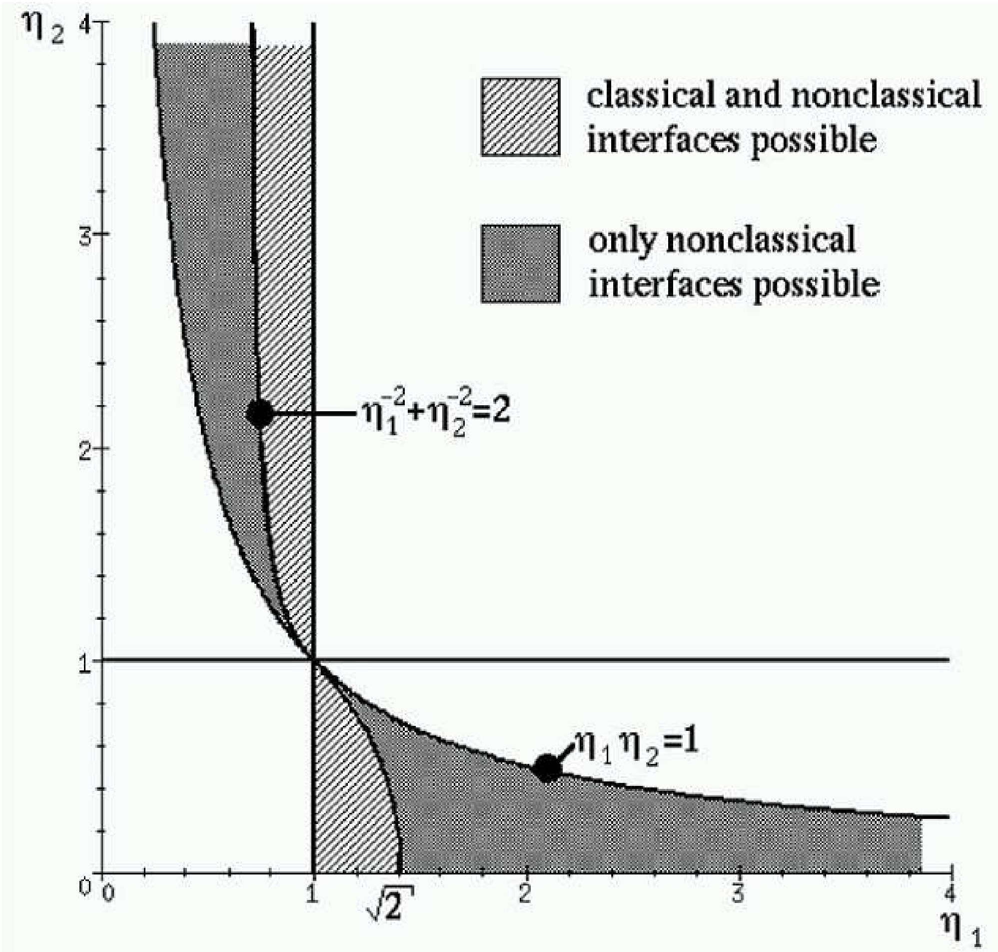
and the necessary conditions become

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

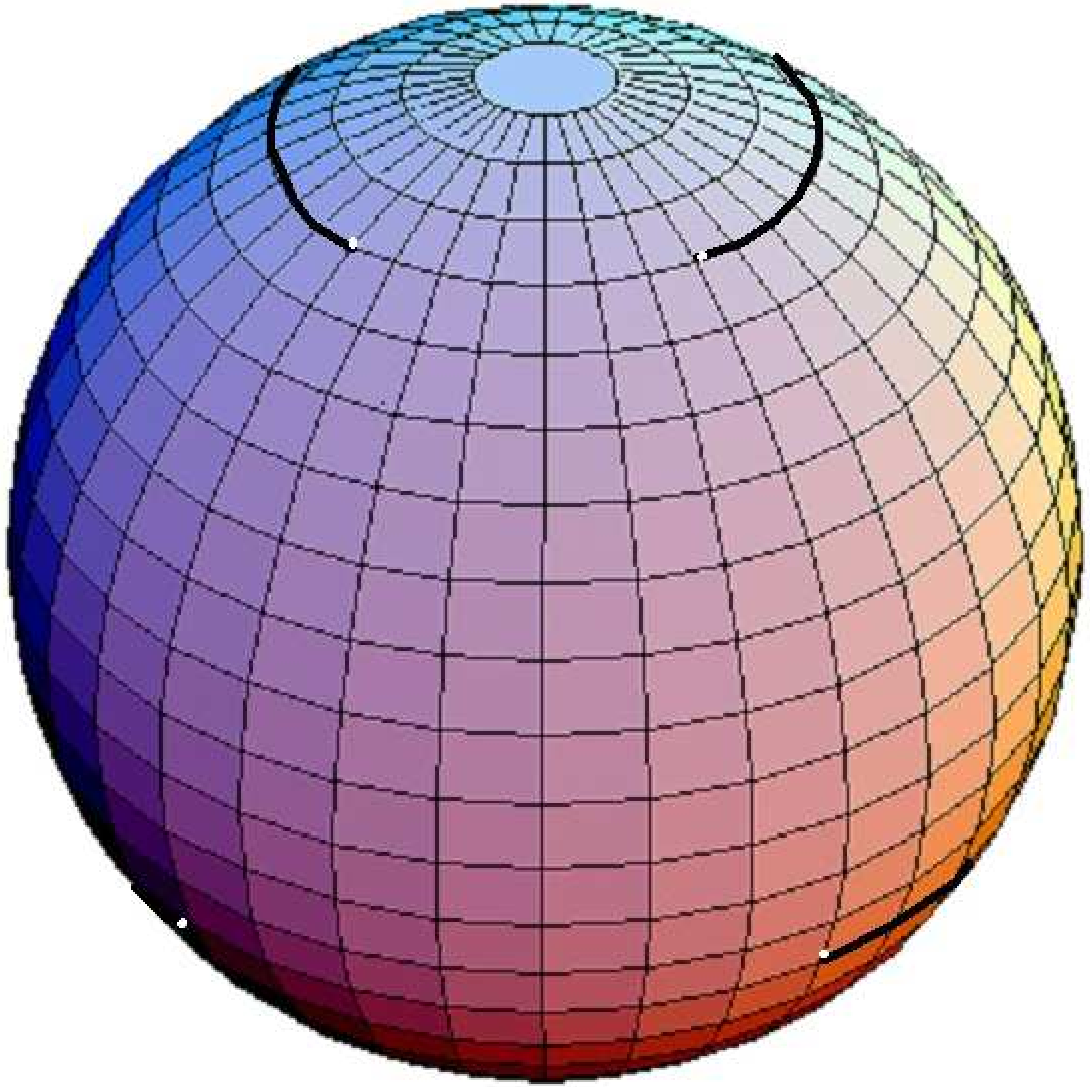
$$\eta_2 \leq \eta_1^{-1} \leq \eta_1 \text{ if } \eta_1 \geq \eta_2.$$

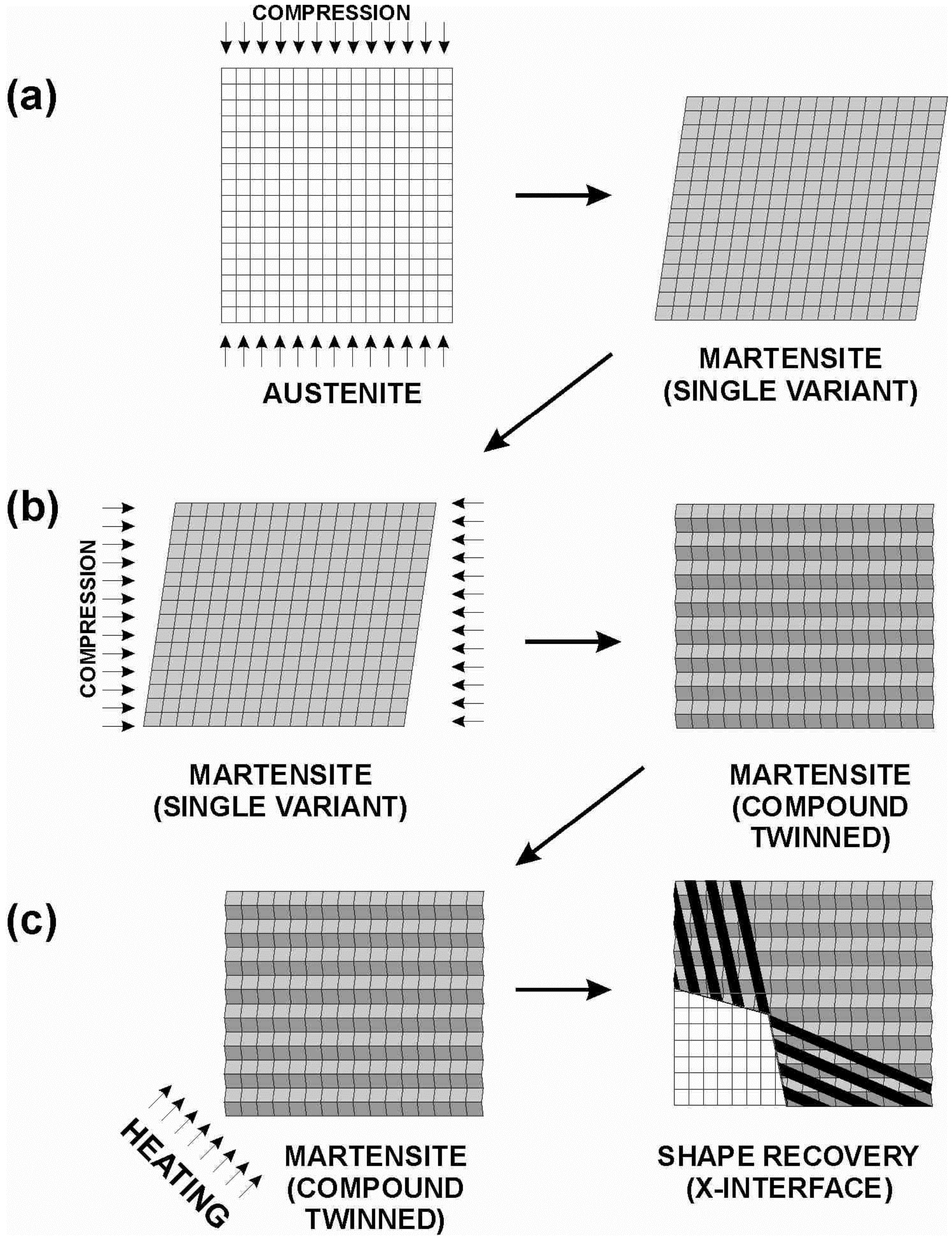
But these turn out to be exactly the conditions given by the two-well theorem to construct a rank-one connection from $(SO(3)U_1 \cup SO(3)U_2)^{qc}$ to the identity! Hence the conditions are sufficient also.

