Harbin Institute of Technology
Summer School on Pure and Applied Mathematics
28 July – 4 August 2015

Mathematics of solid and liquid crystals

John Ball

University of Oxford

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

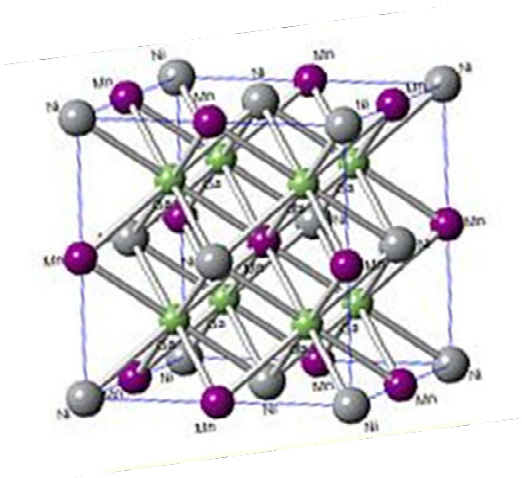
EPSRC Pioneering research and skills

European Research Council Established by the European Commission

THE ROYAL SOCIETY

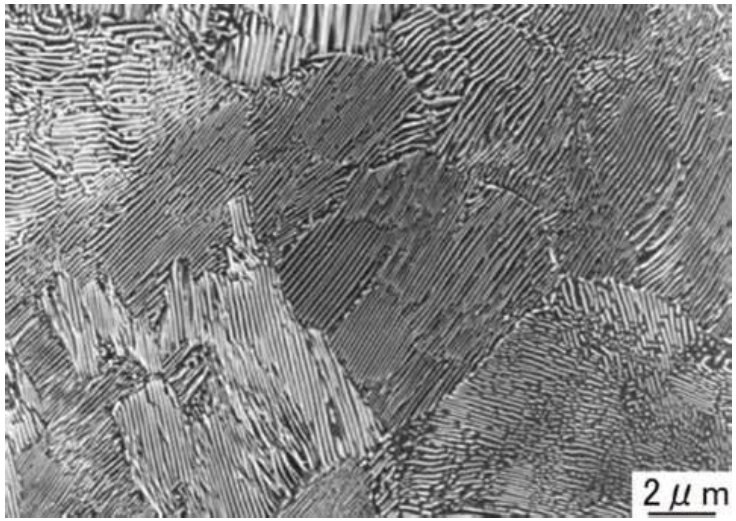
Oxford Centre for Nonlinear PDE

Solid crystals



Ni_2MnGa

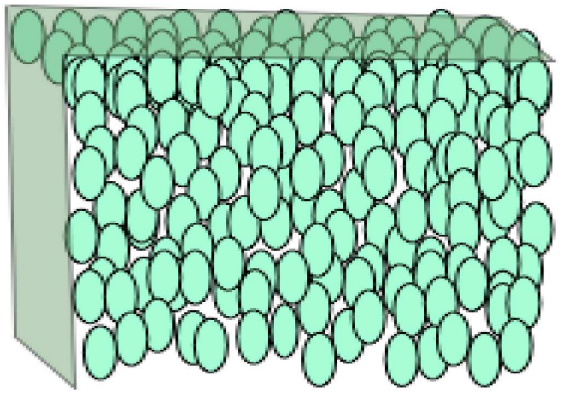
Wikipedia



Pearlite in steel

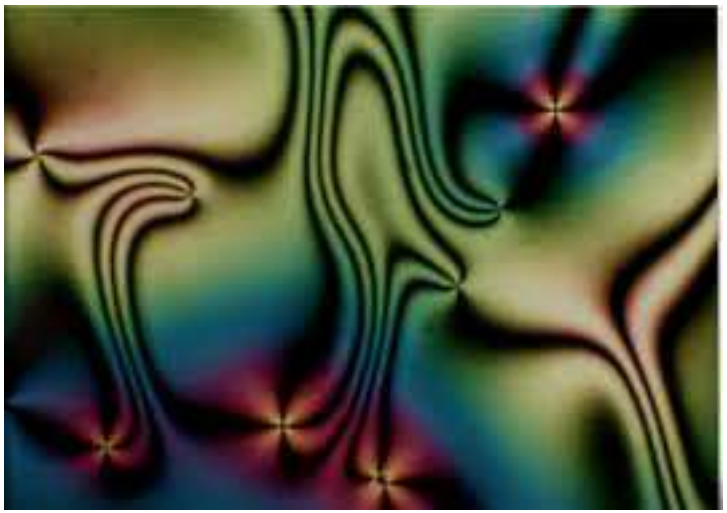
www.spaceflight.esa.int

Liquid crystals



Nematic liquid crystal

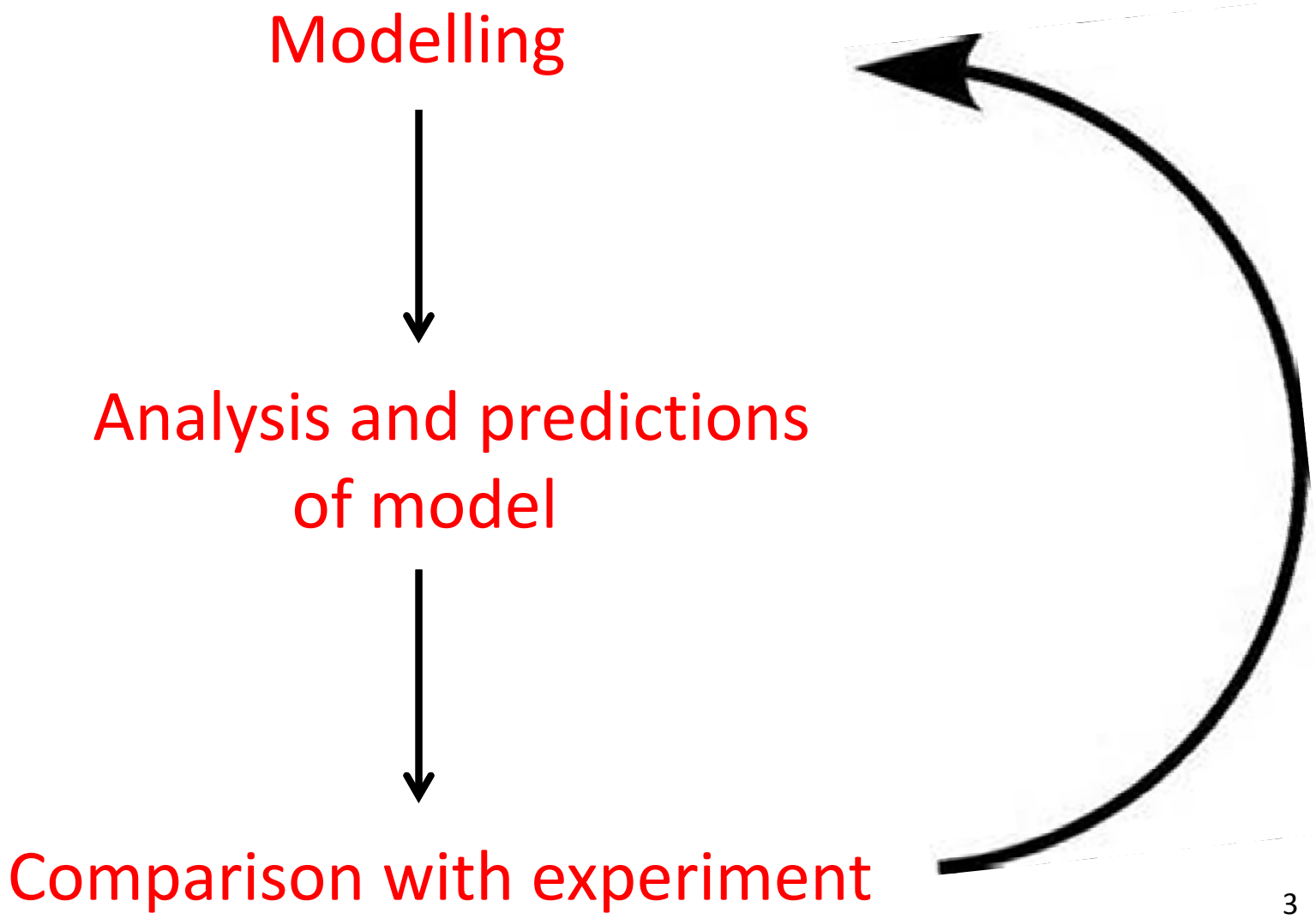
http://chemwiki.ucdavis.edu



Nematic liquid crystal defects

Oleg Lavrentovich (Kent State)

The scientific method for mathematicians



Mathematical areas relevant to the study of solid and liquid crystals

Group theory, linear algebra, invariant theory, nonlinear analysis, partial differential equations, calculus of variations, dynamical systems, probability, statistical mechanics, scientific computation, geometric measure theory, differential geometry, topology, algebraic geometry…

Common variational structure

Minimize a free-energy functional

$m \times n$ matrix

$$I(u) = \int_\Omega f(x, u(x), Du(x))\, dx$$

among $u : \Omega \to \mathbb{R}^m$, $\Omega \subset \mathbb{R}^n$ open, subject to suitable boundary conditions and constraints.

Some questions:

Why minimize I?

In what space of mappings should we look for minimizers, and on what basis do we choose this space?

Do (local or global) minimizers exist?

If so are they smooth or do they have singularities (defects)?

Plan of course

This week:

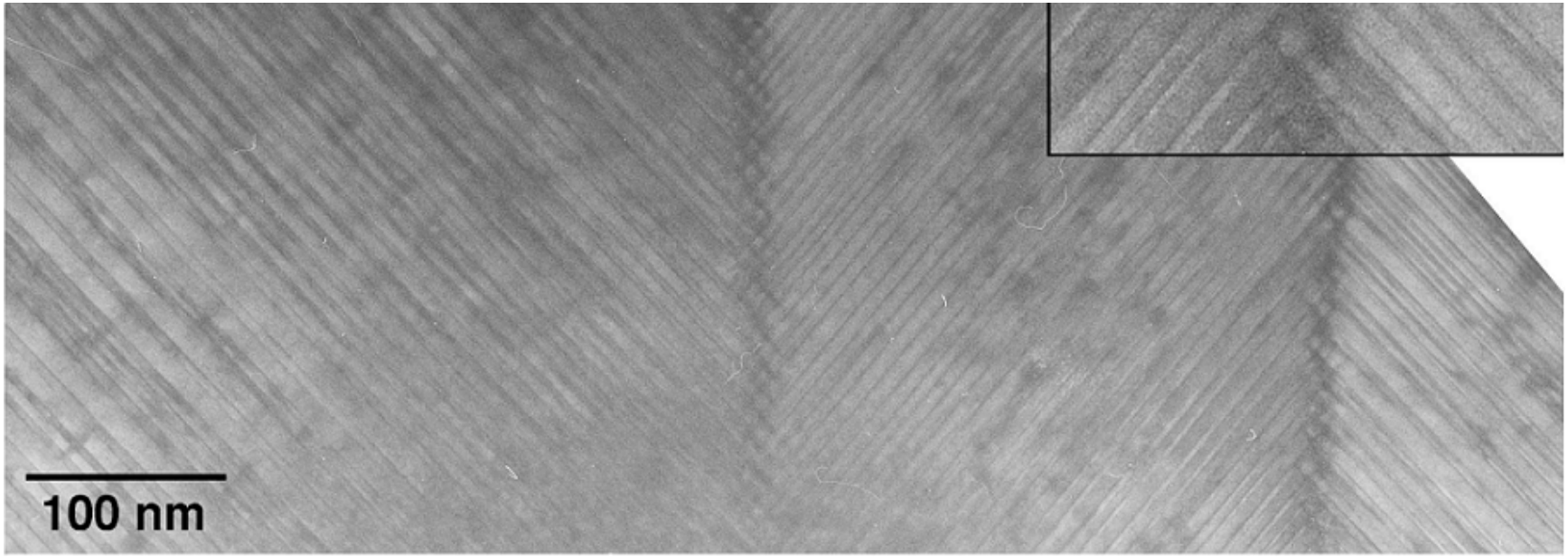
Crystalline solids, interfaces and microstructure

Next week:

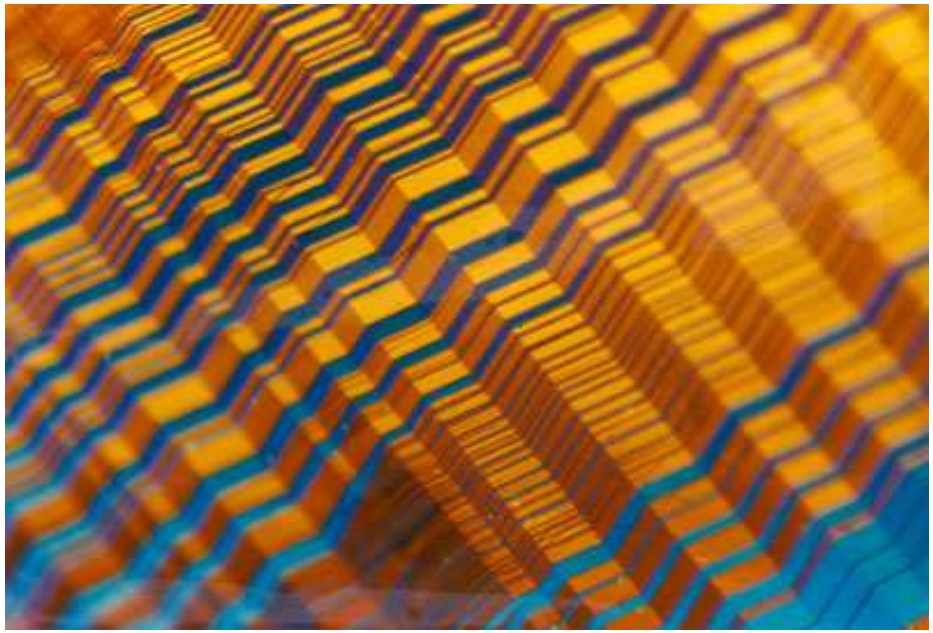
Liquid crystals and the description of defects.