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



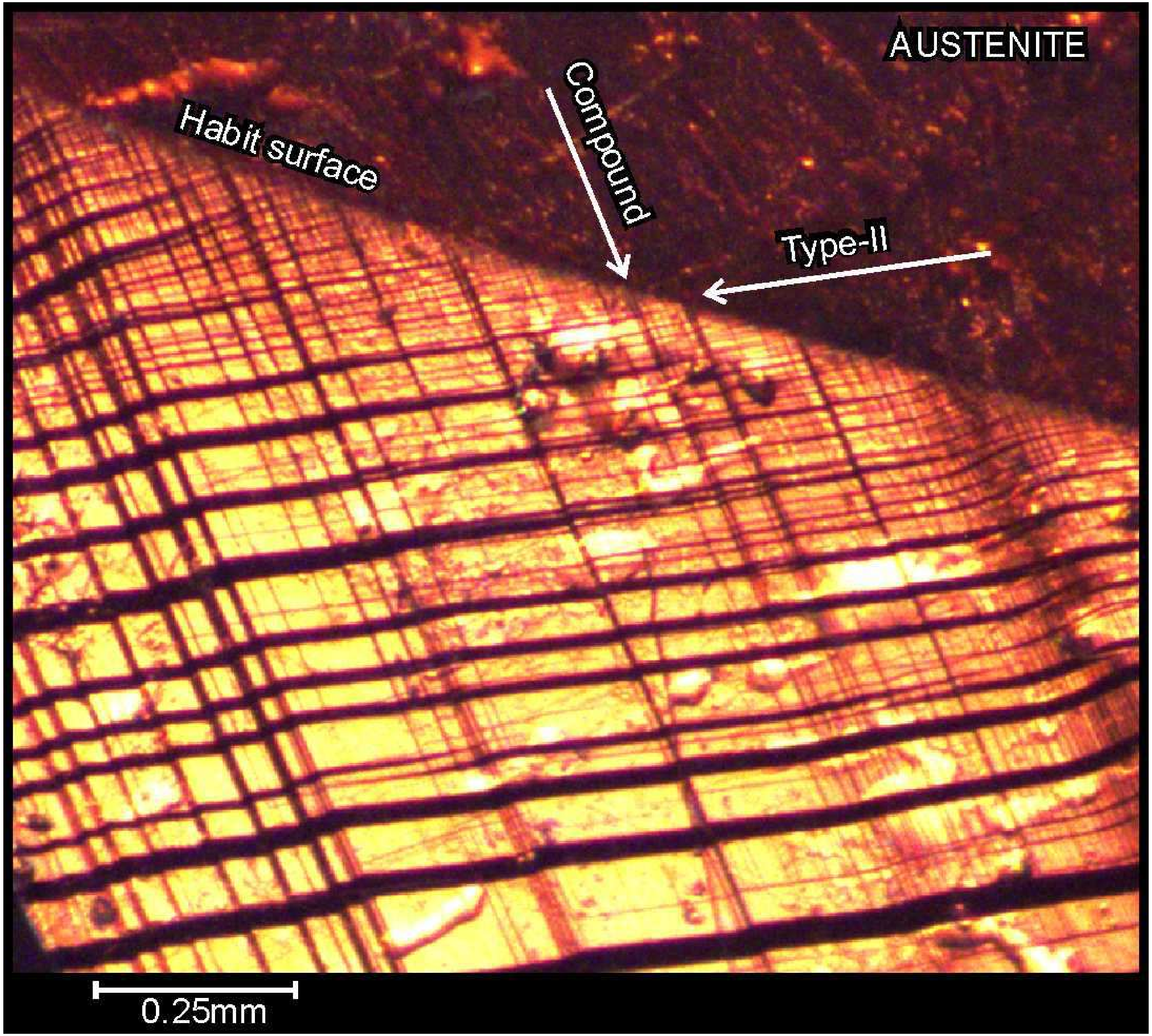
Interface normals



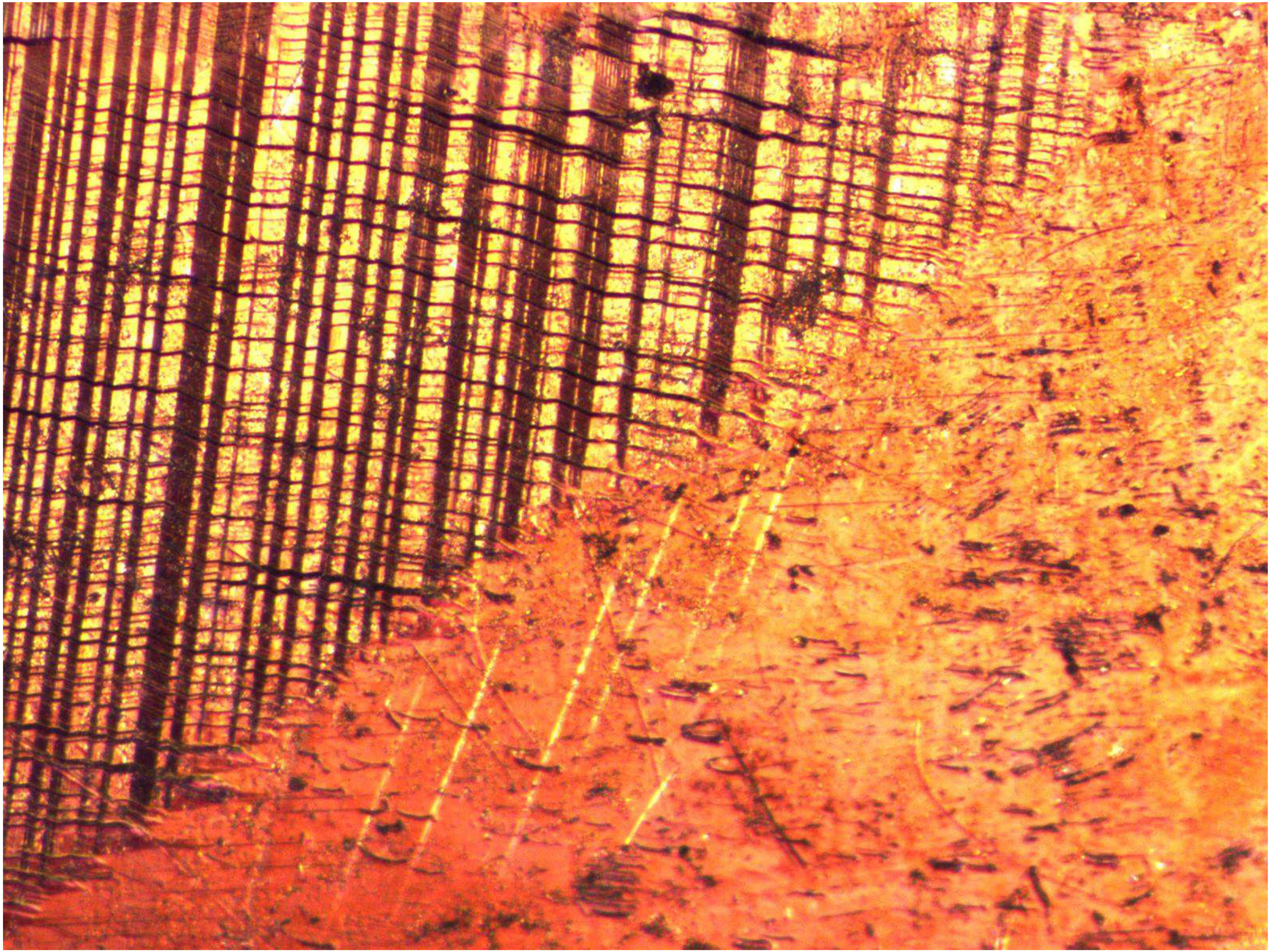


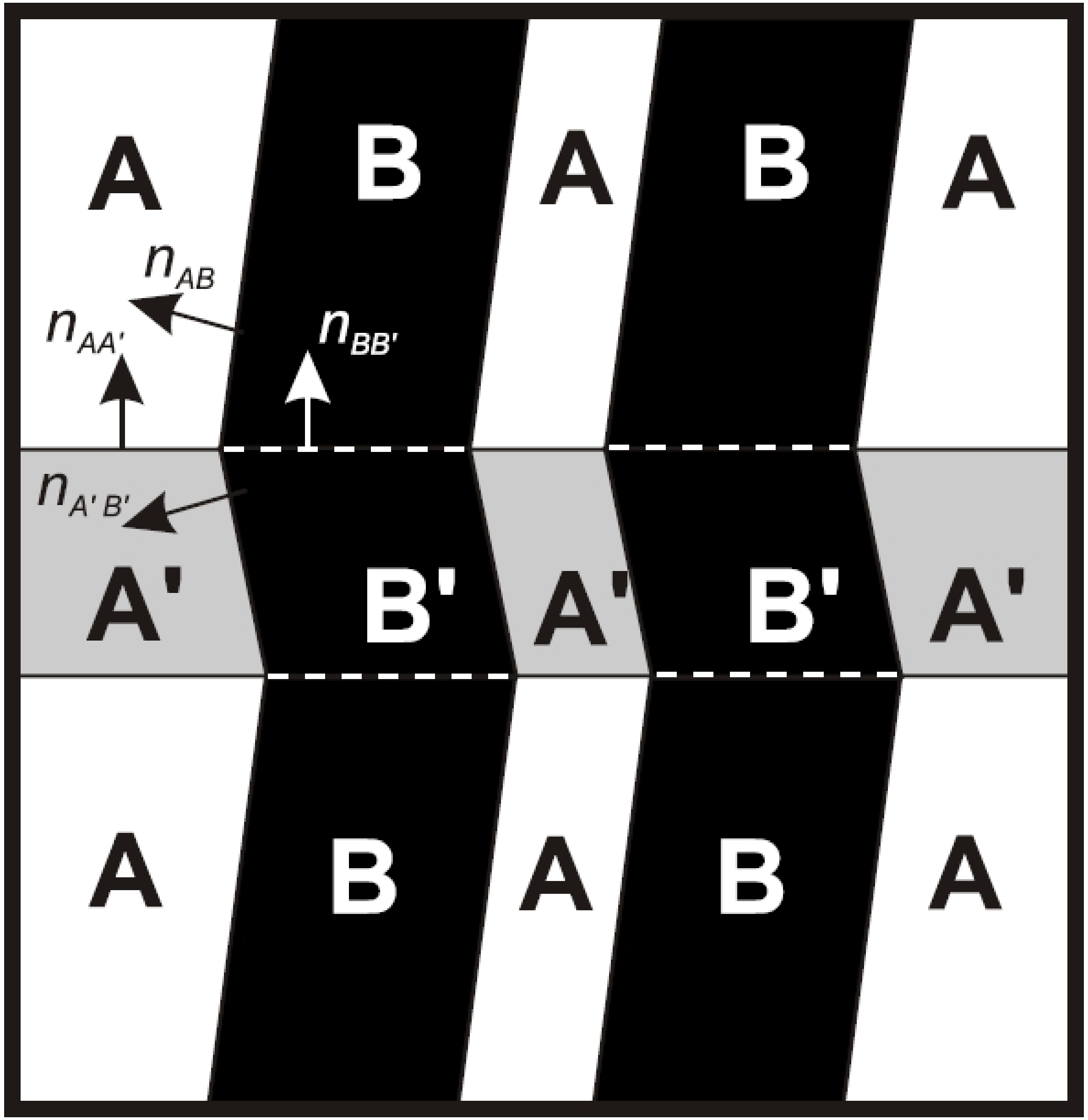
Experimental procedure (H. Seiner)

3.9×3.8×4.2mm CuAlNi single crystal



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

Analysis: JB, K. Koumatos, H. Seiner 2010

Let $U_A, U_{A'}$ and $U_B, U_{B'}$ be two distinct pairs of martensitic variants able to form compound twins (e.g. U_3, U_4 and U_5, U_6). Then the compatibility equations for the parallelogram microstructure are :

$$\begin{aligned} R_{AB}U_B - U_A &= b_{AB} \otimes n_{AB} \\ R_{A'B'}U_{B'} - U_{A'} &= b_{A'B'} \otimes n_{A'B'} \\ R_{AA'}U_{A'} - U_A &= b_{AA'} \otimes n_{AA'} \\ R_{BB'}U_{B'} - U_B &= b_{BB'} \otimes n_{BB'} \\ R_{AB}R_{BB'} &= R_{AA'}R_{A'B'}. \end{aligned}$$

Let $0 \leq \lambda \leq 1$ denote the relative volume fraction of the Type-II twins (the same by the parallelogram geometry), and set

$$\begin{aligned} M_{AB} &= (1-\lambda)U_A + \lambda R_{AB} U_B \\ M_{A'B'} &= (1-\lambda)U_{A'} + \lambda R_{A'B'} U_{B'} \end{aligned}$$

Let $0 \leq \Lambda \leq 1$ be the relative volume fraction of the compound twins. Then the overall macroscopic deformation gradient is