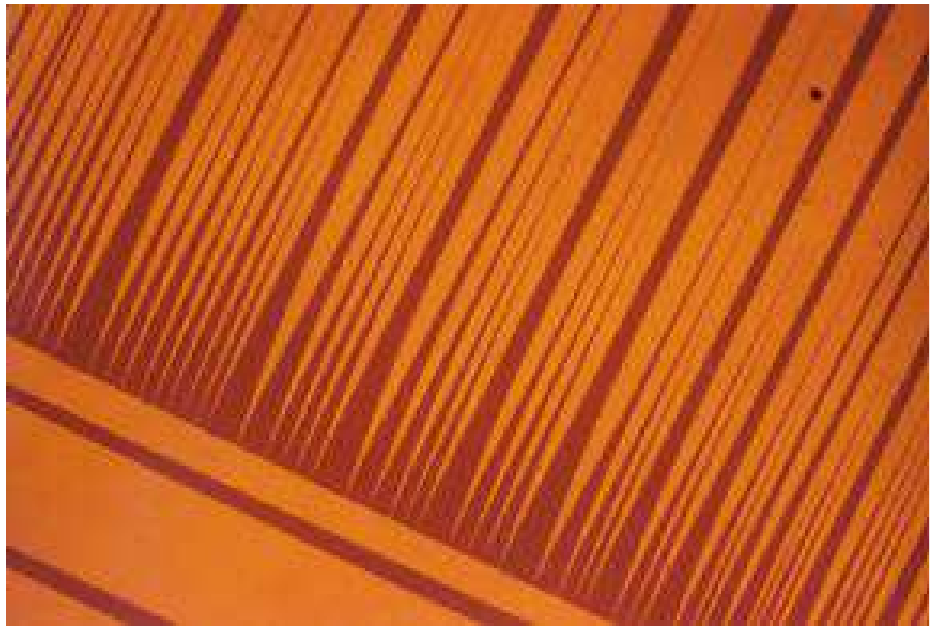
Crystalline solids, interfaces and microstructure

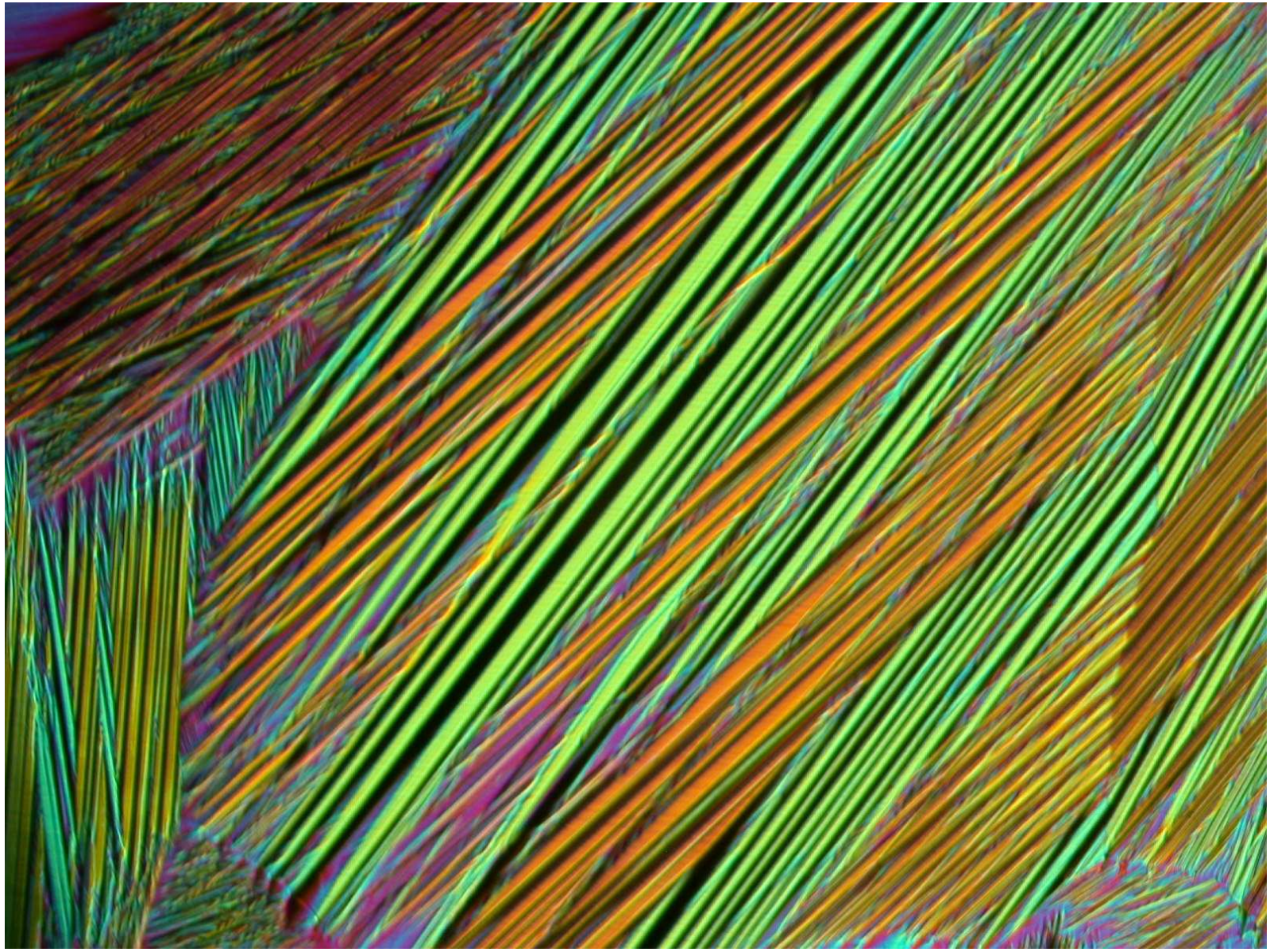
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



Martensitic microstructures in CuAlNi (Chu/James)







CuZnAl microstructure: Michel Morin (INSA de Lyon)

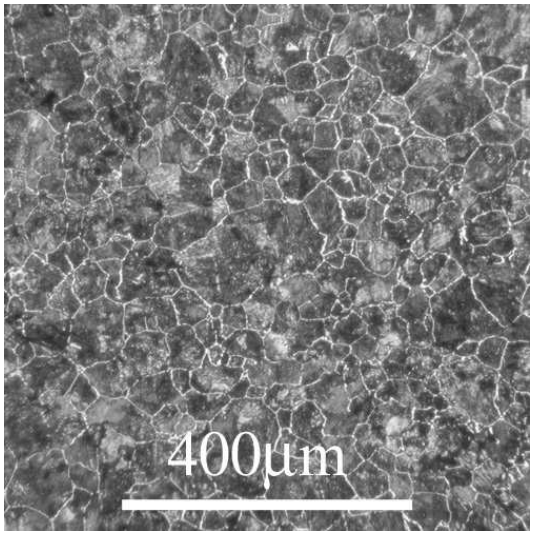
Topics

1. Nonlinear elasticity.
2. Existence of minimizers and analysis tools.
3. Martensitic phase transformations.
4. Microstructure.
5. Austenite-martensite interfaces.
6. Complex microstructures. Nucleation of austenite.
7. Local minimizers with and without interfacial energy.

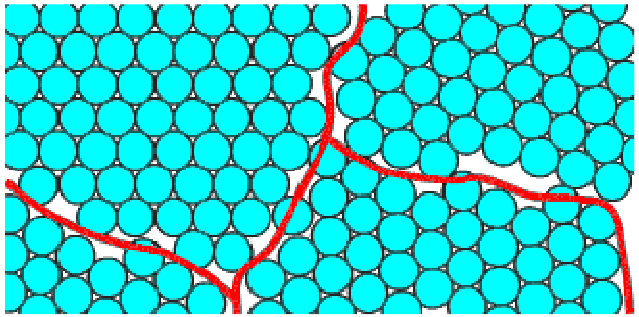
1. Nonlinear elasticity

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.

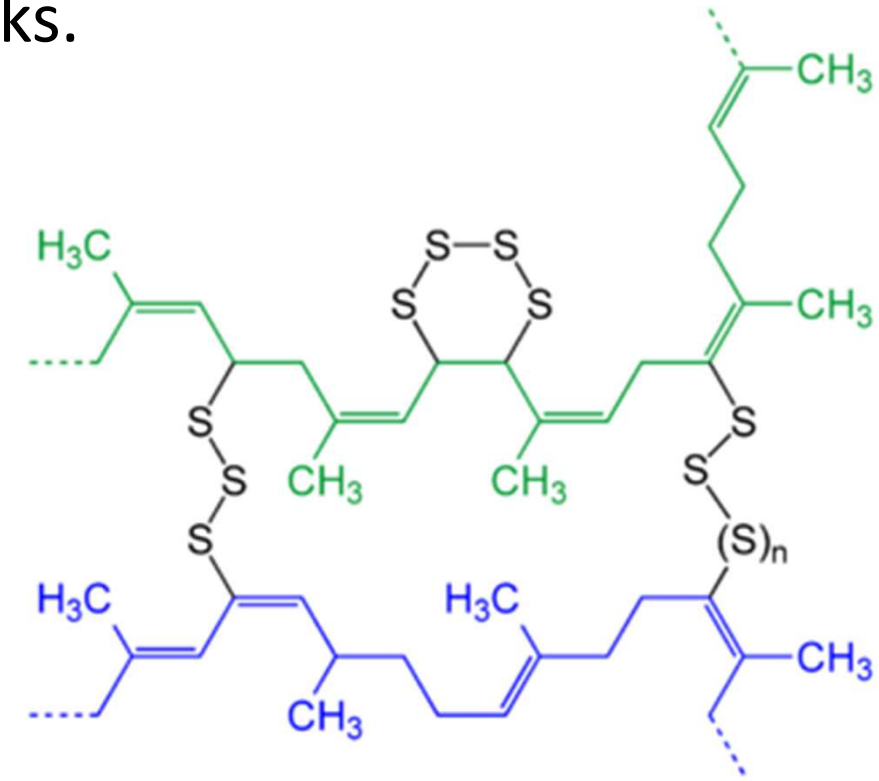


Iron carbon alloy, showing grain structure



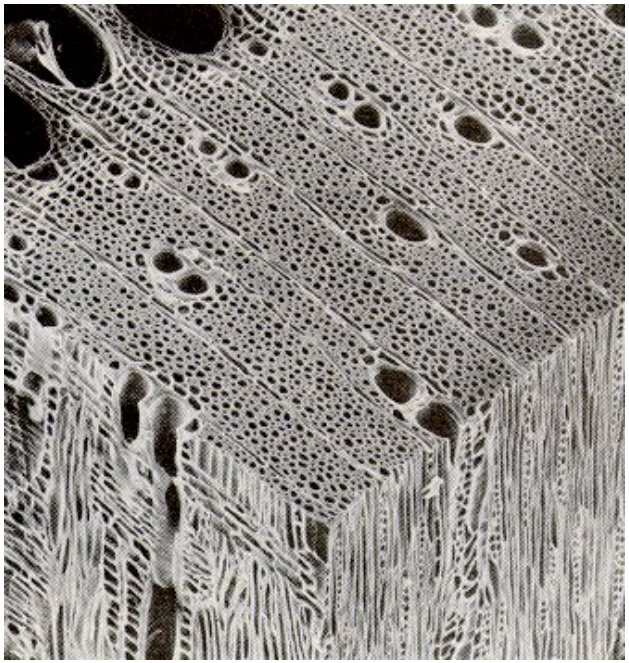
http://www.doitpoms.ac.uk

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.



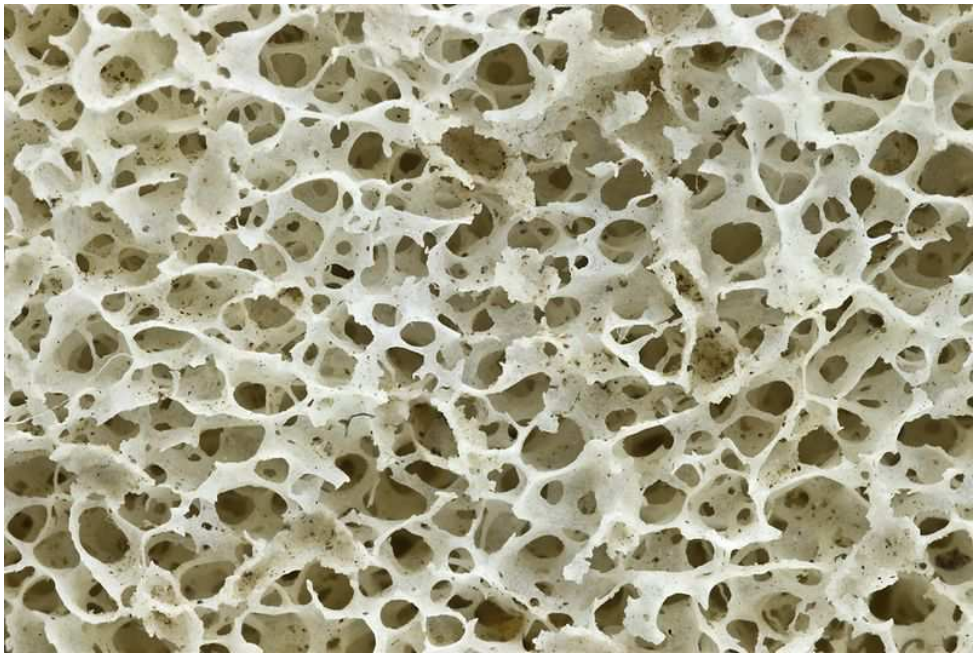
Schematic presentation of two strands (blue and green) of natural rubber after vulcanization with sulphur. (Wikipedia)

Wood and bone have a cellular structure.



White ash

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



Human hip bone

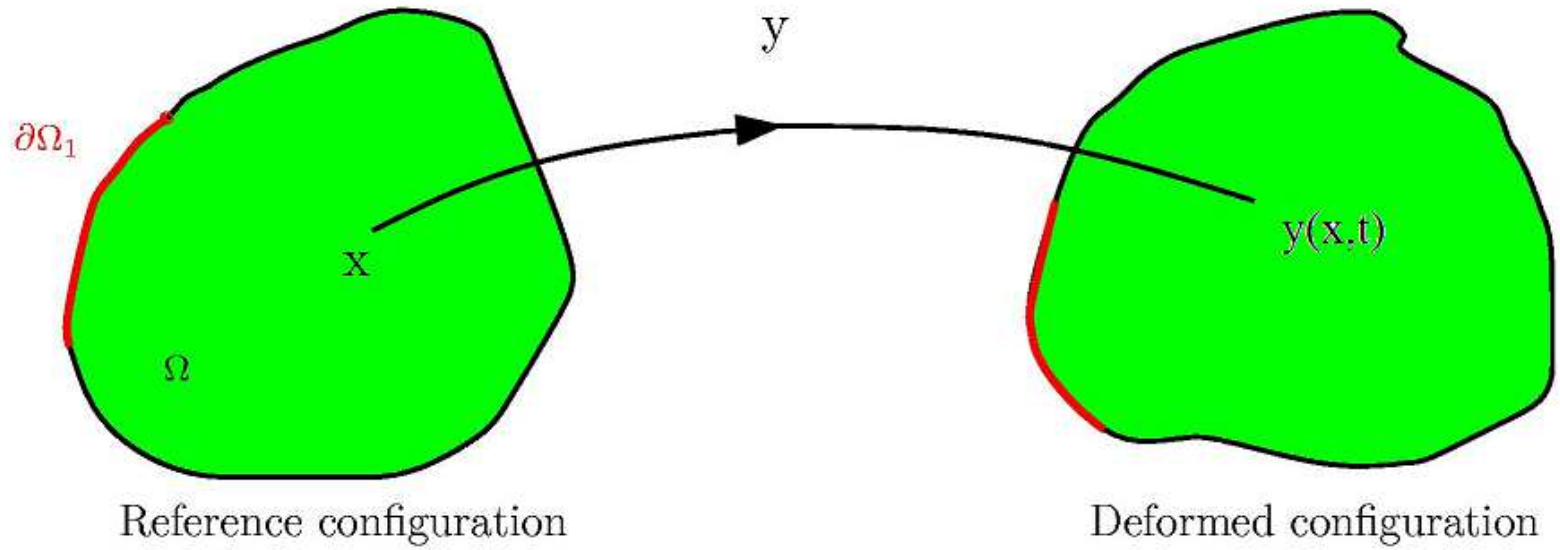
Patrick Siemer, San Francisco, USA

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

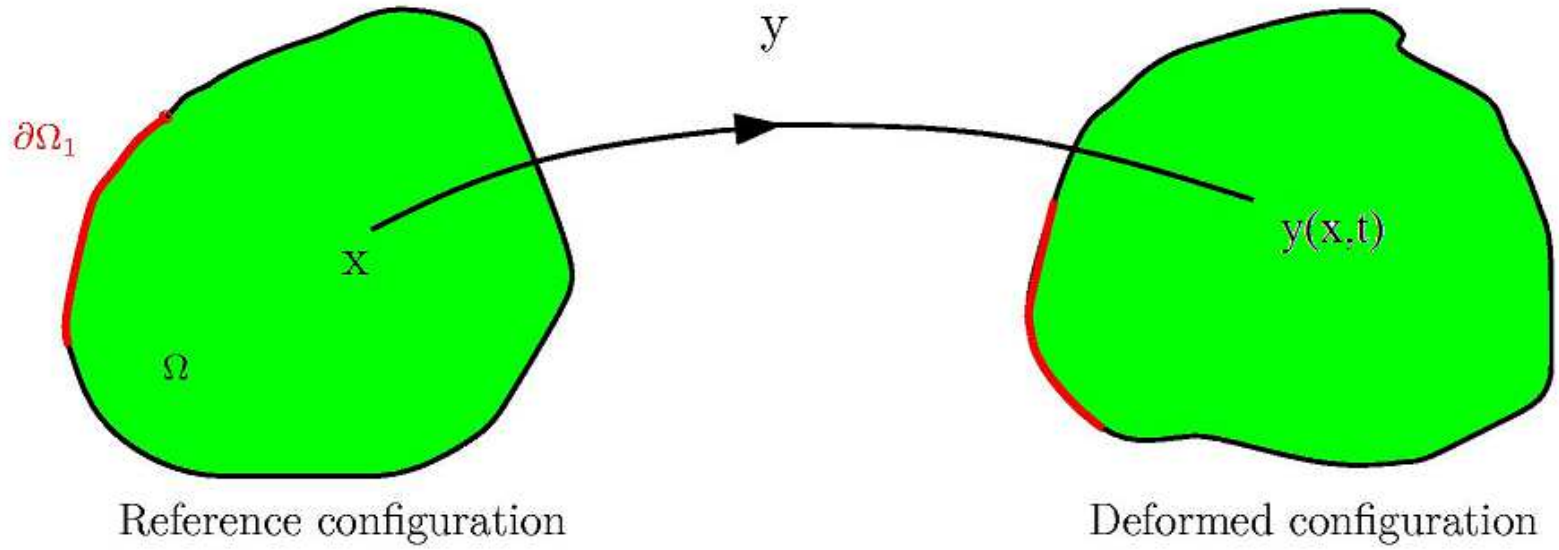
For a long time the nonlinear theory was ignored/forgotten.
1927 A.E.H. Love, Treatise on linear elasticity
1950's R. Rivlin, Exact solutions in *incompressible* nonlinear elasticity (rubber)
1960 - 80 Nonlinear theory clarified by J.L. Ericksen, C. Truesdell …
1980 - Mathematical developments, applications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

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

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

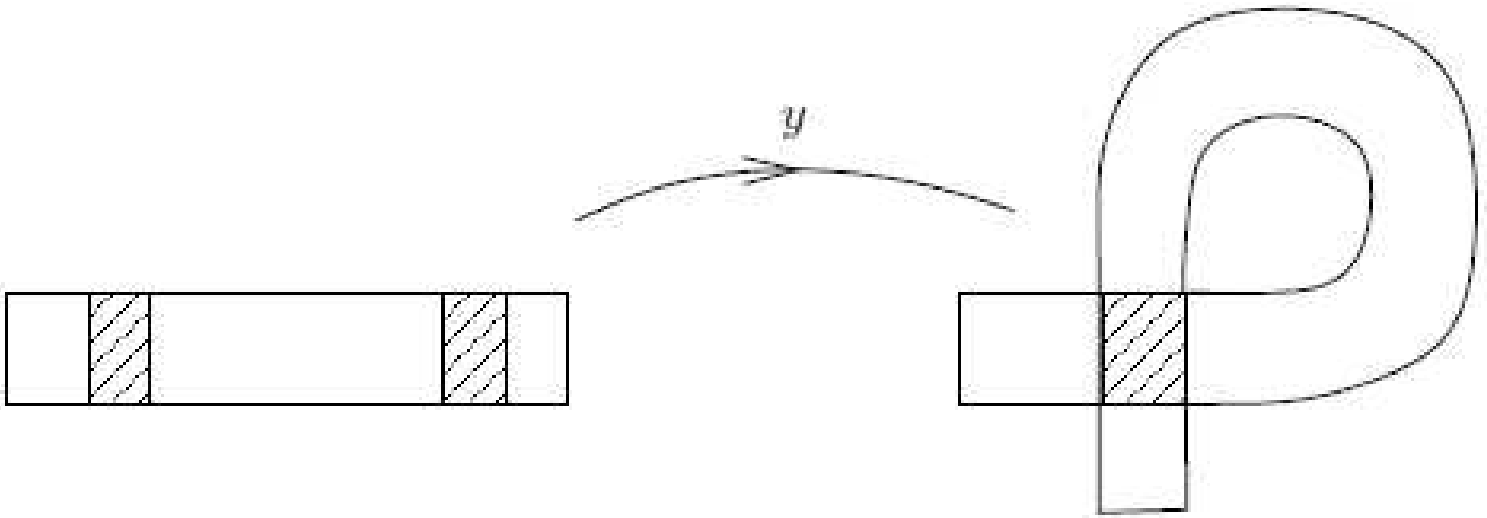
Invertibility

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

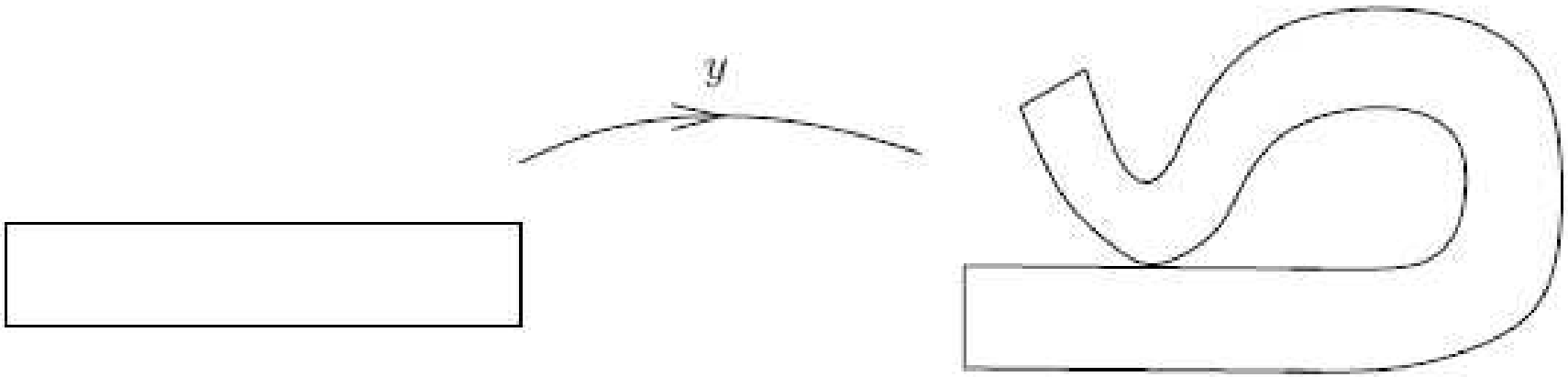
$$J = \det F(x, t) > 0 \quad \text{for } x \in \Omega. \tag{1}$$

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

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

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

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

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

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

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 $B = V^2 = F F^T$ 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

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

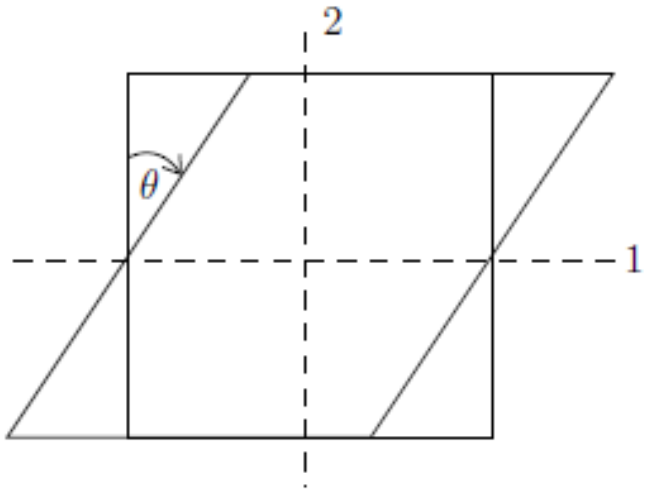
Thus to first order in z the deformation is given by a rotation followed by a stretching of amounts v_i along mutually orthogonal axes, or vice versa. Equivalently, since

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

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

Exercise: simple shear

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



$\gamma = \tan\theta$

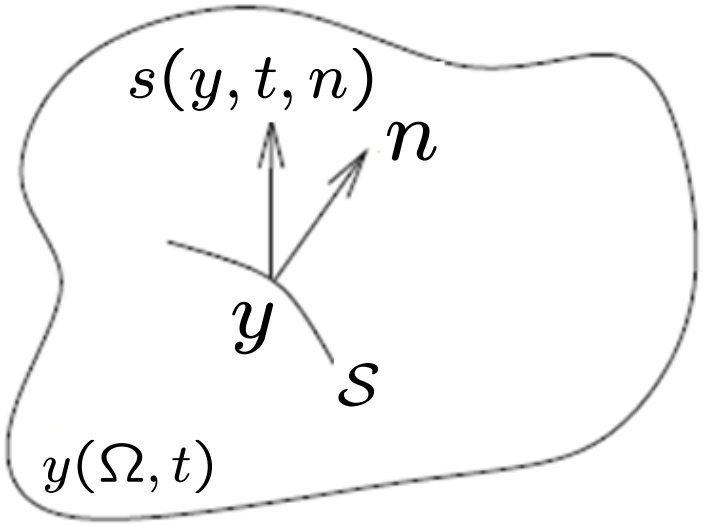
$\theta =$ angle of shear

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 $\frac{1}{\sqrt{2}}(e_1 + e_2), \frac{1}{\sqrt{2}}(e_1 - e_2), e_3$.

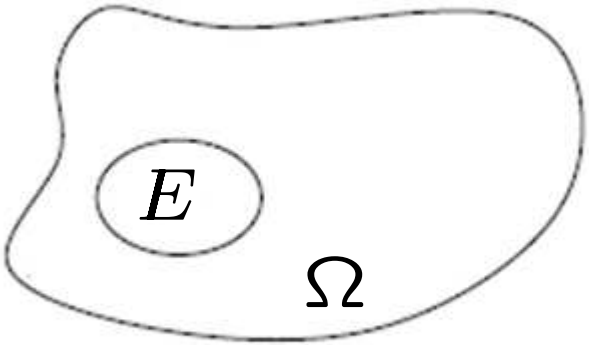
Cauchy's stress hypothesis

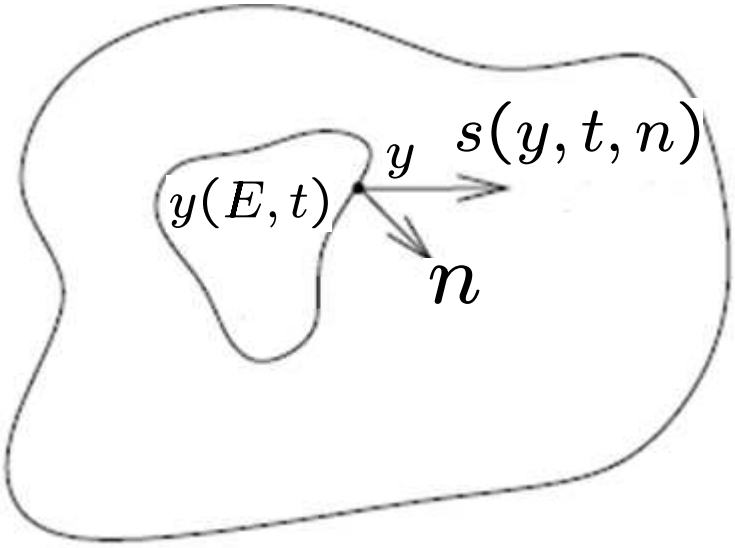


There is a vector field $s(y,t,n)$ (the *Cauchy stress vector*) that gives the force per unit area exerted across a smooth oriented surface $\mathcal{S}$ on the material on the negative side of $\mathcal{S}$ by the material on the positive side.

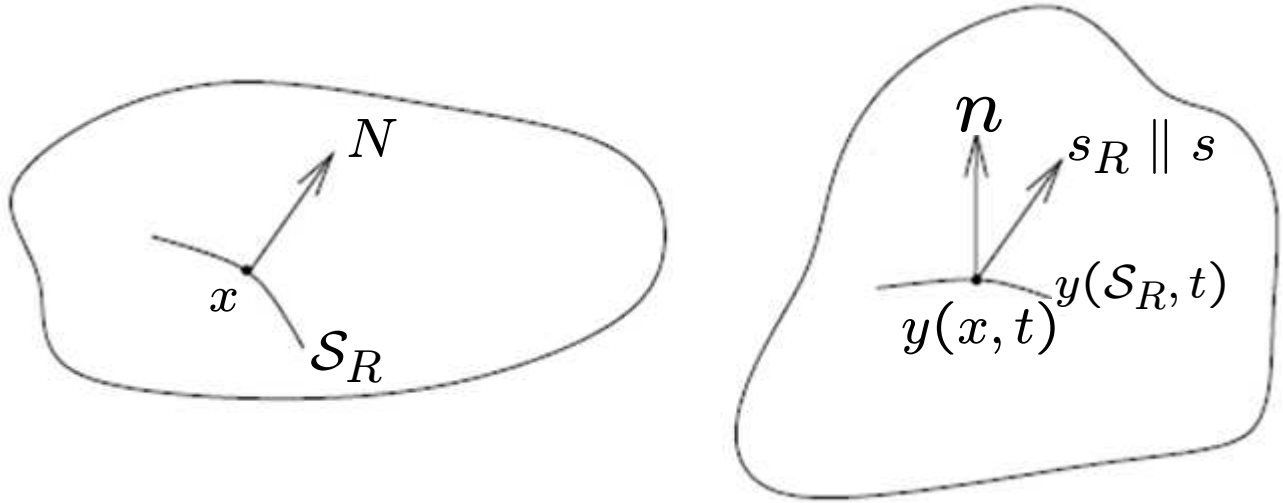
Resultant surface force on $y(E,t)$ is given by

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





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

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

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

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

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

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

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 $b = -\text{grad}_y h(x,y)$,

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

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

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

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 $Ce = 2\mu e + \lambda(\operatorname{tr} e)\,1$, 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).