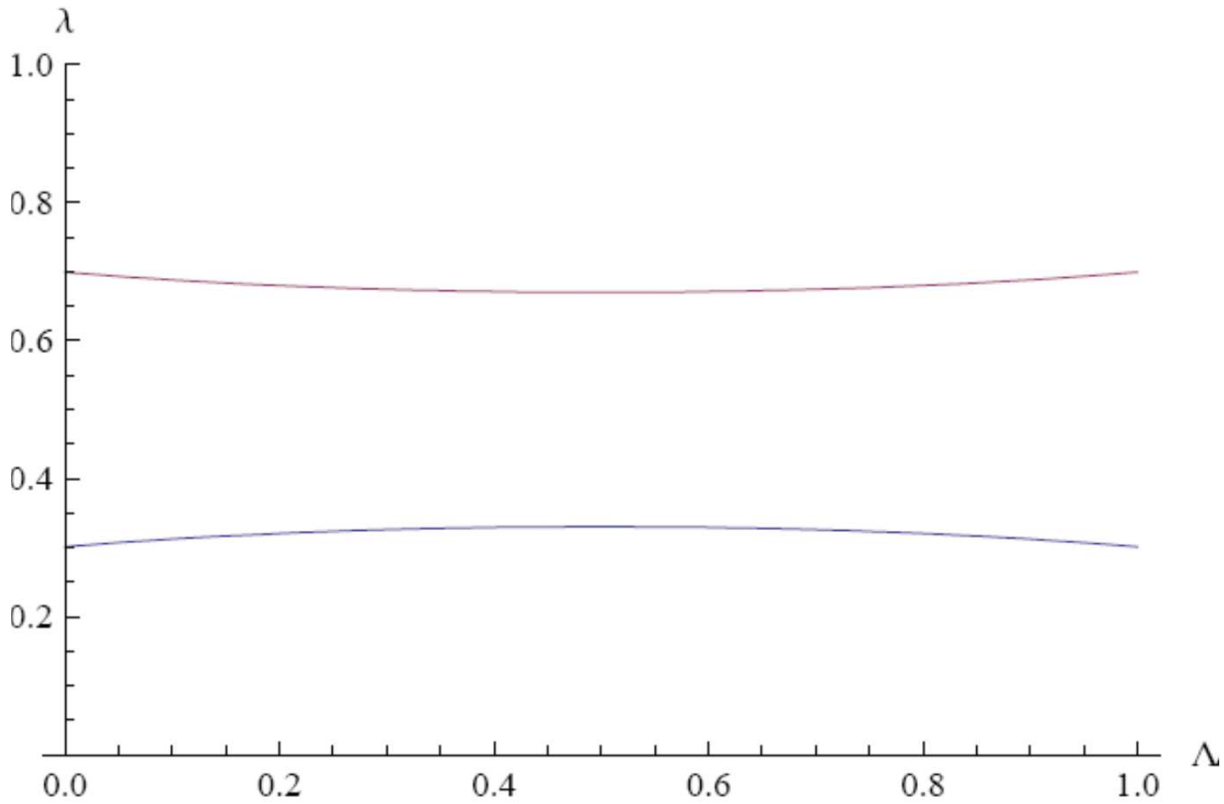
$$M = (1-\Lambda)M_{AB} + \Lambda R_{AA'} M_{A'B'}.$$

For compatibility with the austenite we need

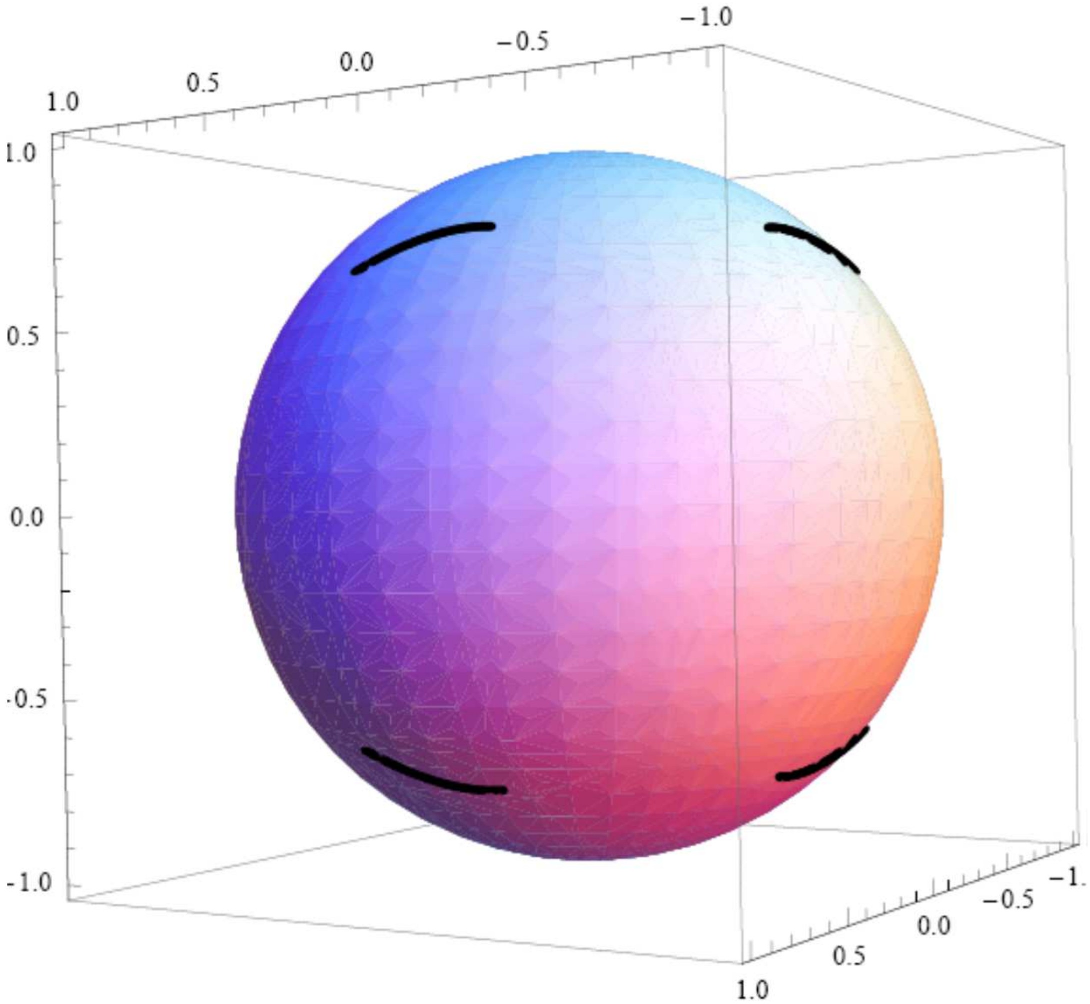
$$\lambda_{\mathsf{mid}}(M^T M) = 1$$

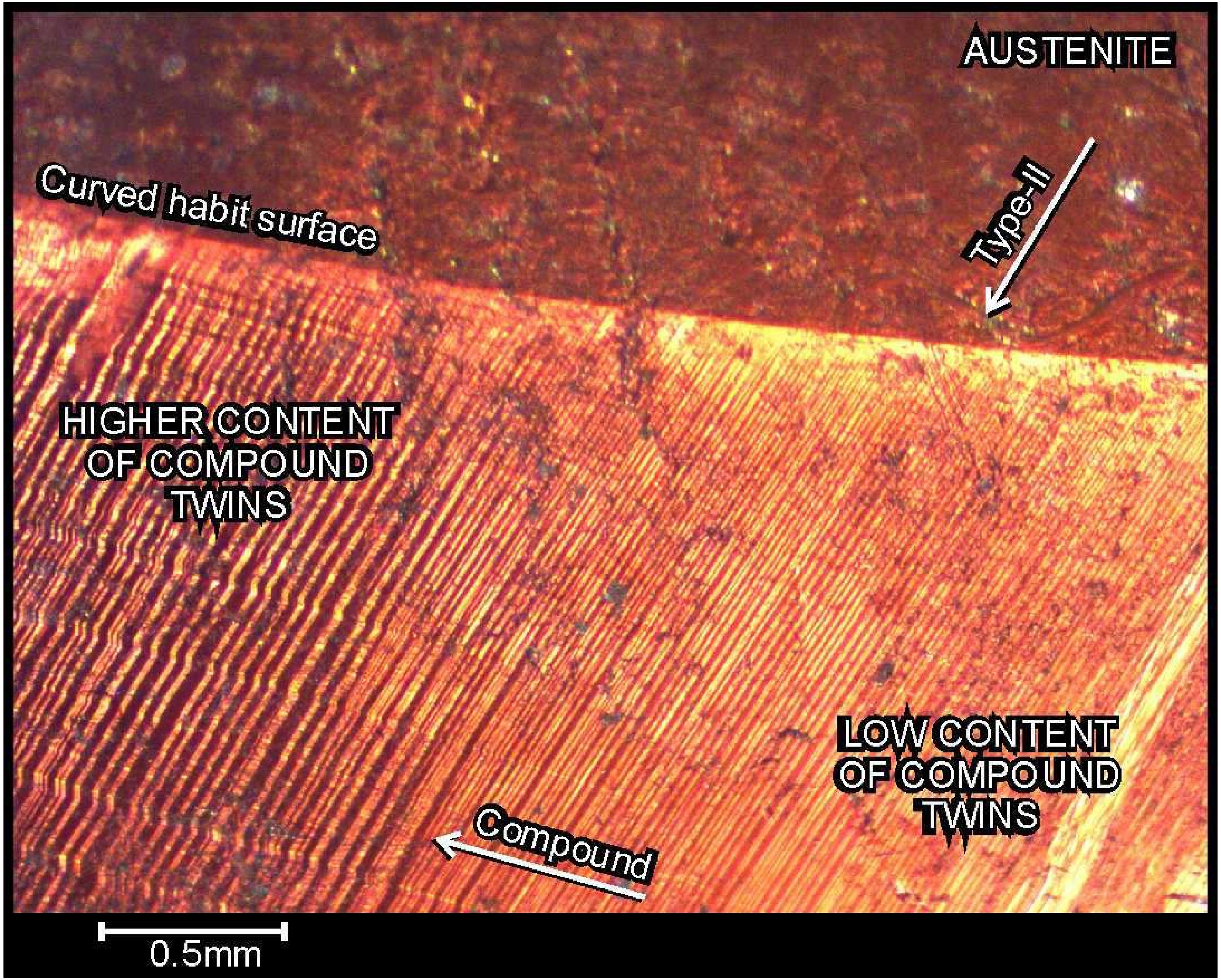
Possible volume fractions

$$\lambda^2 - \lambda = -\frac{a_0 + a_2(\Lambda^2 - \Lambda)}{a_1 + a_3(\Lambda^2 - \Lambda)}.$$



Possible nonclassical interface normals





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

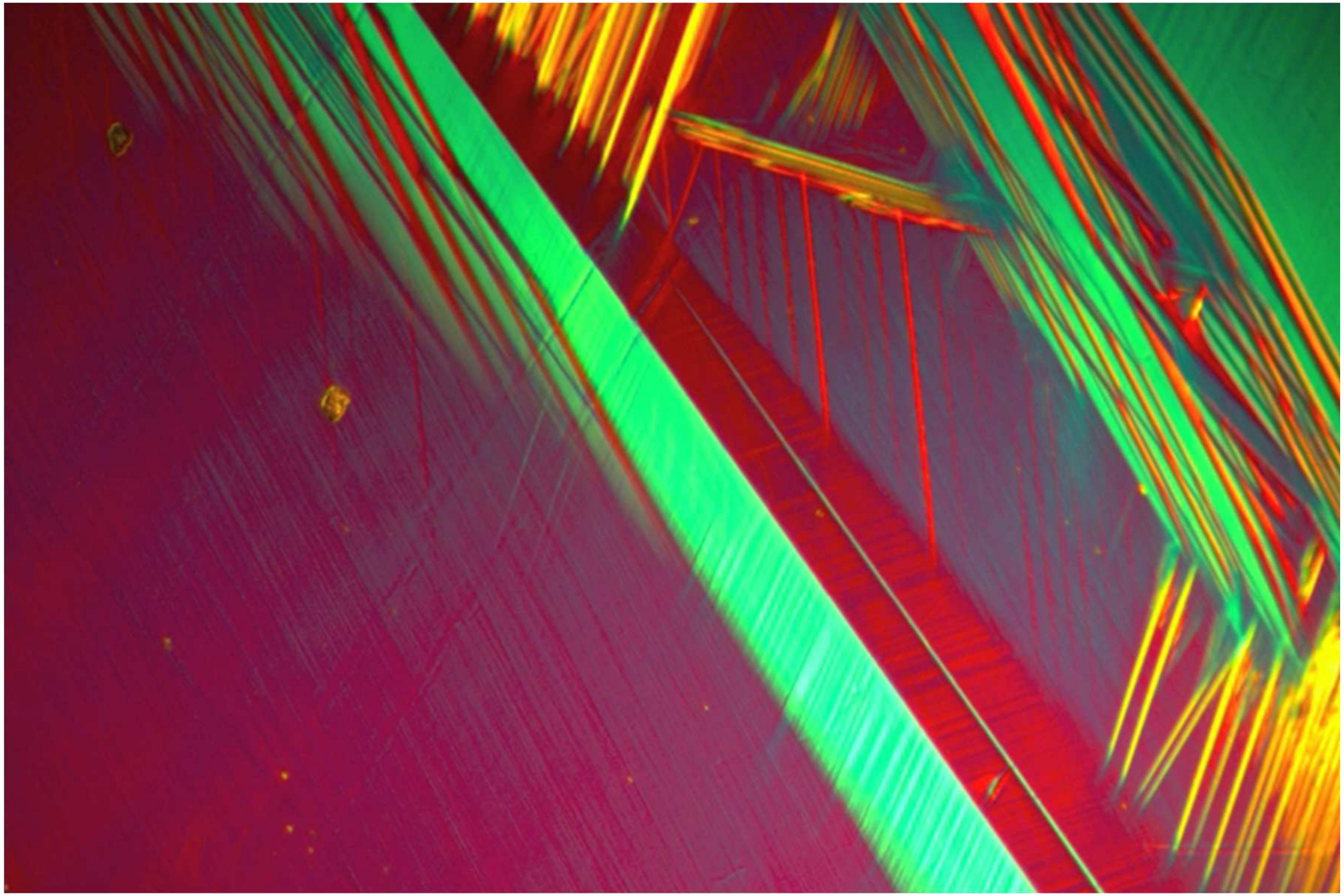
Construction of curved interface

This is possible at zero stress provided $\mathbf{1}$ is rank-one connected to a relative interior point of the set $K = \cup_{i=1}^{N} SO(3)U_i$ of the martensitic wells, where relative is taken with respect to the set $D = \{A : \det A = \det U_i\}$. Such relative interior points are known to exist in the cubic-to-tetragonal case due to a result by Dolzmann and Kirchheim.

JB, K. Koumatos 2014

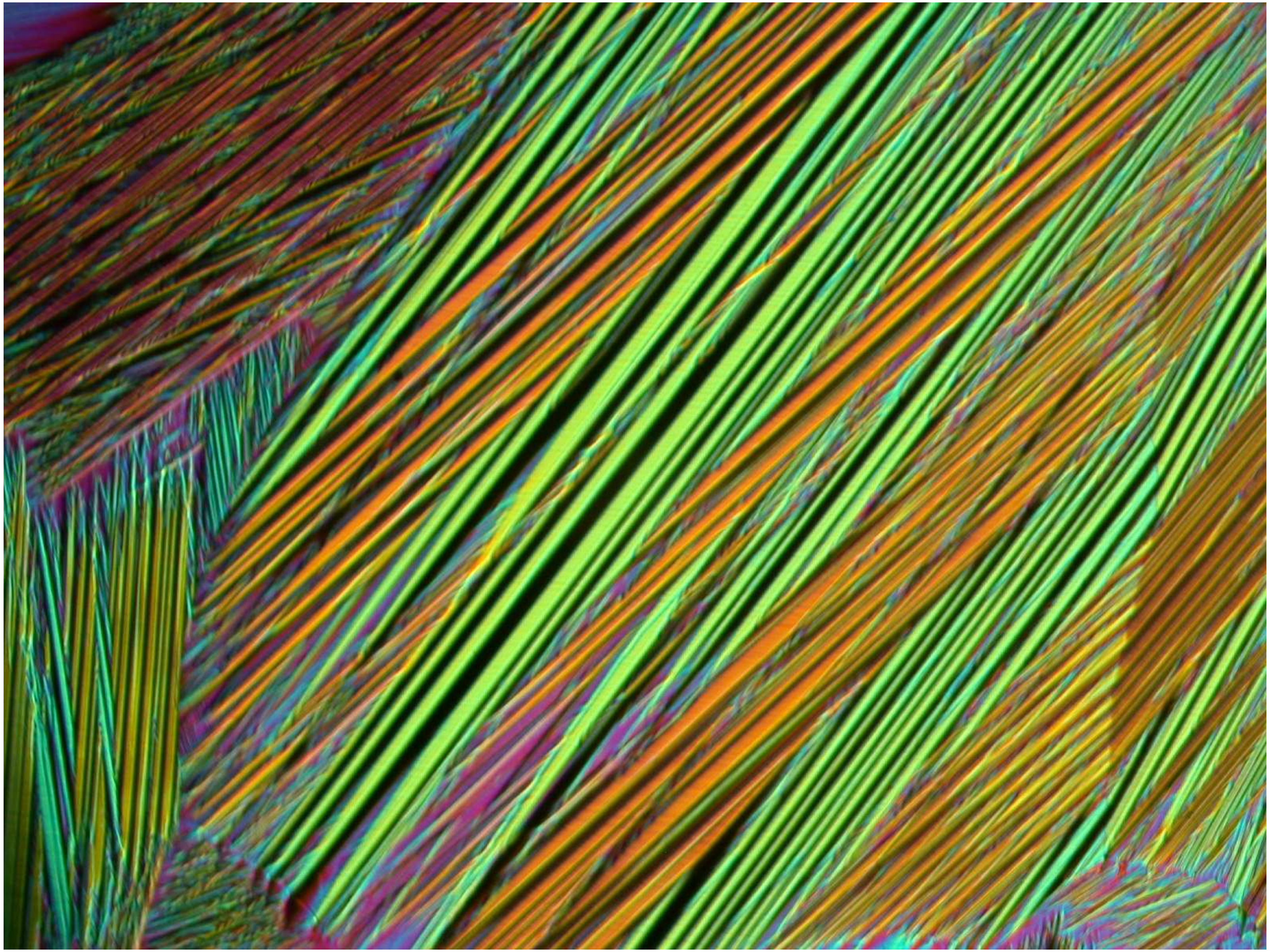
Lecture 6

Complex microstructures. Nucleation of austenite.

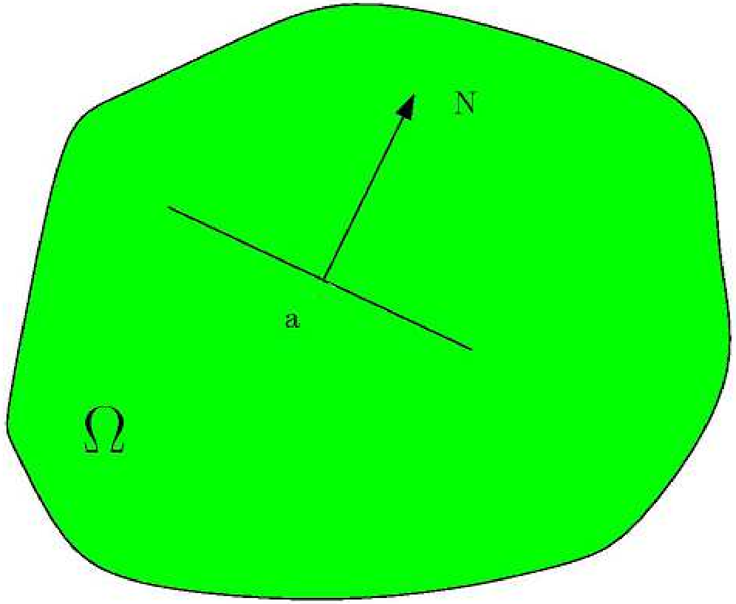


$Zn_{45}Au_{30}Cu_{2}$ ultra low hysteresis alloy

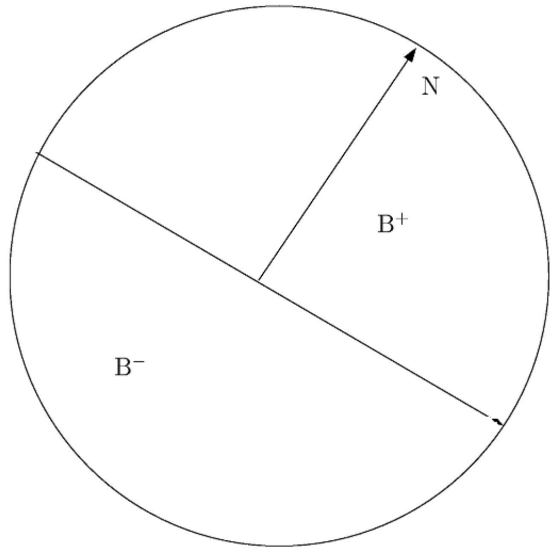
Yintao Song, Xian Chen, Vivekanand Dabade,
Thomas W. Shield, Richard D James, Nature, 502, 85–88 (03 October 2013)



CuZnAl microstructure: Michel Morin (INSA de Lyon)



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, $x \in B(0,1)$.

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

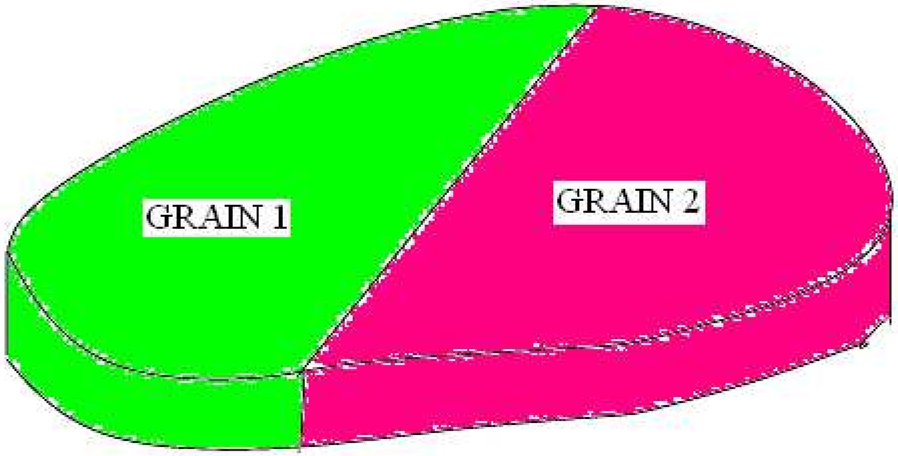
Theorem 1 (B/Carstensen). *There exists $b \in \mathbf{R}^n$ with $b \otimes N \in Dy^{+}(a)^c - Dy^{-}(a)^c$.*

Theorem 2 (B/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)

Application to polycrystals

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



Grain 1

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

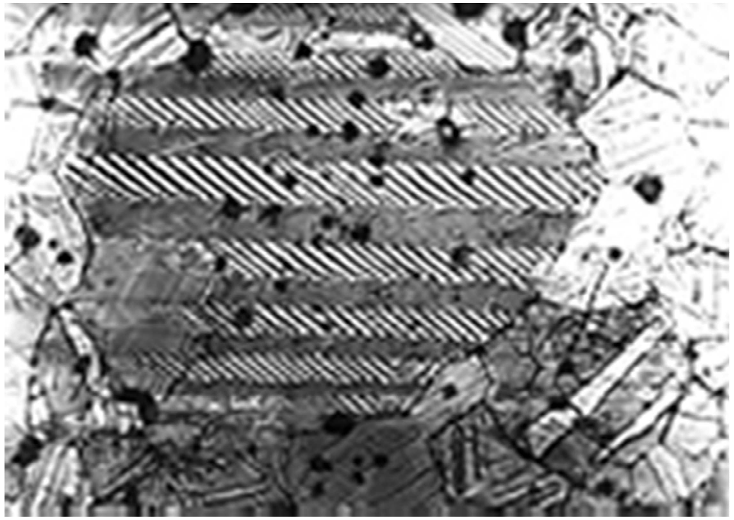
Grain 2

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

$$R_\alpha e_3 = e_3$$

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

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?



Microstructure in polycrystalline $BaTiO_3$ (G. Arlt).

Results 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.

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 interface contains a normal $(\cos\theta, \sin\theta) \in D_1$ and another normal $(\cos\theta', \sin\theta') \in D_2$, 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 the 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.