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

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

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

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

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

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

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

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

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

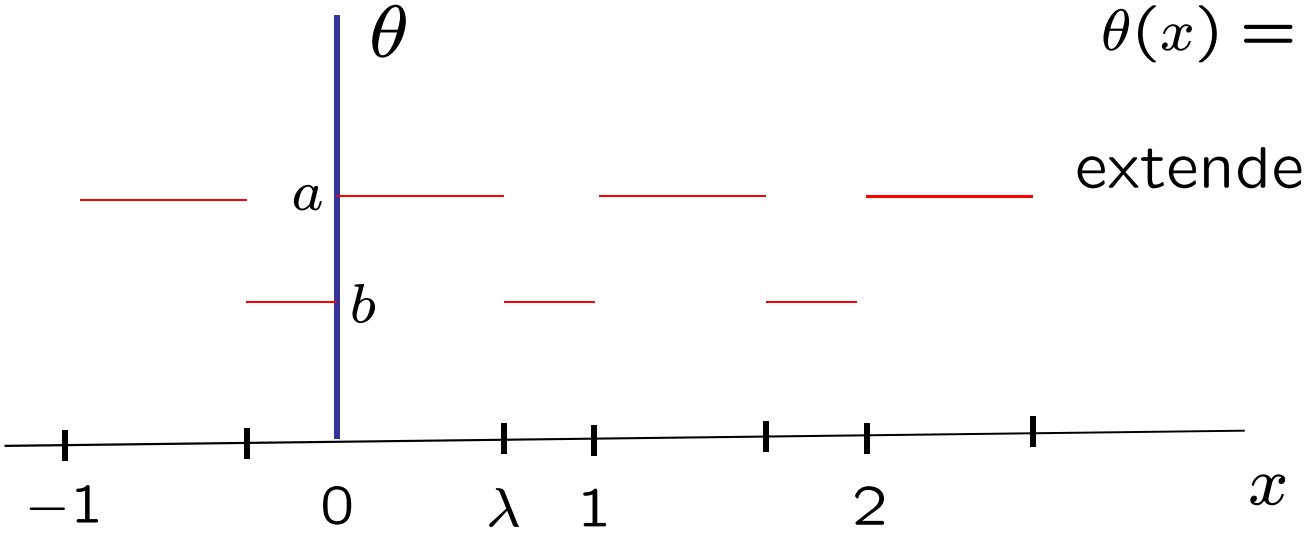
where $\frac{1}{p} + \frac{1}{p'} = 1$.

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.



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

extended periodically to $\mathbb{R}$.

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

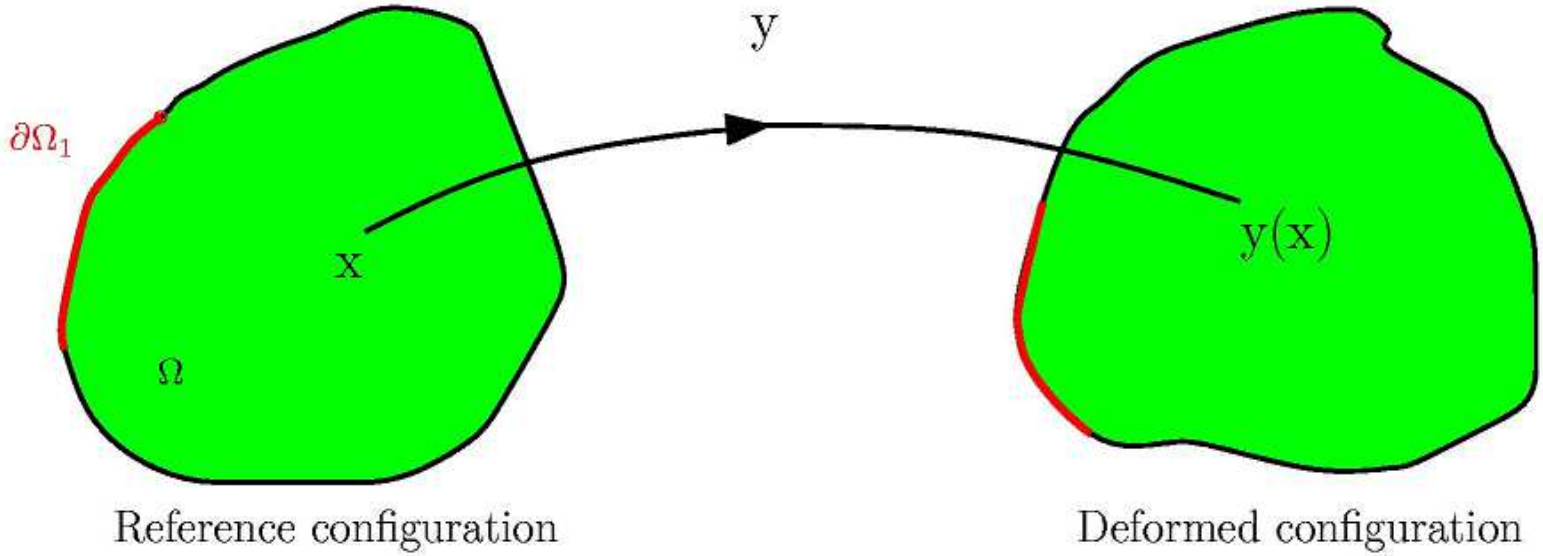
(i) Prove that $\theta^{(j)} \overset{*}{\rightharpoonup} \lambda a + (1-\lambda)b$ in $L^\infty(0,1)$

(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, $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$.

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

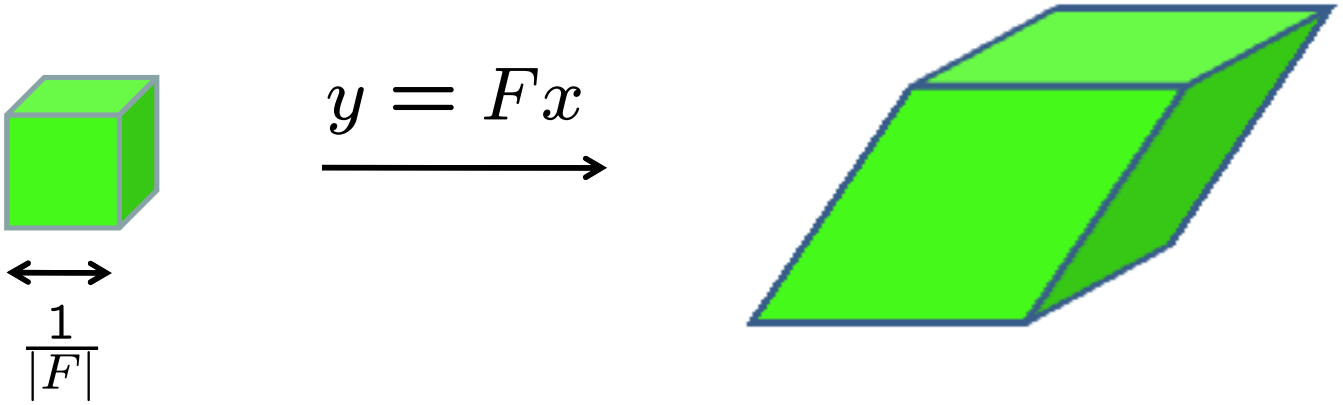
(H2) $W(F) \to \infty$ as $\det F \to 0+$,

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

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

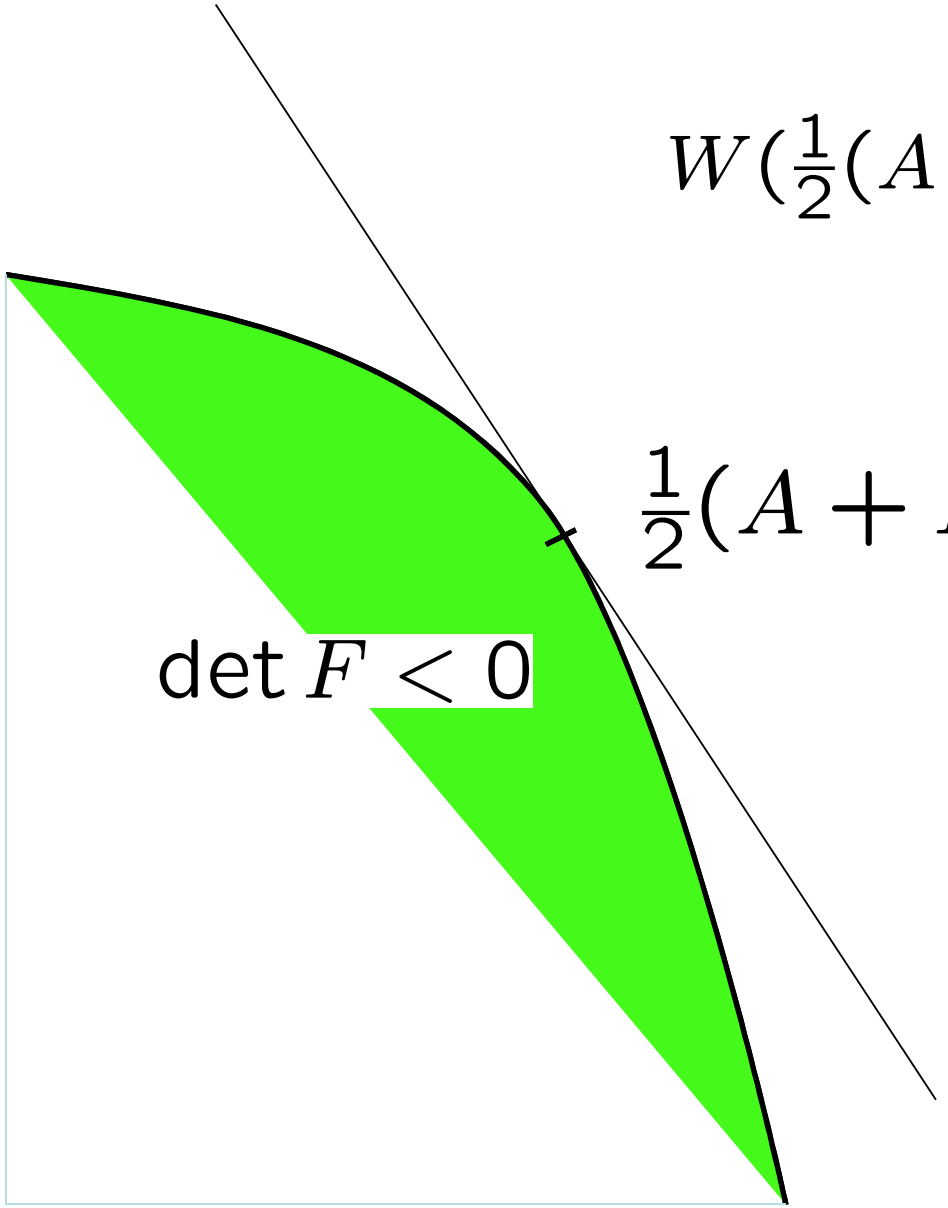
1. Convexity of W is inconsistent with (H2) because $M_+^{3\times 3}$ is not convex.

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

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

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

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



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

$\det F < 0$

$\det F > 0$

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

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.

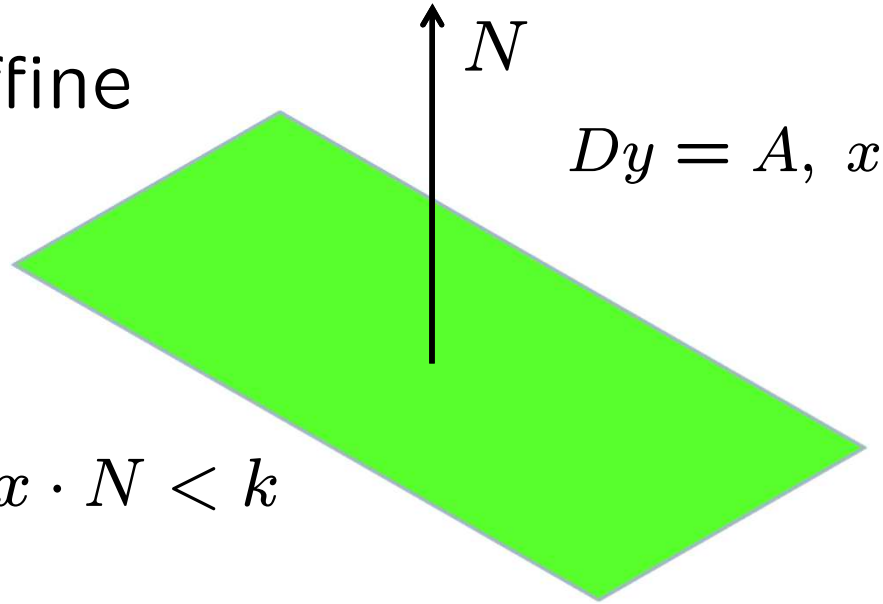
$$I(z) = \int_\Omega W(Dz)\, dx \geq$$

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

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

Rank-one matrices and the Hadamard jump condition

y piecewise affine

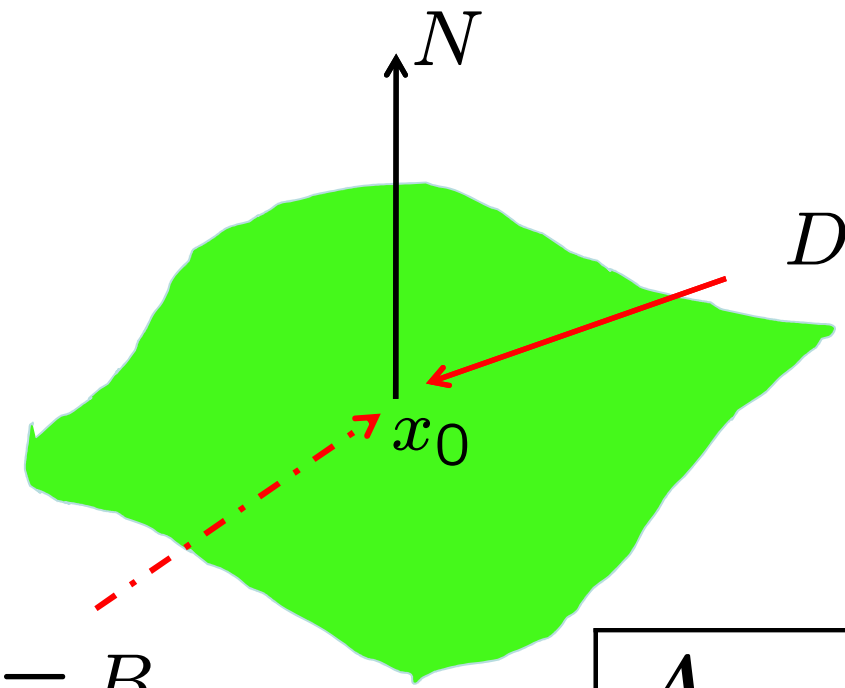


Let $C = A - B$. Then $Cx = 0$ if $x \cdot N = 0$. Thus $C(z - (z \cdot N)N) = 0$ for all z, and so $Cz = (CN \otimes N)z$. Hence

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

Hadamard jump condition

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



$Dy^+(x_0) = A$

$Dy^-(x_0) = B$

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

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

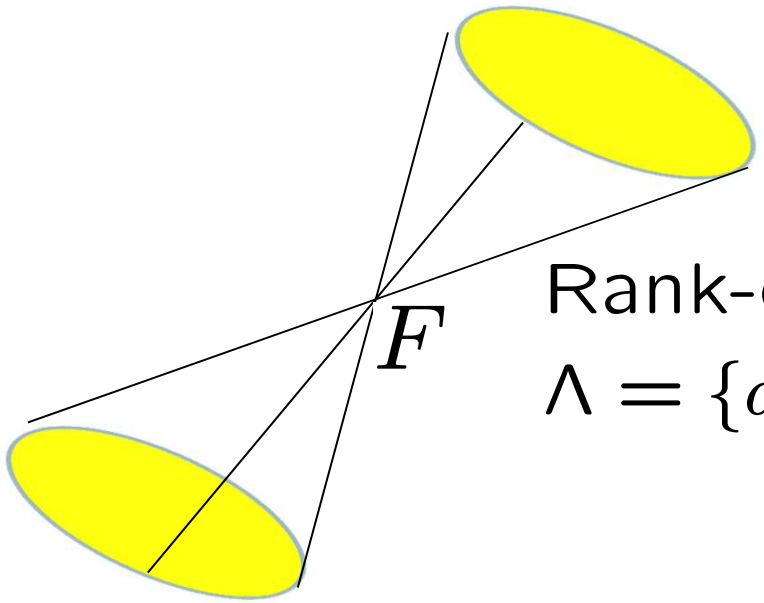
W is *rank-one convex* if the map $t \mapsto W(F + ta \otimes N)$ is convex for each $F \in M^{3\times 3}$ and $a \in \mathbb{R}^3, N \in \mathbb{R}^3$.

(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 $M^{3\times 3}_+$ is rank-one convex
(i.e. if $F, G \in M^{3\times 3}_+$ with $F - G = a \otimes N$ then $\lambda F + (1-\lambda)G \in M^{3\times 3}_+$.)

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

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

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

definition independent of Ω

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

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

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 $\frac{1}{\text{meas}\,Q}\int_Q Dy\,dx = F$.

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

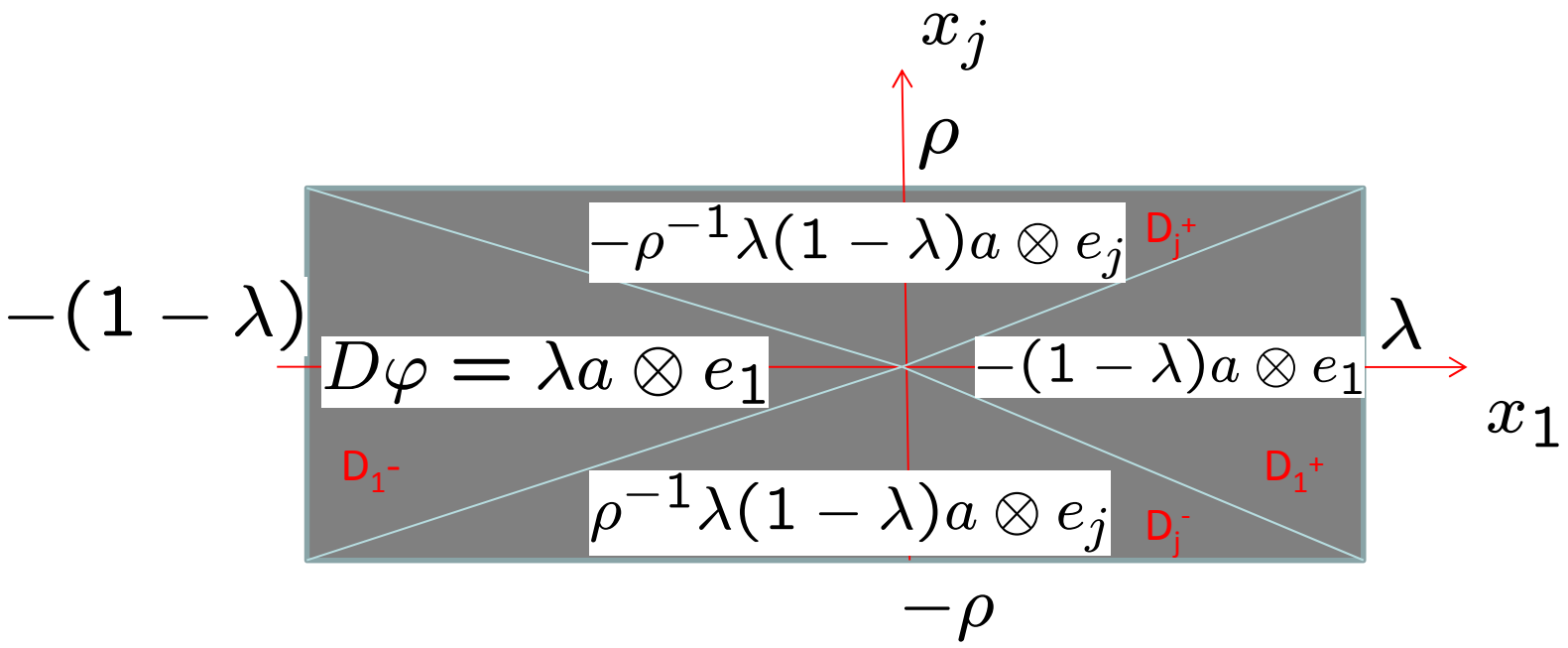
We prove that

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

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

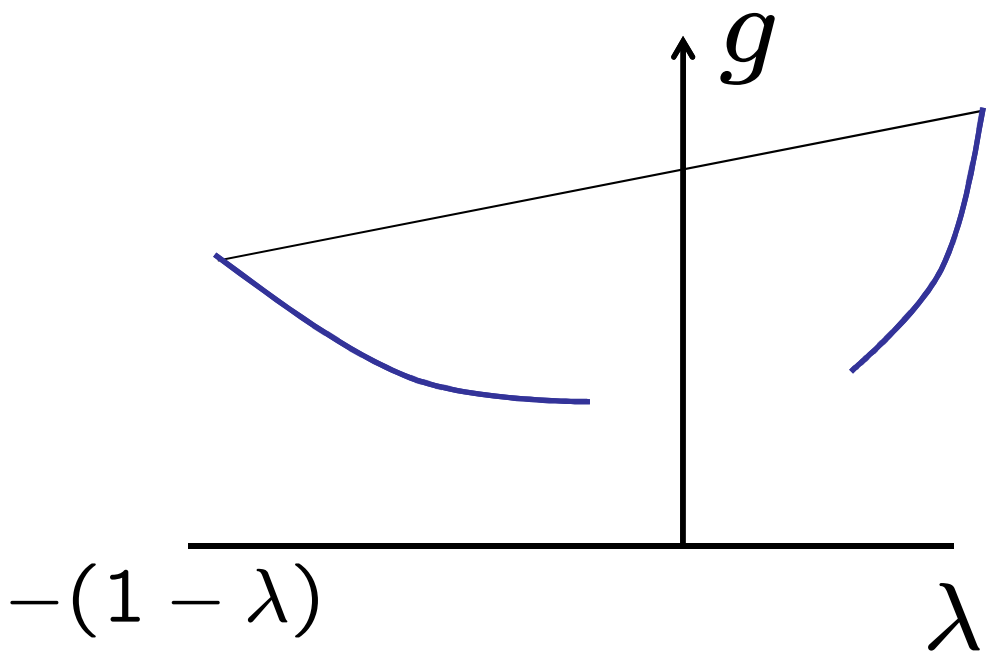
$$(2\rho)^{n-1}W(F) \leq \frac{(2\rho)^{n-1}\lambda}{n}W(F-(1-\lambda)a\otimes e_1) + \frac{(2\rho)^{n-1}(1-\lambda)}{n}W(F+\lambda a\otimes e_1) + \sum_{j=2}^{n}\frac{(2\rho)^{n-1}}{2n}[W(F+\rho^{-1}\lambda(1-\lambda)a\otimes e_j) + W(F-\rho^{-1}\lambda(1-\lambda)a\otimes e_j)]$$

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

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

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

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

$$\int_\Omega J(Dv)\varphi \, dx = \int_\Omega [v_1 v_{2,1}\varphi_{,2} - v_1 v_{2,2}\varphi_{,1}] \, dx. \qquad 87$$

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

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

$$\downarrow L^1 \qquad \downarrow L^{p'} \downarrow L^p \quad \downarrow L^{p'} \downarrow L^p$$

$$\chi \qquad u_1\ u_{2,1} \quad u_1\ u_{2,2}$$

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

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

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

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

$$W \text{ convex} \Rightarrow W \text{ polyconvex} \Rightarrow W \text{ quasiconvex}$$

$\not\Leftarrow W = \det$ and $\not\Leftarrow$ Zhang

$$\Rightarrow W \text{ rank-one convex.}$$

$\not\Leftarrow$ Šverák

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

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

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),

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

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.)

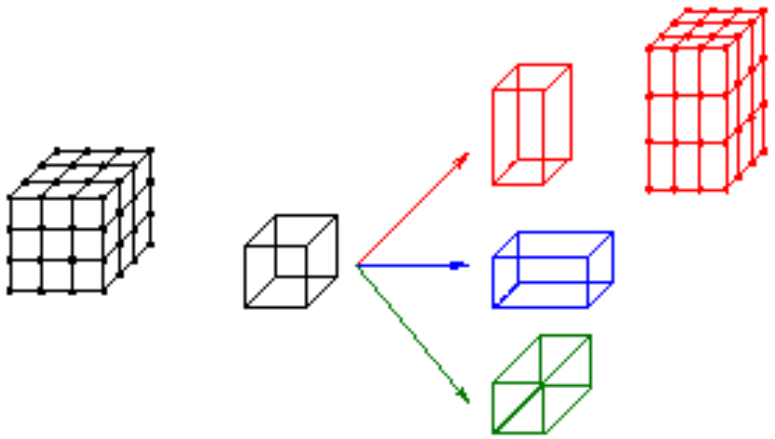
3. Martensitic phase transformations

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

e.g. cubic to tetragonal

$\theta > \theta_c$

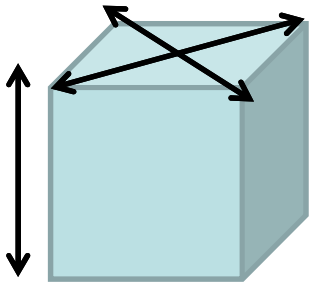
cubic austenite



$\theta < \theta_c$

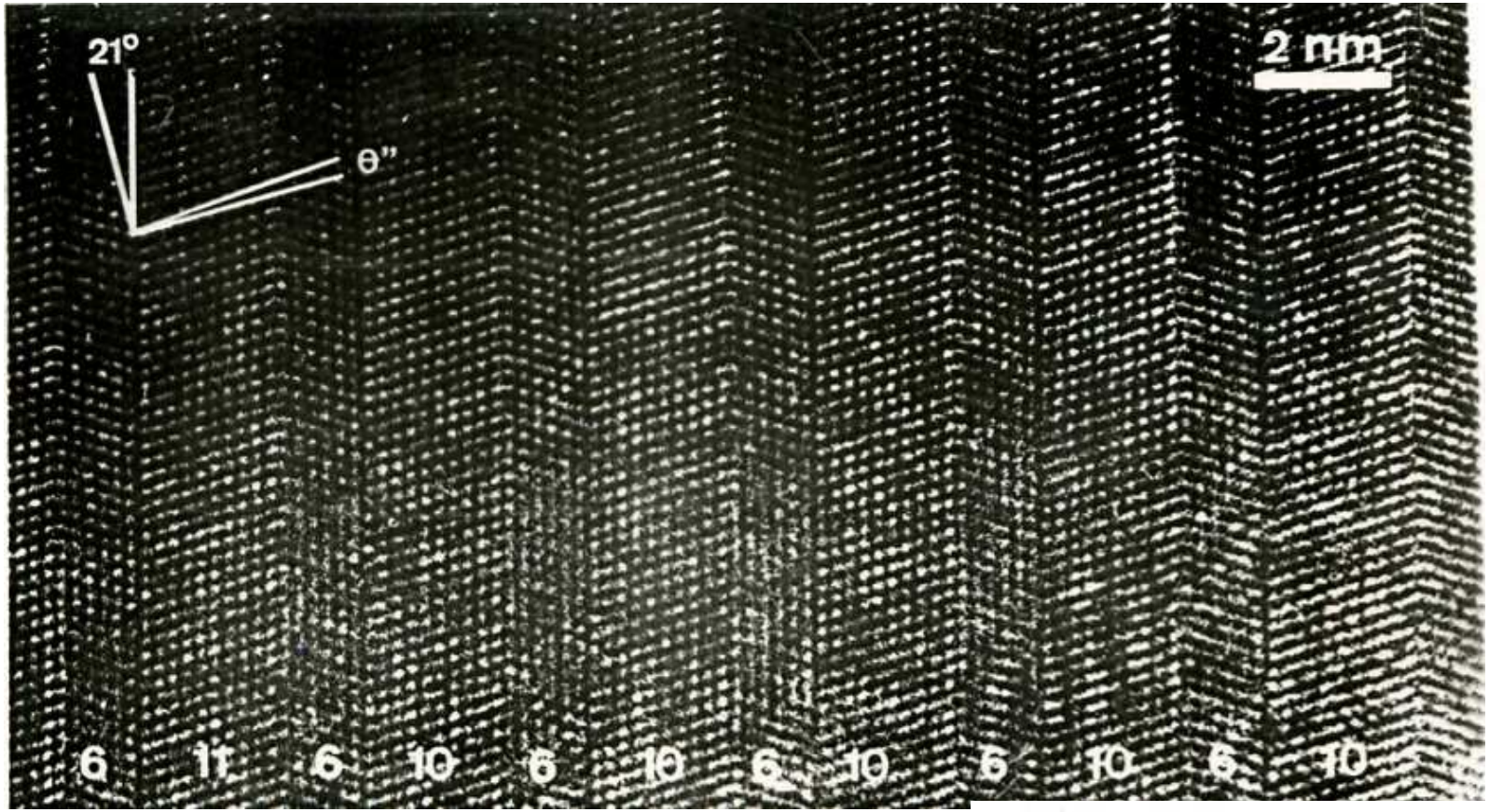
three tetragonal variants of martensite

cubic to orthorhombic (e.g. CuAlNi)



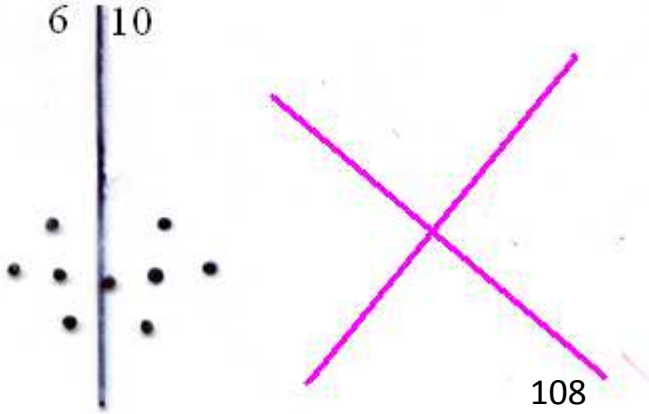
$\theta < \theta_c$

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 $A \in M^{3\times 3}_+$, 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