Nucleation of austenite in martensite

JB, Konstantinos Koumatos, Hanus Seiner

2012, 2013

Experimental observations

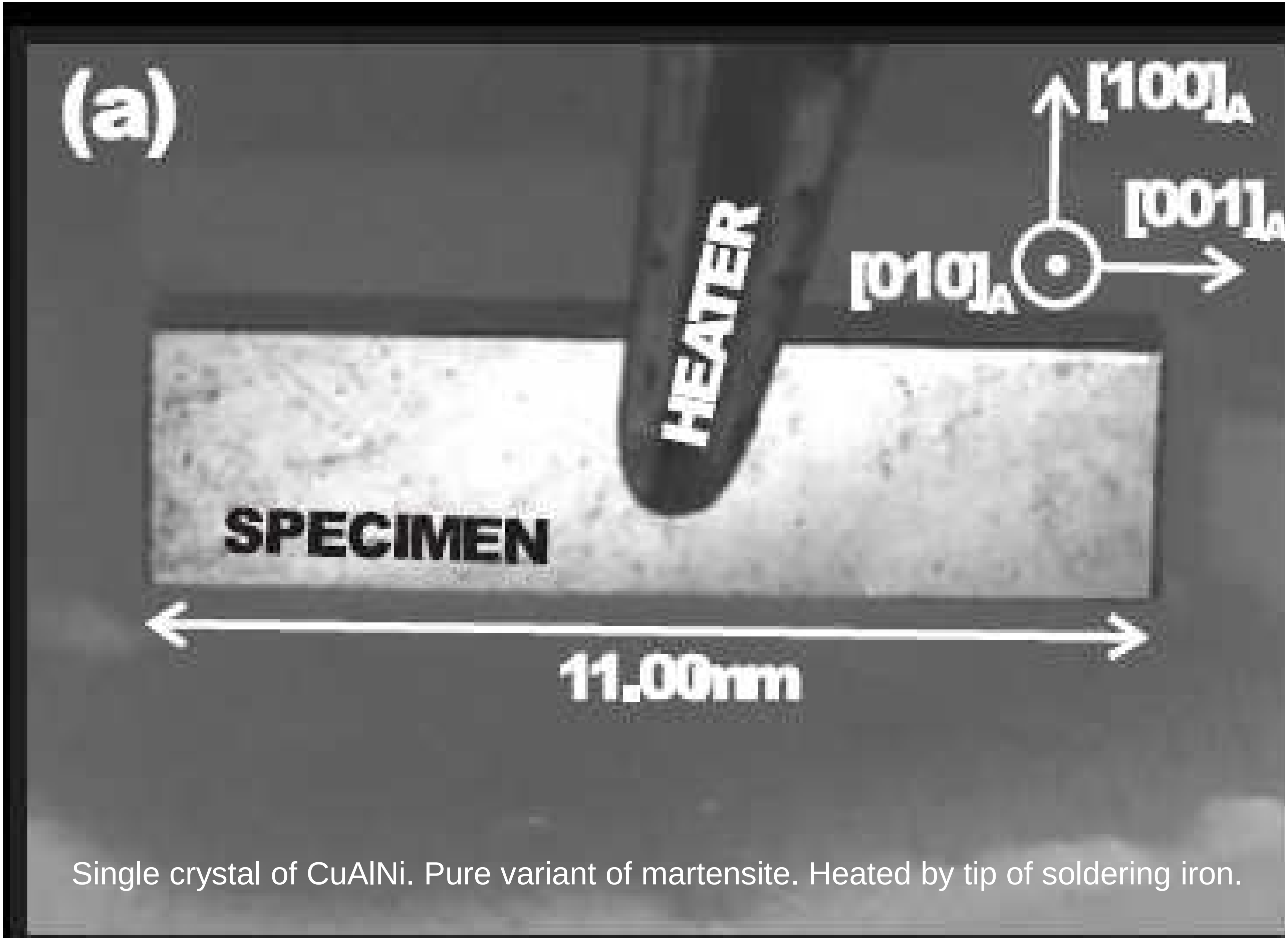
Specimen: single crystal of CuAlNi prepared by the Bridgeman method in the form of a prismatic bar of dimensions $12 \times 3 \times 3\text{mm}^3$ in the austenite with edges approximately along the principal cubic directions.

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.

The martensite-to-austenite transition temperatures were $A_S = -6°$C and $A_F = 22°$C. The critical temperature T_C for the transition from the stabilized martensite induced by homogeneous heating for this specimen was $\sim$60°C. This was estimated from optical observations of the transition with one of the specimen faces laid on and thermally contacted with a gradually heated Peltier cell, using a heat conducting gel.

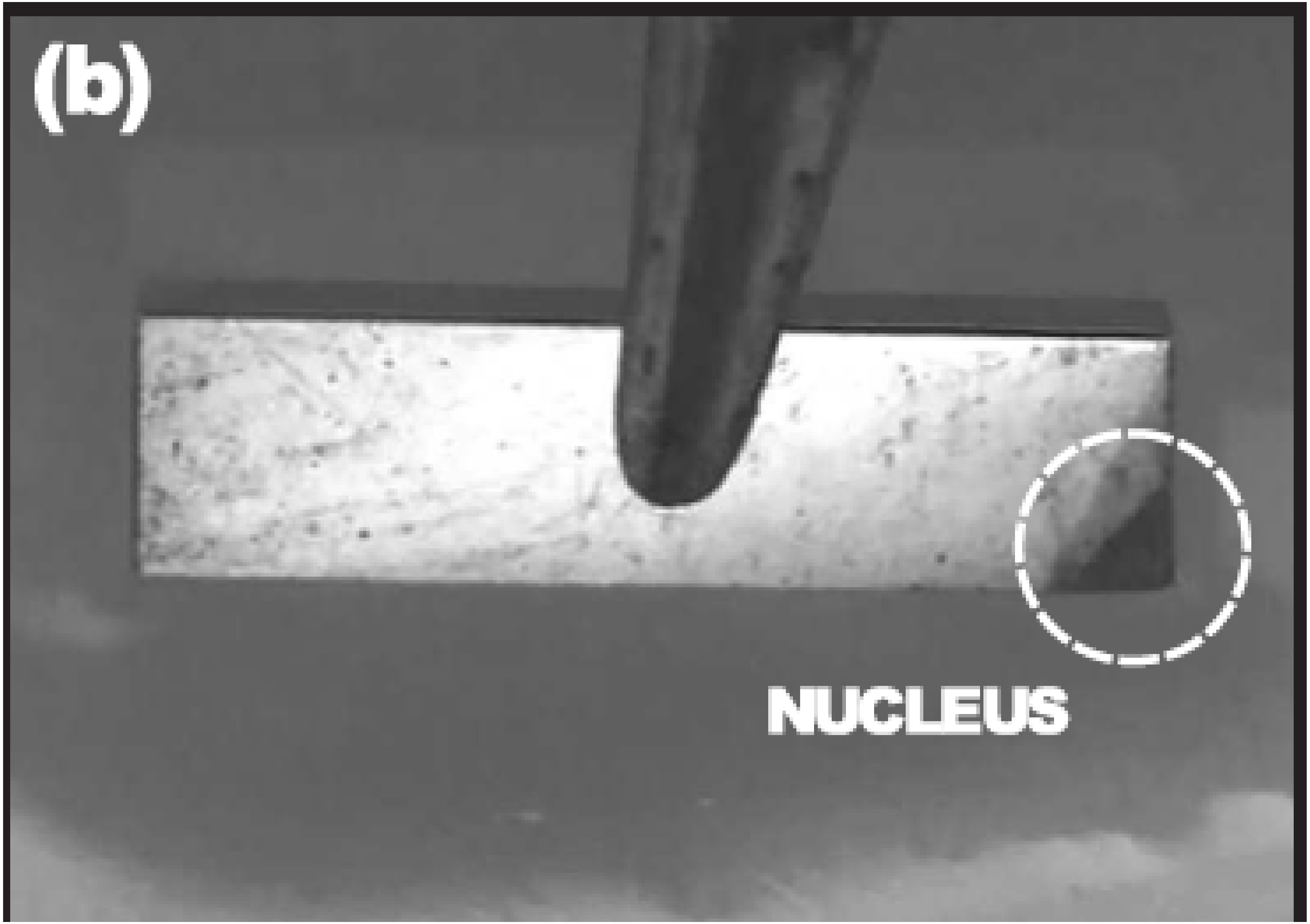
Localized heating experiment

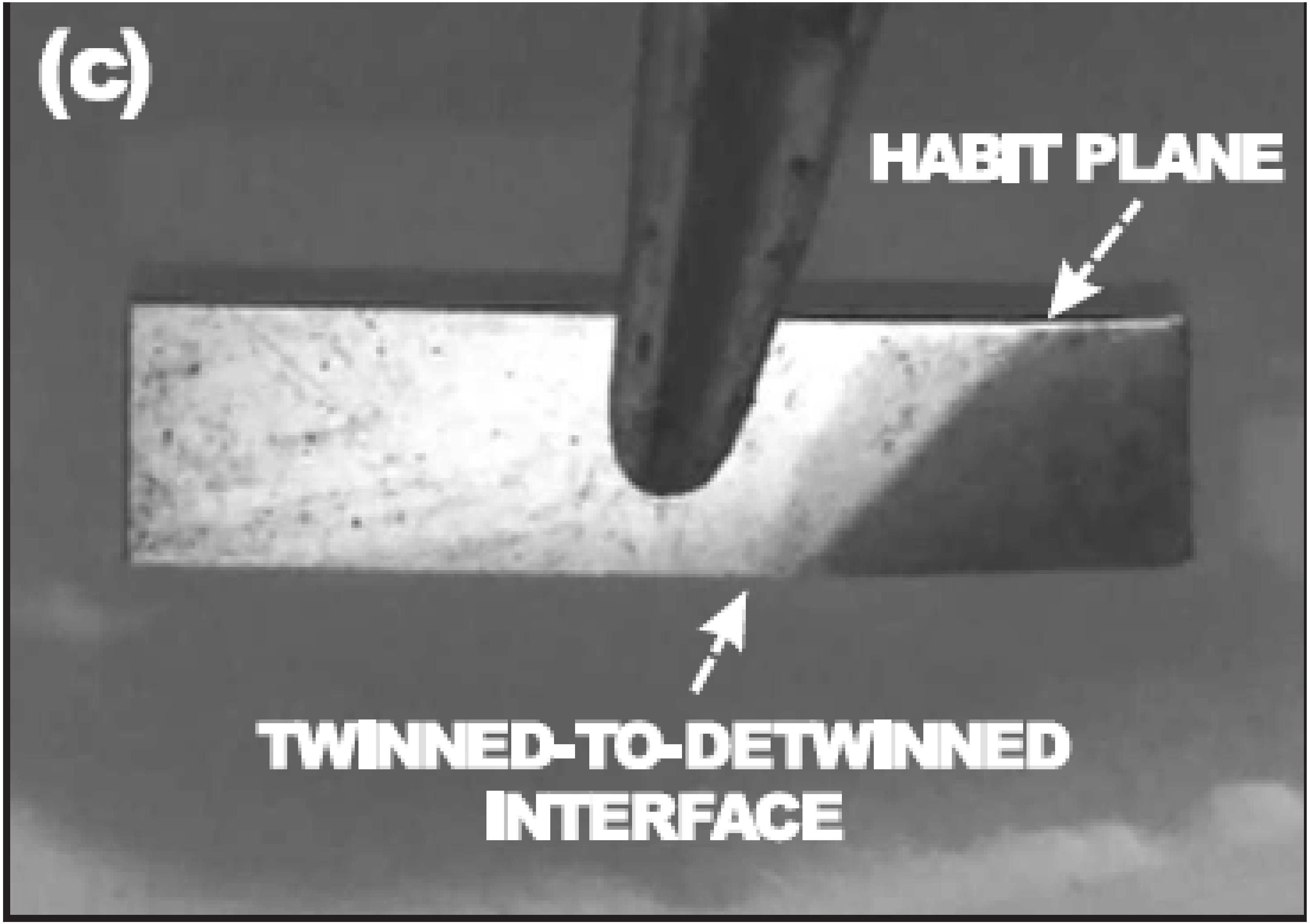
The specimen was freely laid on a slightly pre-stressed, free-standing polyethylene (PE) foil to ensure minimal mechanical constraints, then locally heated by touching its surface with an ohmically heated tip of a (digital) soldering iron with temperature electronically controlled to be 200°C, i.e. significantly above the A_S and T_C temperatures.



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

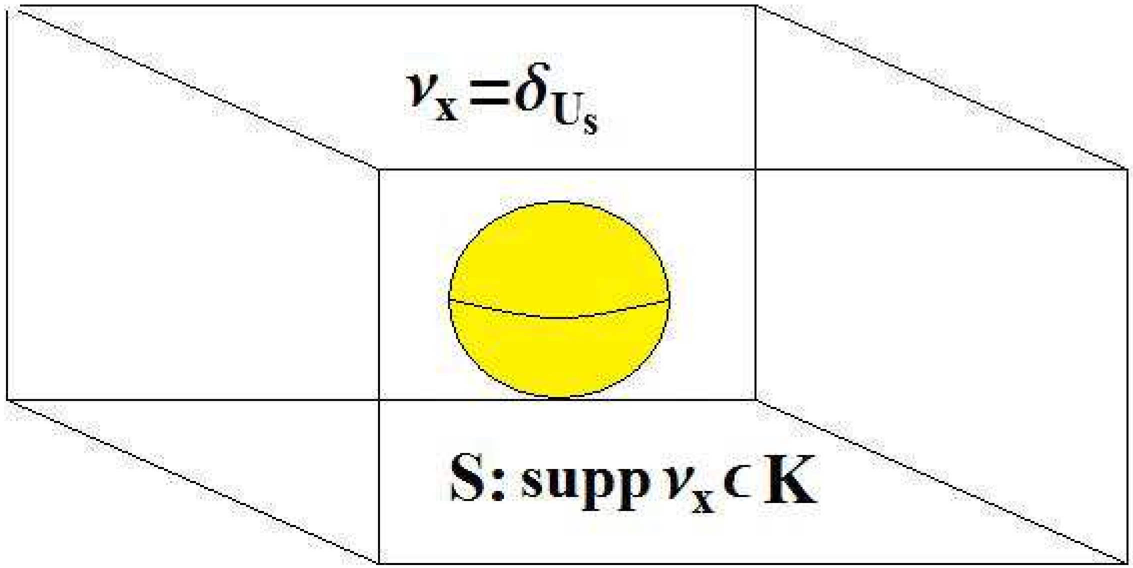
$$W(A) = \begin{cases} -\delta & A \in SO(3) \\ 0 & A \in \bigcup_{i=1}^{6} SO(3)U_i \\ +\infty & \text{otherwise} \end{cases},$$

and $\delta > 0$.