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

For cubic to orthorhombic $N = 6$ and

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

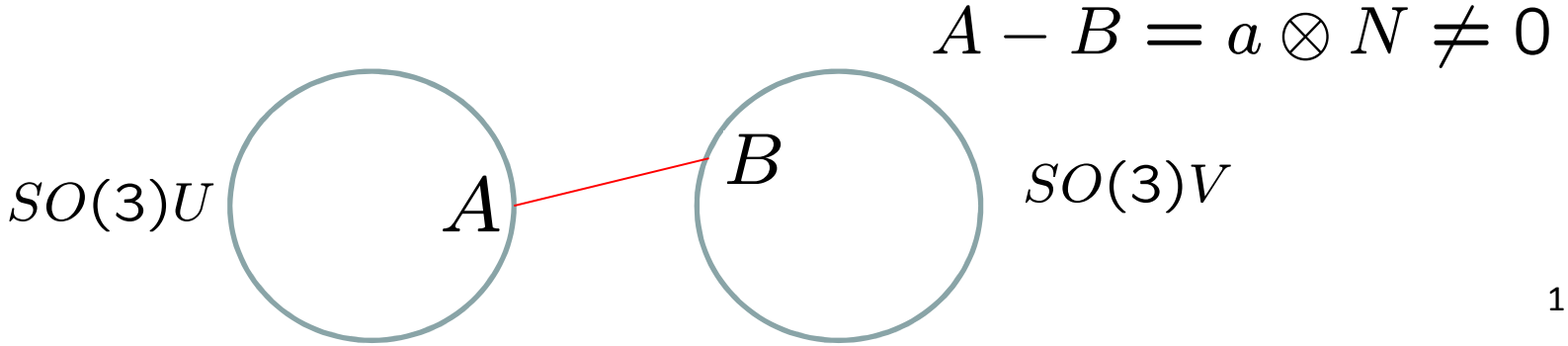
$$U_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},\quad U_5 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2}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

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



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

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

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

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

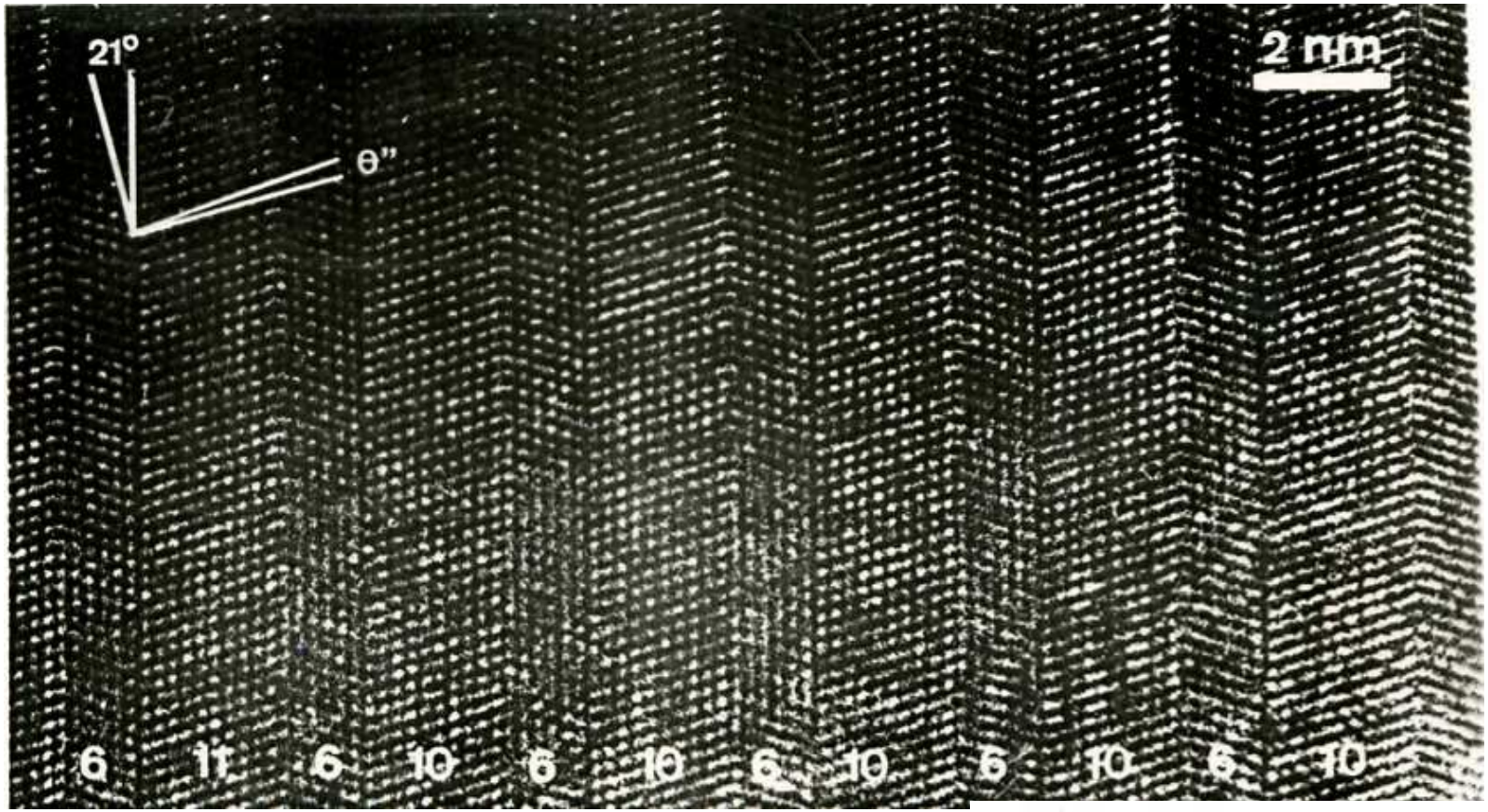
Proof. If there is a rank-one connection then 1 is an eigenvalue since $\det(U_i^2 - 1) = 0$.

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

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

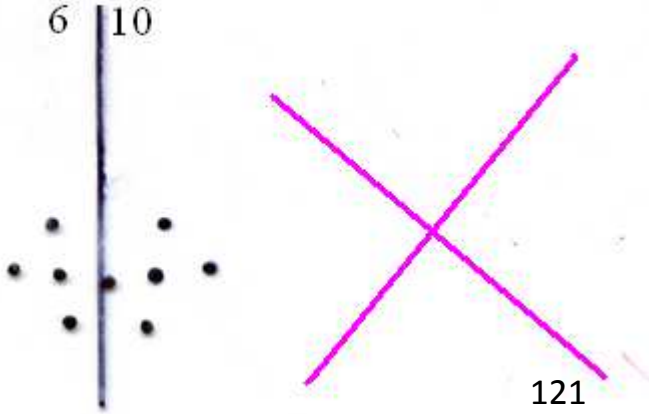
where $\alpha = \sqrt{\frac{1-\lambda_1^2}{\lambda_3^2-\lambda_1^2}}, \beta = \sqrt{\frac{\lambda_3^2-1}{\lambda_3^2-\lambda_1^2}}$.

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

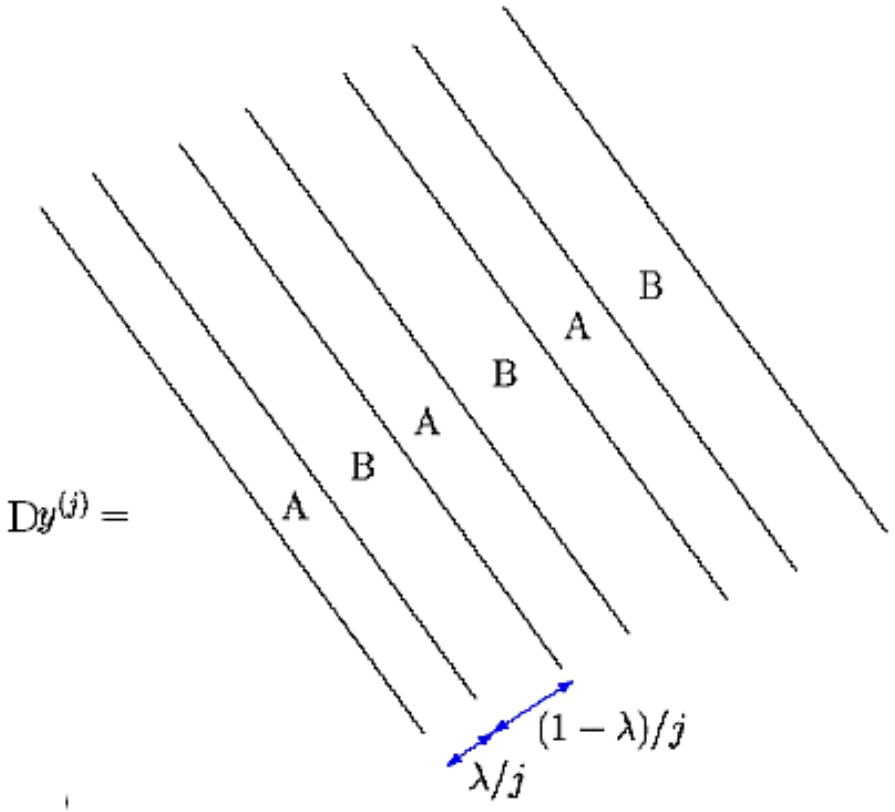


Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

Baele, van Tenderloo, Amelinckx



Layering twins



Simple laminate

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

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

4. Microstructure

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).

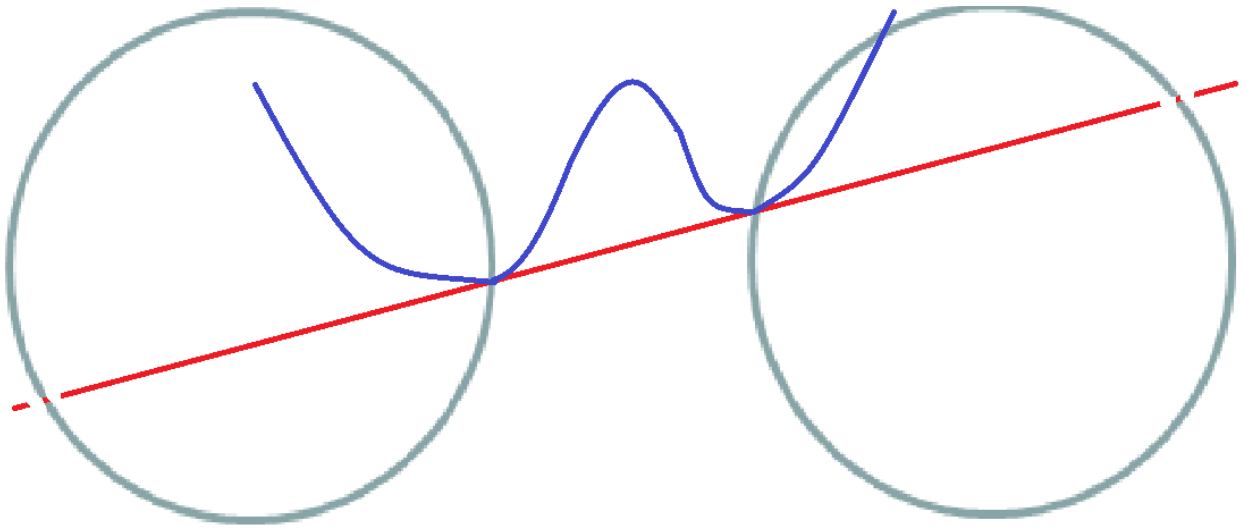
In trying to understand why we see some microstructures and not others, we will use methods based on energy minimization. However, the formation of microstructure is obviously a pattern formation problem, which really should be treated using an appropriate dynamical model.

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.

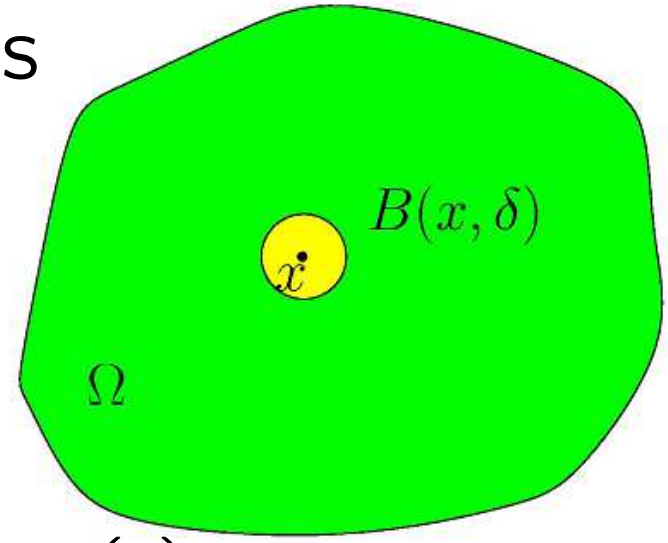


So we expect the minimum of the energy in general not to be attained, with minimizing sequences $y^{(j)}$ in general generating infinitely fine microstructures.