So $W(A) < \infty$ on

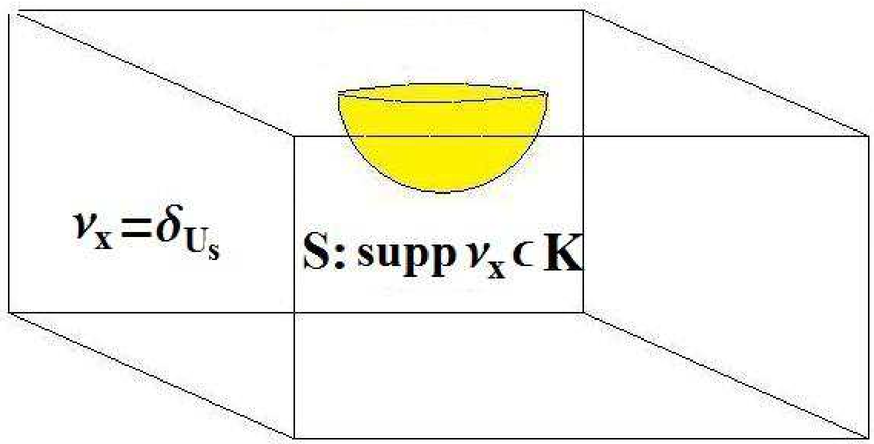
$$K = SO(3) \cup \bigcup_{i=1}^{6} SO(3)U_i$$

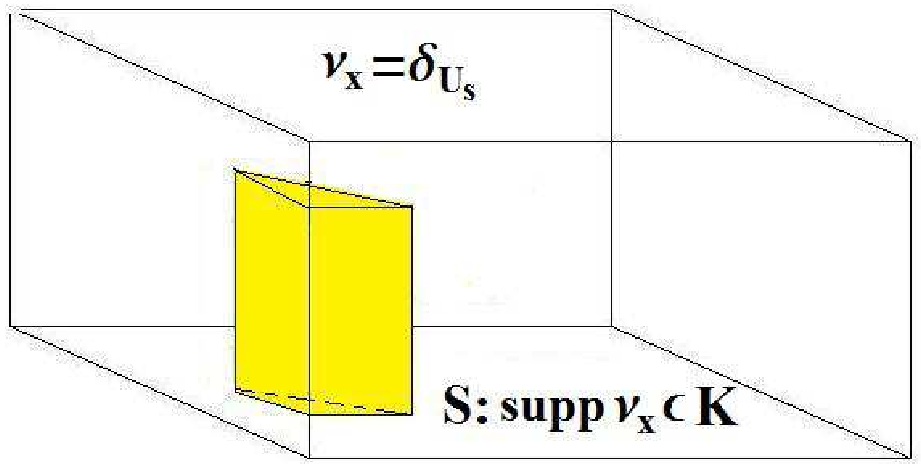
Nucleation impossible in the interior



Theorem $I(\nu) \geq I(\delta_{U_s})$
(quasiconvexity at U_s)

Nucleation impossible at faces or edges

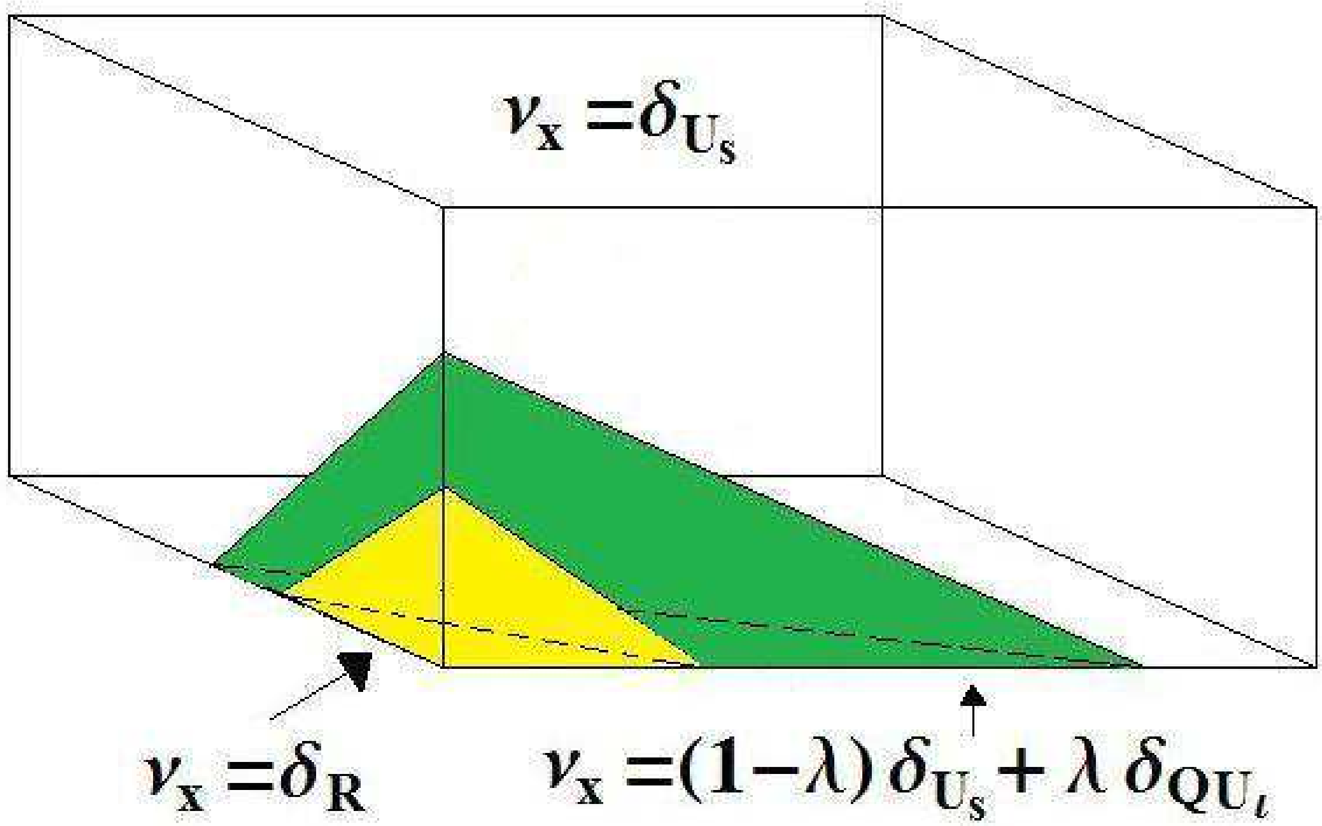




Similarly in these cases we have

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

Nucleation possible at a corner



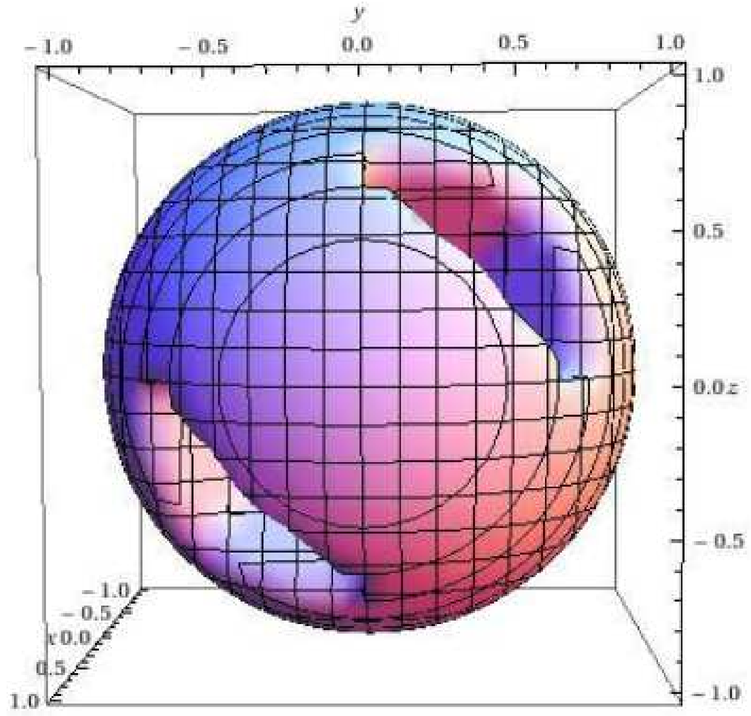
$I(\nu) < I(\delta_{U_s})$

I *not* quasiconvex at such a corner.

Remarks

1. We are able to prove quasiconvexity at faces with most, but not all, normals. What would happen for a specimen that was a ball?

Possible face normals for which we can prove quasiconvexity, using deformation parameters for Seiner's specimen.



2. We have shown that a *localized* nucleation can only occur at a corner, but one could hope to show using methods of Grabovsky & Mengesha (2009) that any ν sufficiently close to δ_{U_s} with $I(\nu) < I(\delta_{U_s})$ must involve nucleation at a corner.

Mechanical stabilization

Above $A_S = -6^\circ$C the energy of the austenite is less than that of the martensite. So why doesn't the transition from the stabilized martensite to austenite by homogeneous heating take place at a much lower temperature than $T_c \sim 60^\circ$C? In other words, what is the explanation for the mechanical stabilization effect?

One piece of evidence is that under homogeneous heating the nucleation still takes place at a corner, suggesting the relevance of the quasiconvexity calculations.

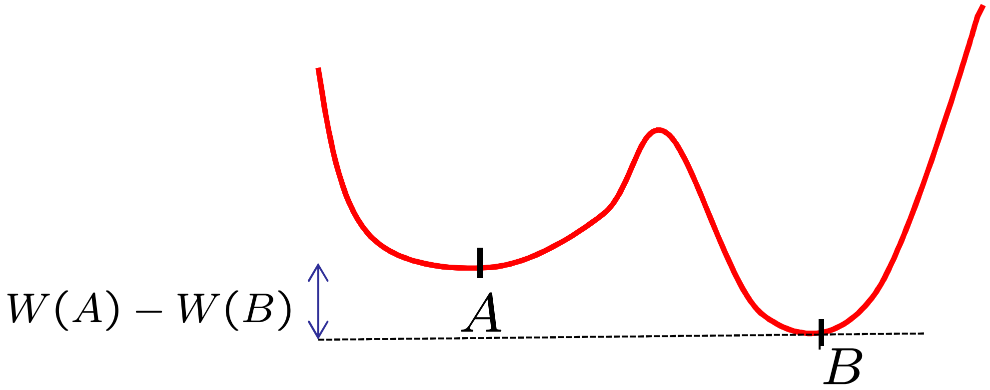
While a general explanation is lacking, a relevant consideration is the following: if we nucleate a small volume V of austenite from a single laminate of martensite (idealizing the thermally induced martensite) by introducing an austenite-martensite interface at a corner, we reduce the energy by δV *plus* a term proportional to V, representing the energy of the interfaces between twins in the laminate which are no longer there in the austenite.

Lecture 7

Local minimizers with and without interfacial energy

Incompatibility-induced hysteresis

JB/James 2014



Example.

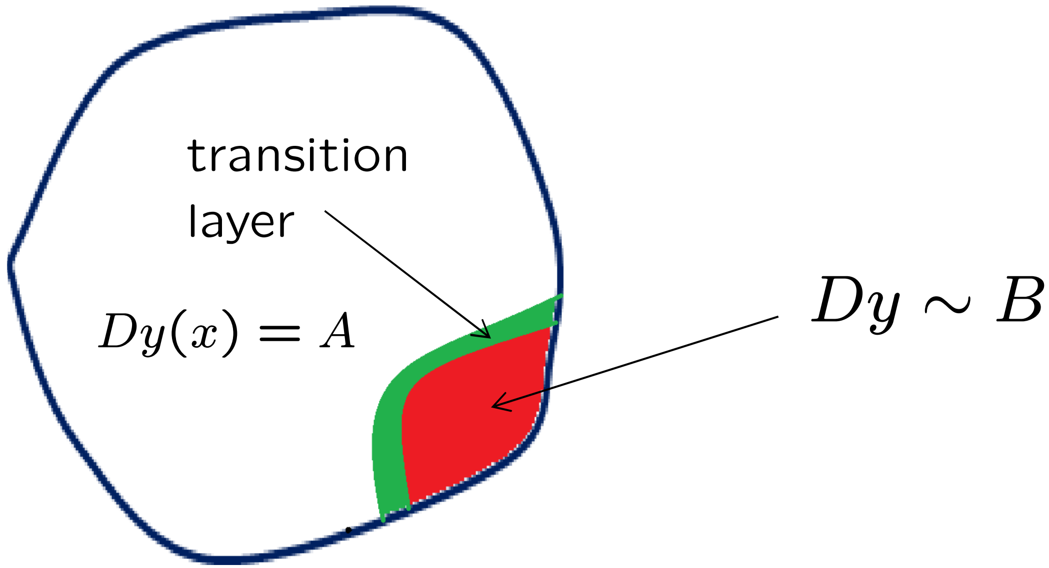
Consider the integral

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

where $W : M^{3\times 3} \to \mathbb{R}$ and W has two local minimizers at A, B with 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.