Gradient Young measures

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

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

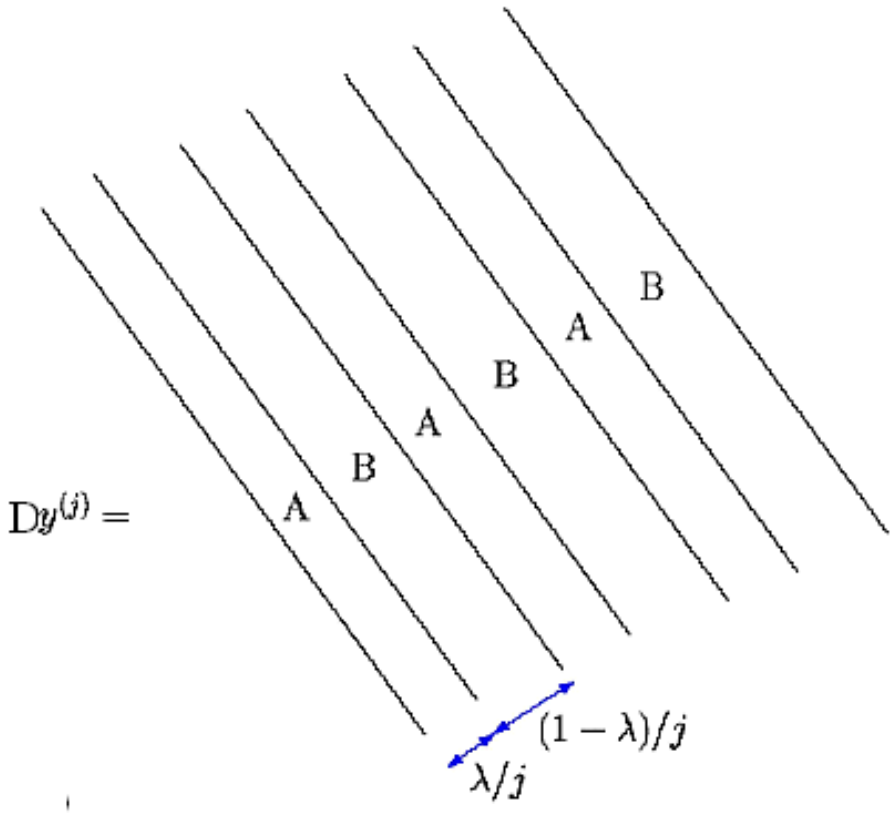


$$\nu_{x,j,\delta}(E) = \frac{\text{vol } \{z \in B(x,\delta) : Dy^{(j)}(z) \in E\}}{\text{vol } B(x,\delta)}$$

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

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

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

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

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

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

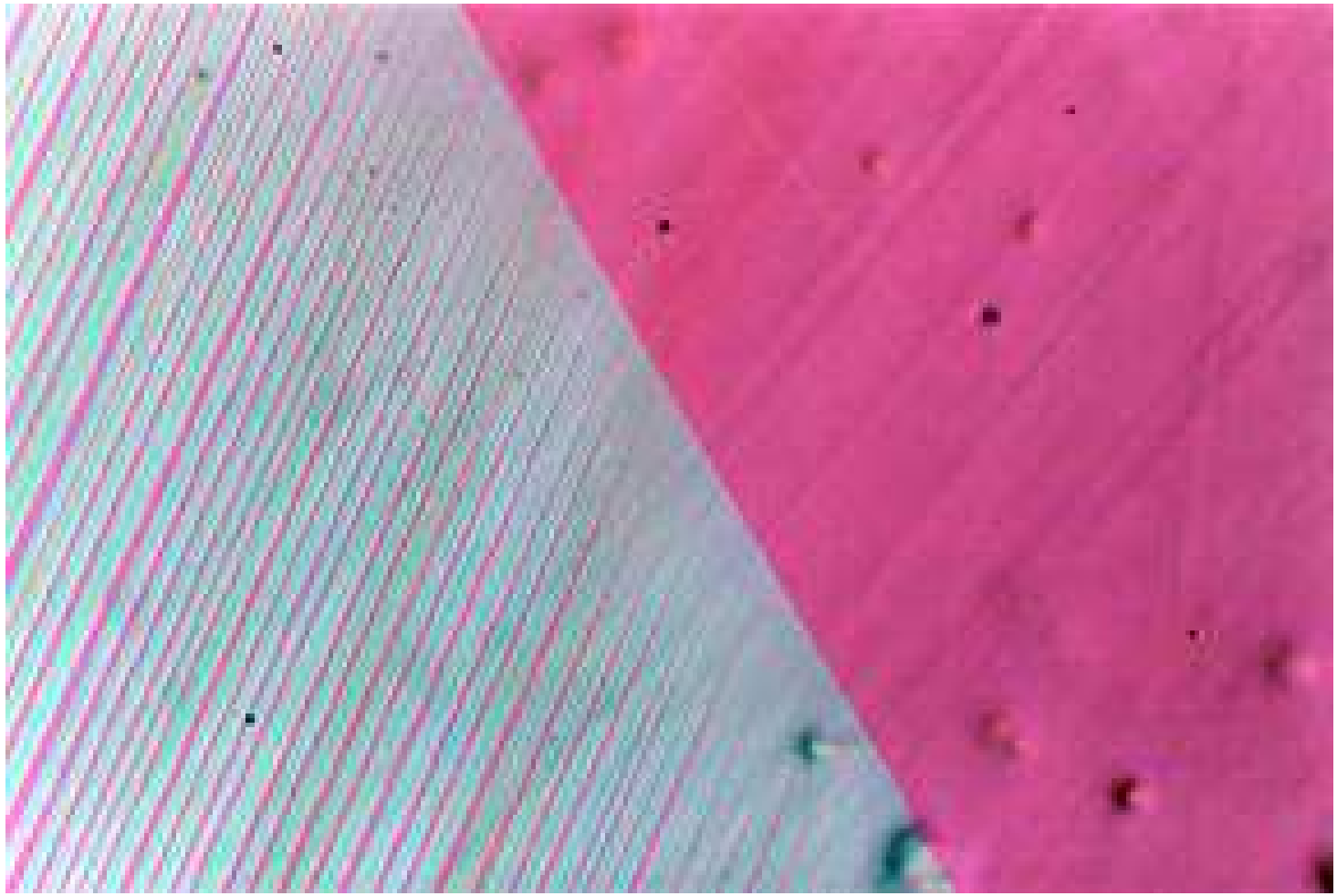
How does austenite transform to martensite as θ passes through θ_c?

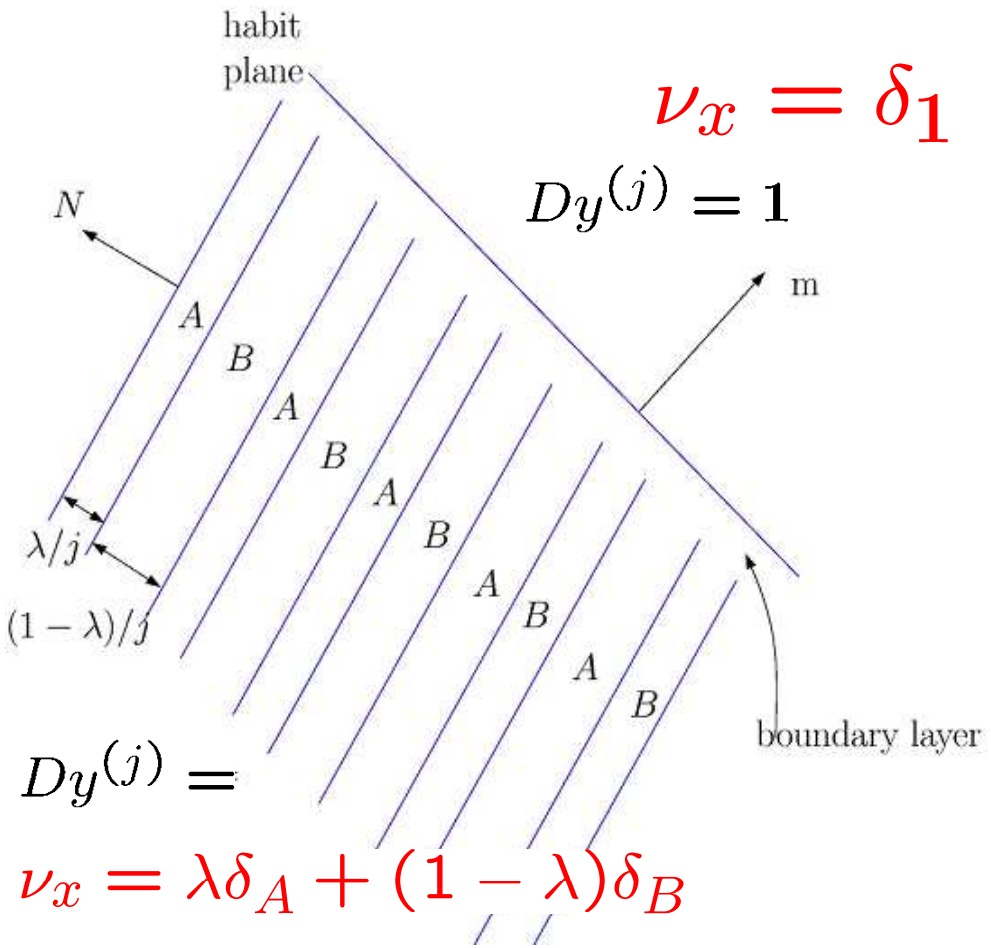
It cannot do this by means of an exact interface between austenite and martensite, because this requires the middle eigenvalue of U_i to be one, which in general is not the case (but see studies of James et al on low hysteresis alloys).

So what does it do?

(Classical) austenite-martensite interface in CuAlNi

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

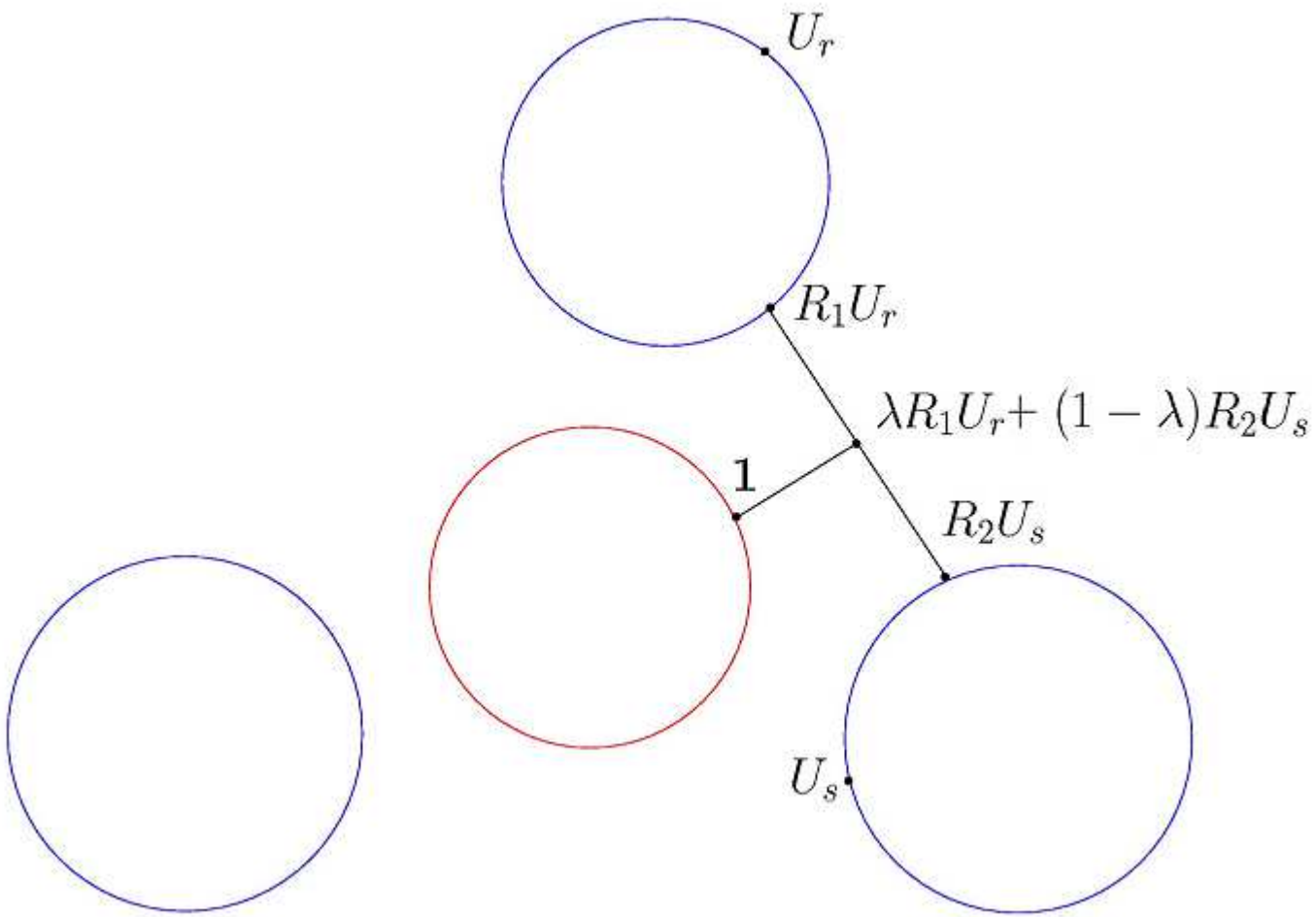


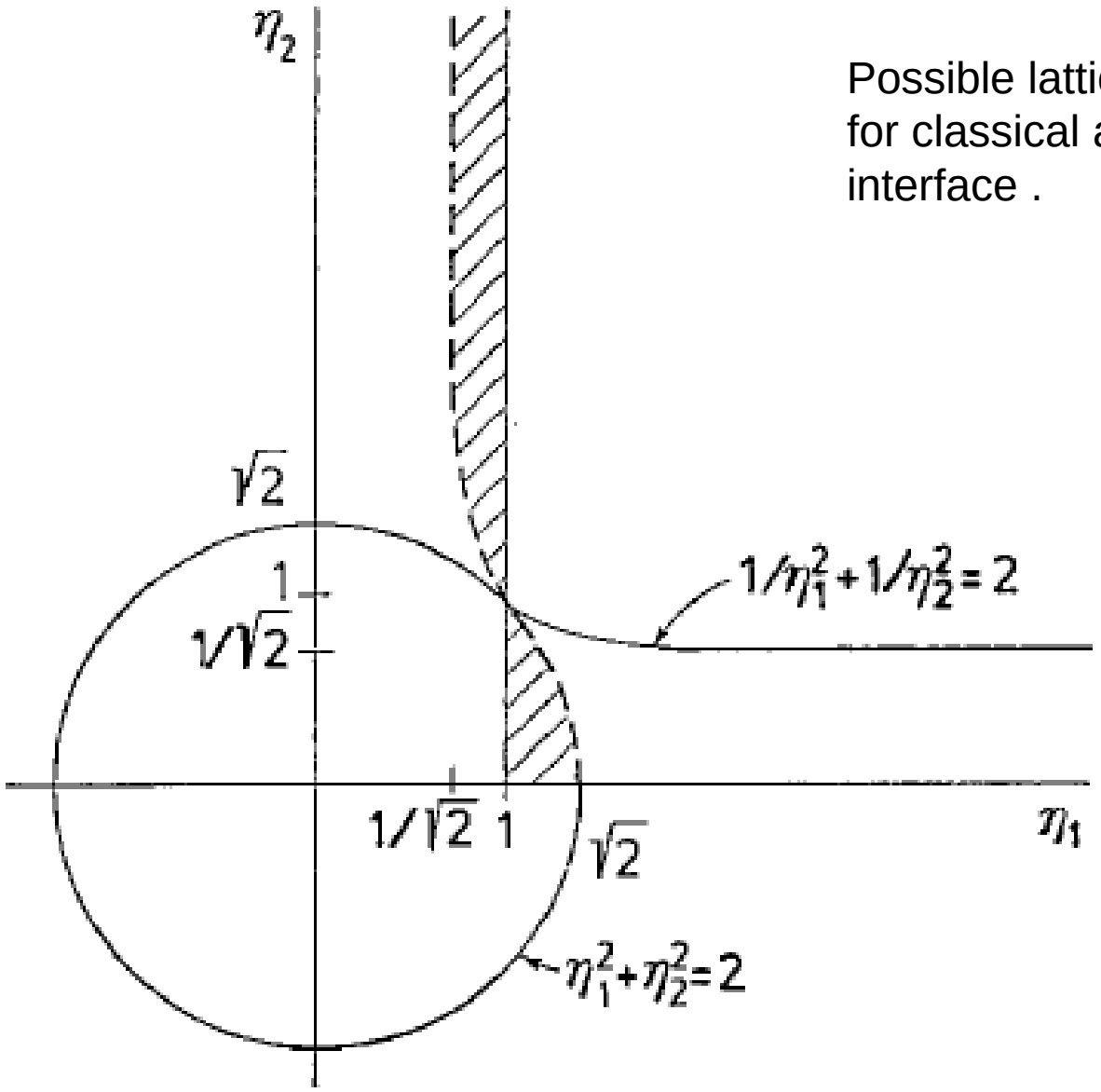


Gives formulae of the crystallographic theory of martensite (Wechsler, Lieberman, Read)