Definition. Let $K_1, \ldots, K_N$ be nonempty, disjoint, compact subsets of $M^{m\times n}$. Then the $\{K_i\}$ are incompatible if whenever $(\nu_x)_{x\in\Omega}$ is a gradient Young measure with

$$\text{supp } \nu_x \subset \bigcup_{i=1}^{N} K_i \ \text{ a.e. } x \in \Omega$$

then

$$\text{supp } \nu_x \subset K_r \ \text{ a.e. } x \in \Omega$$

for some r.

Otherwise, the $\{K_i\}$ are compatible.

Example 1

$K_1 = \{A_1\}, \ldots, K_N = \{A_N\}, \;\; A_i \in M^{m\times n}$.

A necessary condition for the sets $K_1, \ldots, K_N$ to be incompatible is that

$$\text{rank}\,(A_i - A_j) > 1, \;\; \text{for all } i \neq j.$$

This is sufficient iff $N \leq 3$.

$N = 2$ B/James

$N = 3$ Šverák

$N = 4$ Counterexample of Tartar/Scheffer.

Contrast with case of exact gradients.
If $N \leq 4$ then

$$Dy(x) \in \bigcup_{i=1}^{N} \{A_i\} \text{ a.e.}$$

implies

$$Dy(x) = A_r \text{ a.e. for some } r$$

(Chlebik/Kirchheim) but this is false for $N \geq 5$ (Kirchheim/Preiss).

Example 2

Let $m = n$,

$$K_1 = \mathrm{SO}(n)U_1, \ldots, K_N = \mathrm{SO}(n)U_N$$

$U_i = U_i^T > 0$ distinct.

A necessary condition for the sets $K_1, \ldots K_N$ to be incompatible is that there are no rank-one connections between the K_i.

Sufficient if $n = 2$ (Šverák) and for $n = 3, N = 2$ for certain classes of U_1, U_2 (Matos, Kohn/Lods, Dolzmann/Kirchheim/Müller/Šverák).

However the

Conjecture (Kinderlehrer)
K_1, K_2 are incompatible iff K_1, K_2 not rank-one connected.

is unresolved.

A function $f : M^{m\times n} \to \mathbf{R} \cup \{+\infty\}$ is quasiconvex if there exists a nondecreasing sequence $f^{(j)} : M^{m\times n} \to \mathbf{R}$ of quasiconvex functions with

$$f(A) = \lim_{j\to\infty} f^{(j)}(A) \text{ for all } A \in M^{m\times n}.$$

Theorem

$K_1, \ldots, K_N$ are incompatible iff
(i) the sets K_i^{qc} are gradient incompatible
(ii) for each $i = 1, \ldots, N$ the functions $\phi_i : M^{m\times n} \to [0, \infty]$ defined by

$$\phi_i(A) = \begin{cases} 1 & \text{if } A \in K_i^{\text{qc}} \\ 0 & \text{if } A \in \bigcup_{j\neq i} K_j^{\text{qc}} \\ +\infty & \text{otherwise} \end{cases}$$

are quasiconvex.

Transition layer estimate:

Suppose $K_1, K_2 \subset M^{m\times n}$ incompatible, $\Omega \subset \mathbb{R}^n$ a bounded Lipschitz domain. Let $1 < p < \infty$. Then there exist constants $\varepsilon_0(K_1, K_2, p, \Omega) > 0$, $\gamma_0(K_1, K_2, p, \Omega) > 0$ such that if $0 \leq \varepsilon \leq \varepsilon_0$, $y \in W^{1,p}(\Omega; \mathbb{R}^m)$ then

$$\int_{T_\varepsilon(y)} [1 + |Dy|^p]\, dx \geq \gamma_0 \min\{\mathcal{L}^n(\Omega_{1,\varepsilon}(y)), \mathcal{L}^n(\Omega_{2,\epsilon}(y))\},$$

where

$$\Omega_{i,\varepsilon}(y) = \{x \in \Omega : Dy(x) \in N_\varepsilon(K_i)\}$$

$$T_\varepsilon(y) = \{x \in \Omega : Dy(x) \notin N_\varepsilon(K_1) \cup N_\varepsilon(K_2)\}$$

Hence one can prove a metastability theorem for microstructures with a pair of incompatible sets K_1, K_2 replacing the matrices A, B.

Applications:

1. Biaxial experiments on CuAlNi of Chu &James.

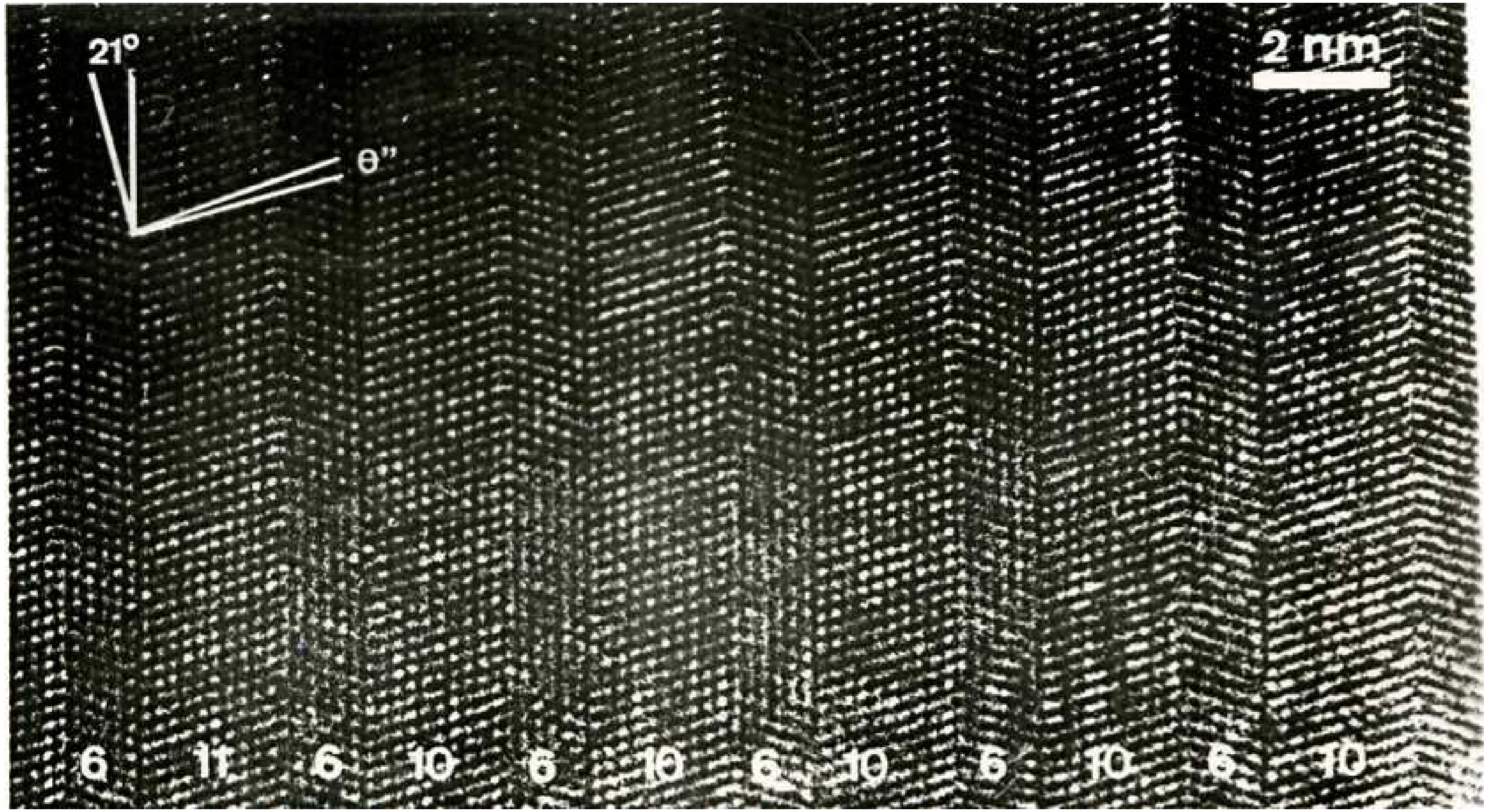
2. Pure dilatational transformations with energy wells $SO(3)$ and $kSO(3)$ with $k > 0$.

3. Terephthalic acid. Huge transformation strain

$$U = \begin{pmatrix} 0.970 & 0.038 & -0.121 \\ 0.038 & 0.835 & -0.017 \\ -0.121 & -0.017 & 1.298 \end{pmatrix}$$

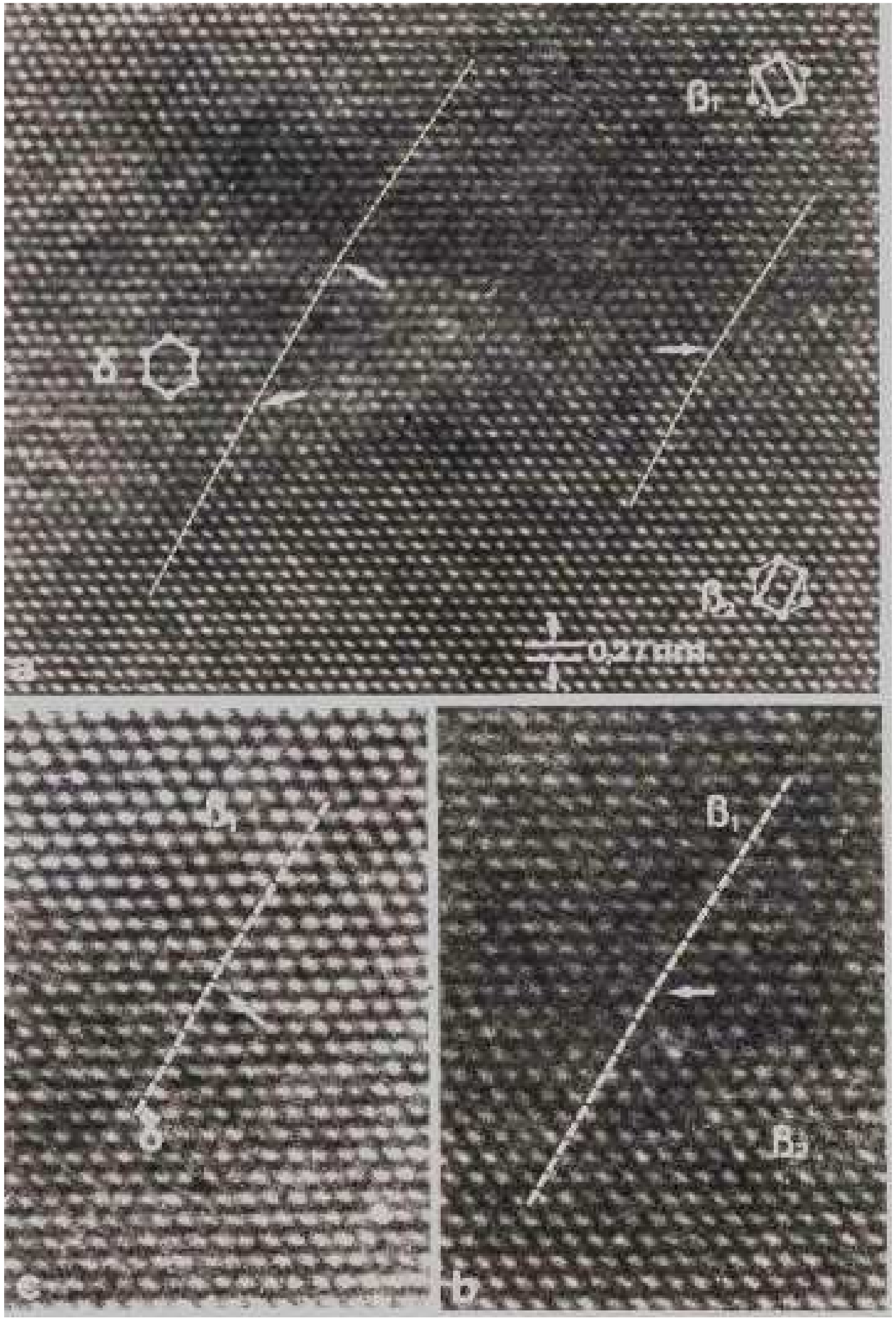
Interfacial energy

Some interfaces are atomistically sharp



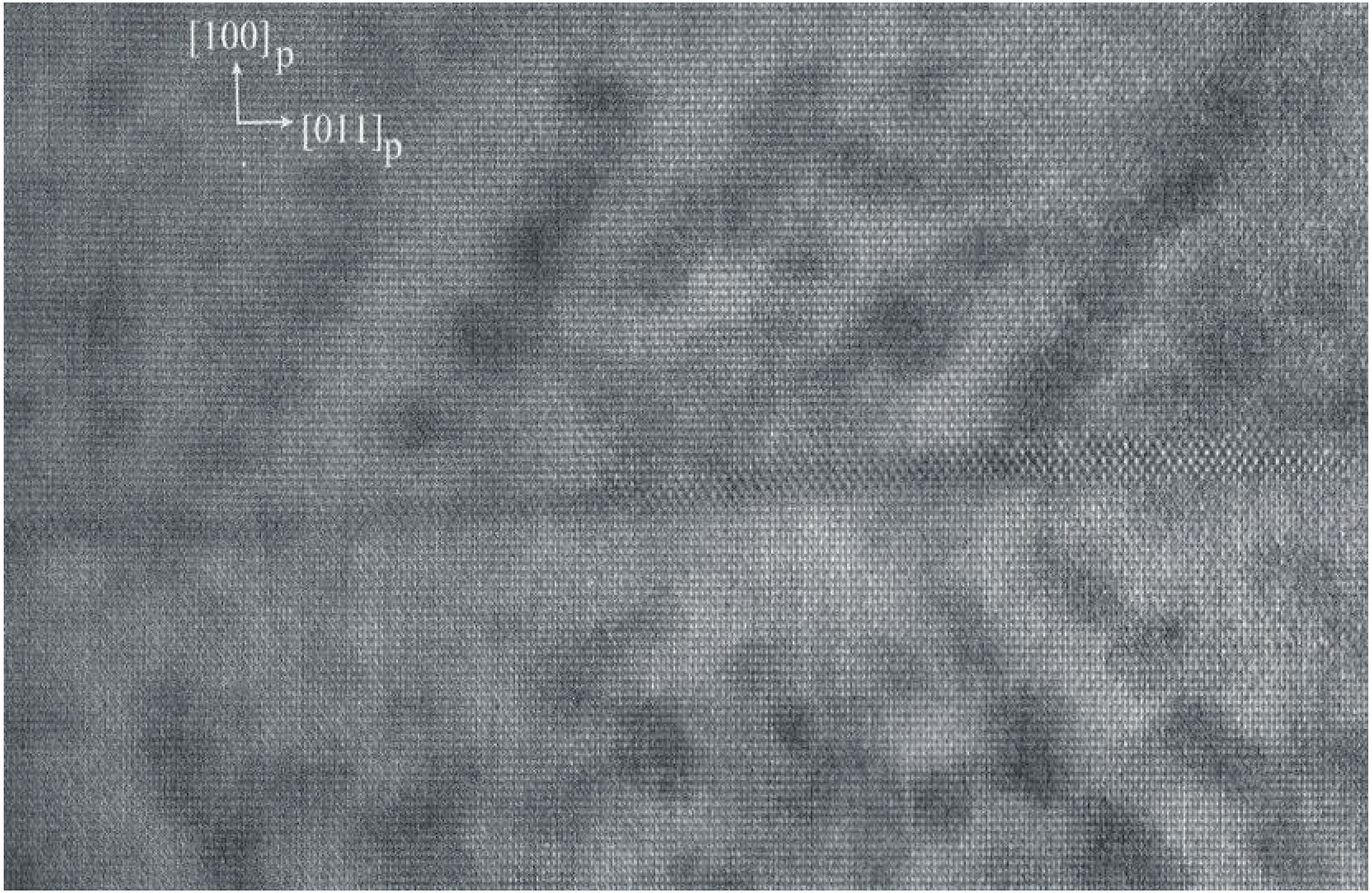
NiMn Baele, van Tenderloo, Amelinckx

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

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

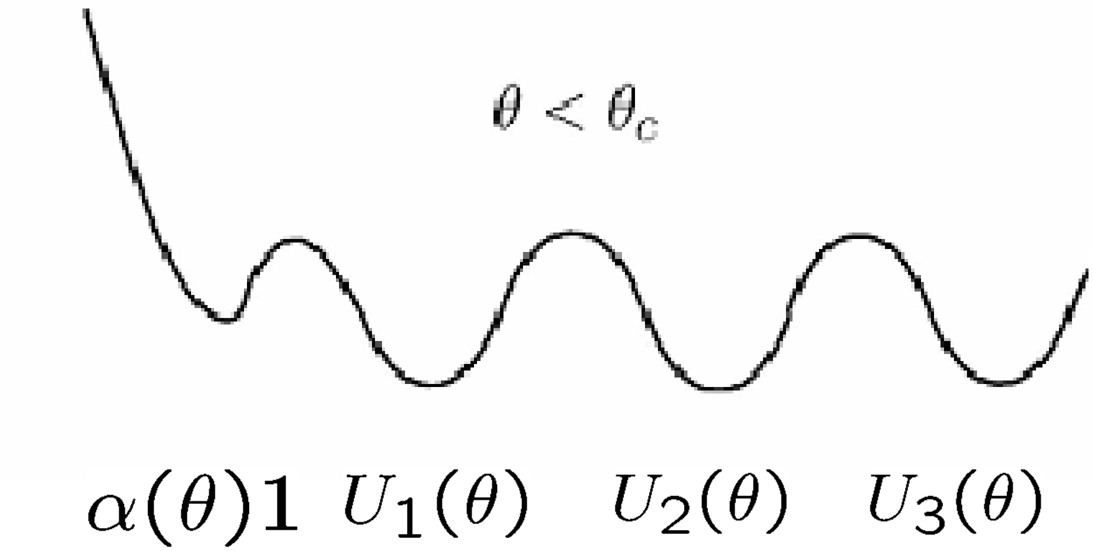
in $W^{1,\infty}(\Omega;\mathbf{R}^3)$.

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 $\to$ 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.

Sharp interface models

A natural idea is to minimize an energy such as

$$I(y) = \int_\Omega W(Dy)\,dx + \kappa\mathcal{H}^2(S_{Dy}),$$

where $\kappa > 0$ and S_{Dy} denotes the jump set of Dy.

However this is not a sensible model, because if we have a sharp interface and approximate y by a smooth deformation, then the interfacial energy disappears and the elastic energy hardly changes. Thus a minimizer can never have a sharp interface.

A model allowing smooth and sharp interfaces JB/ Carlos Mora-Corral (Madrid)

If we combine the smooth and sharp interface models we get a model that is well posed and in fact allows both kind of interface. In the simplest case we minimize

$$I(y) = \int_\Omega (W(Dy) + \varepsilon^2 |\nabla^2 y|^2)\, dx + \kappa \mathcal{H}^2(S_{Dy})$$

in the set

$$\mathcal{A} = \{y \in W^{1,p} : Dy \in GSBV, y|_{\partial\Omega_1} = \bar{y}\}.$$

Here $\nabla^2 y$ denotes the weak approximate differential of Dy.

More generally we can suppose the energy is given by

$$\begin{aligned} I(y) &= \int_\Omega W(Dy, \nabla^2 y)\, dx + \\ &\qquad \int_{S_{Dy}} \gamma(Dy^+(x), Dy^-(x), \nu(x))\, d\mathcal{H}^2(x). \end{aligned}$$

One-dimensional case

Minimize

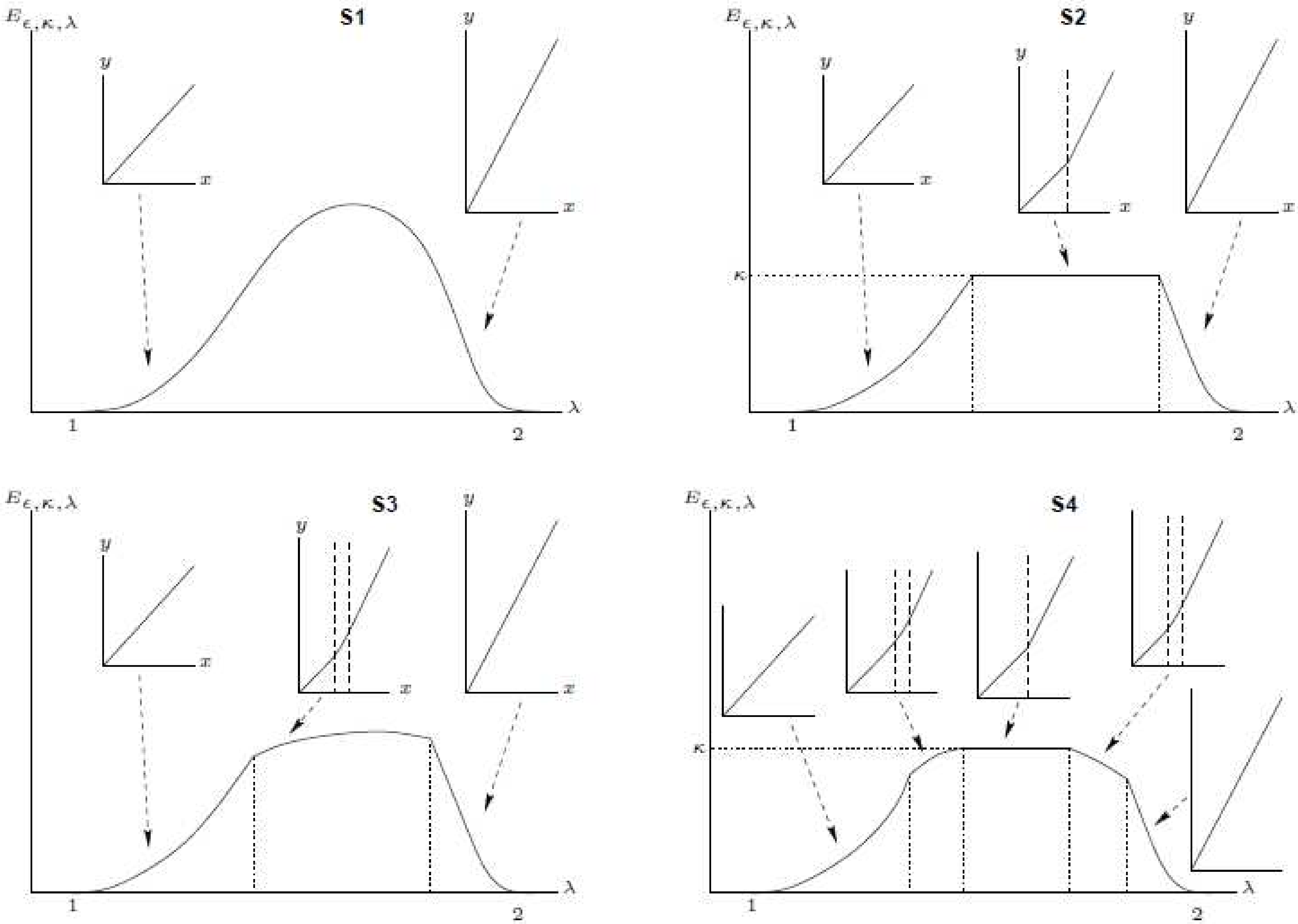
$$I_{\varepsilon,\kappa}(y) = \int_0^1 (W(y') + \varepsilon^2 |\nabla^2 y|^2)\, dx + \kappa \mathcal{H}^0(S_{y'})$$

in

$$\begin{aligned}\mathcal{A}_\lambda &= \{y \in W^{1,1}(0,1) : y(0) = 0, y(1) = \lambda, \\ &\qquad y' \in SBV(0,1), y' > 0 \text{ a.e.}\}\end{aligned}$$

Assume $W(1) = W(2) = 0, W(p) > 0$ if $p \neq 0, 1$. Let

$$E_{\varepsilon,\kappa,\lambda} = \inf_{y \in \mathcal{A}_\lambda} I_{\varepsilon,\kappa}(y)$$


S1
S2
S3
S4
$E_{\epsilon,\kappa,\lambda}$
y
x
κ
λ
1
2