24 habit planes for cubic-to-tetragonal

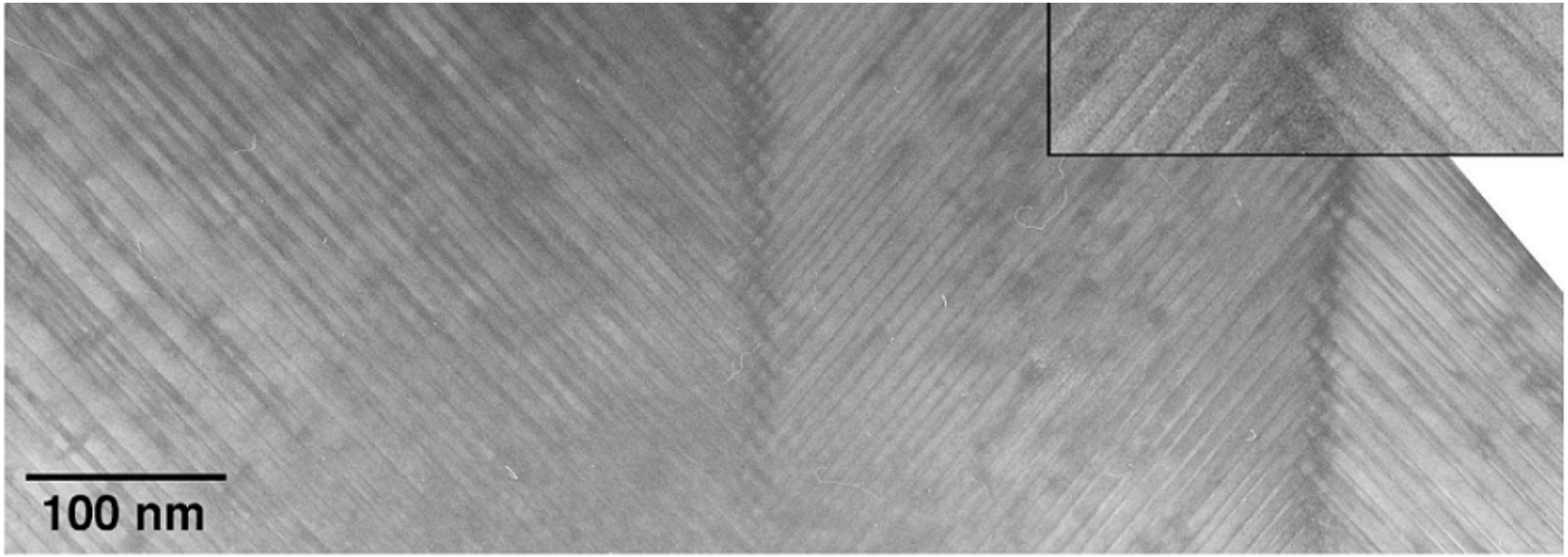
Rank-one connections for A/M interface



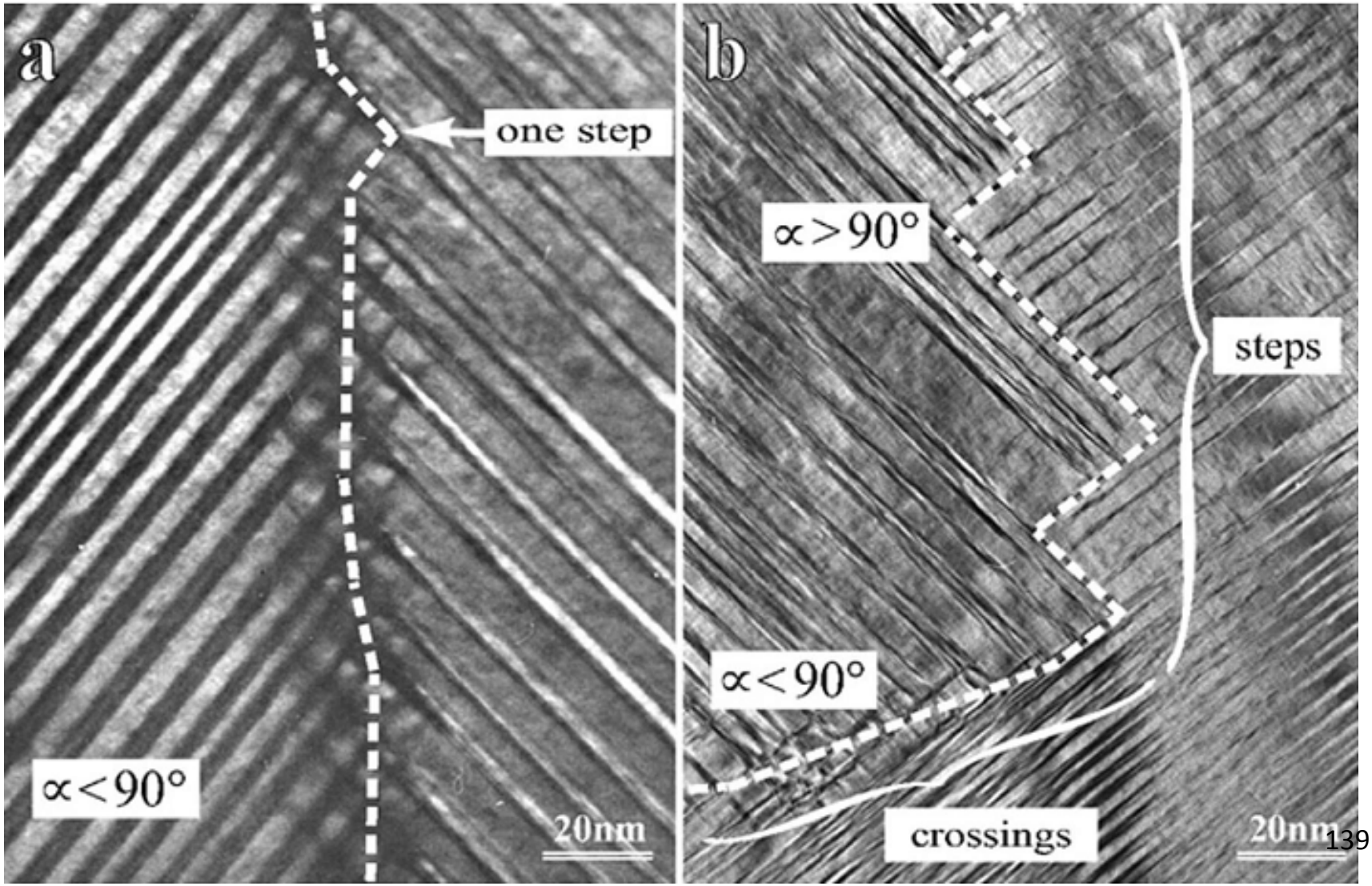


Possible lattice parameters
for classical austenite-martensite
interface .

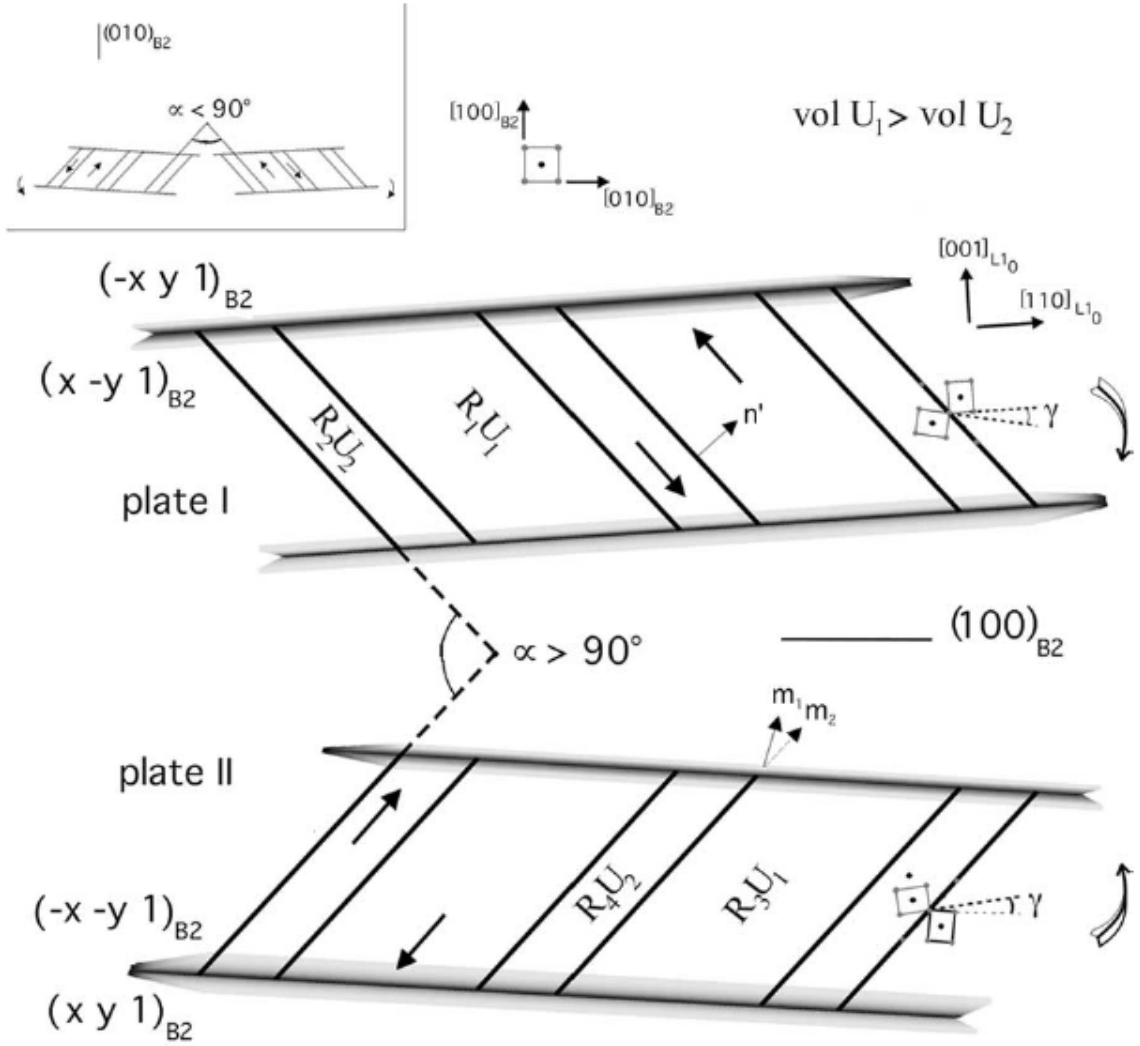
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)

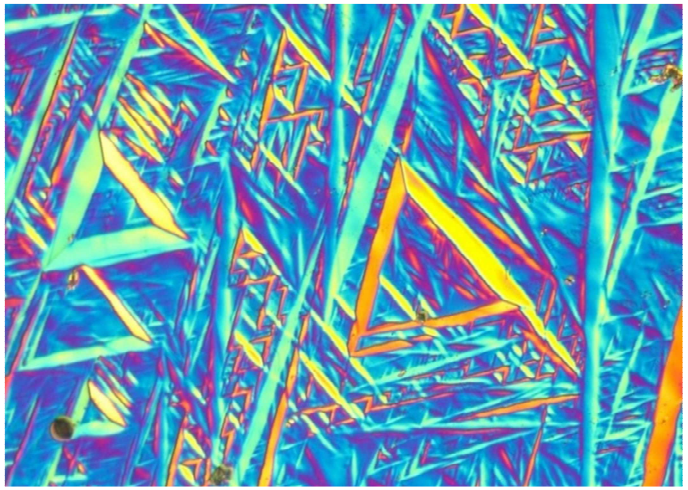


Crossings and steps



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

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

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

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

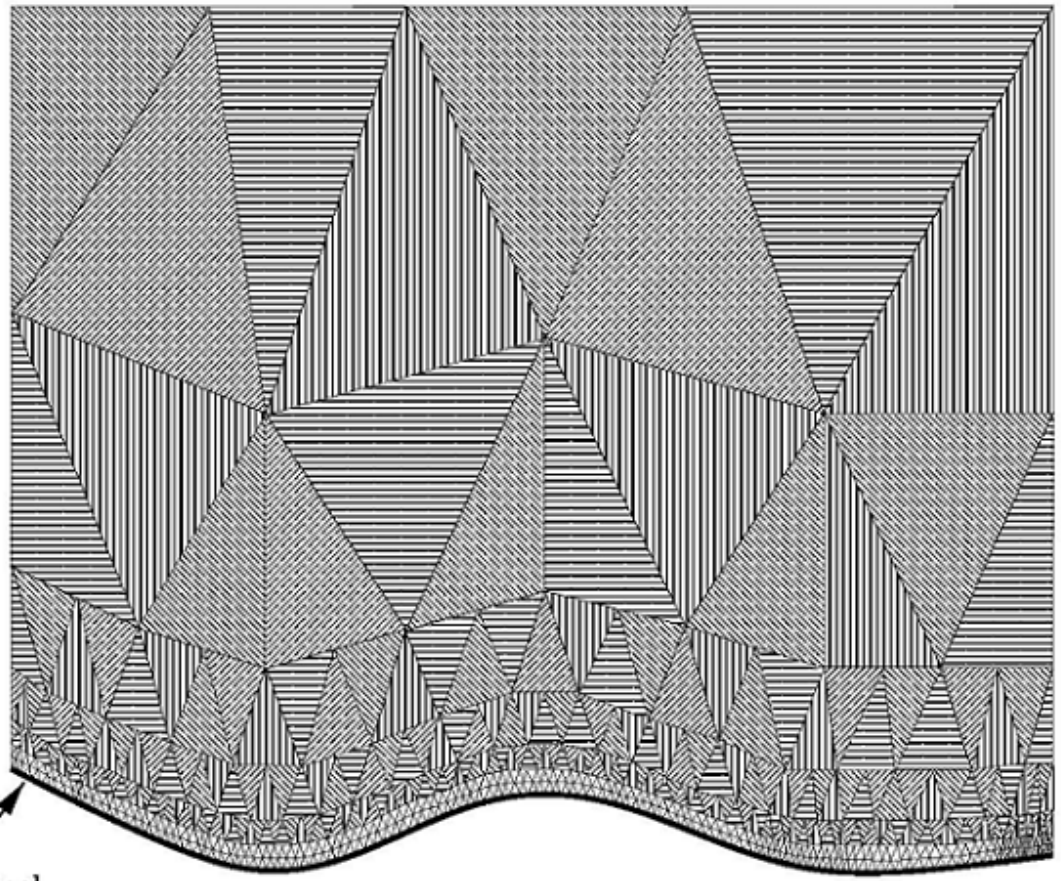
B/Schryvers 2003

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)

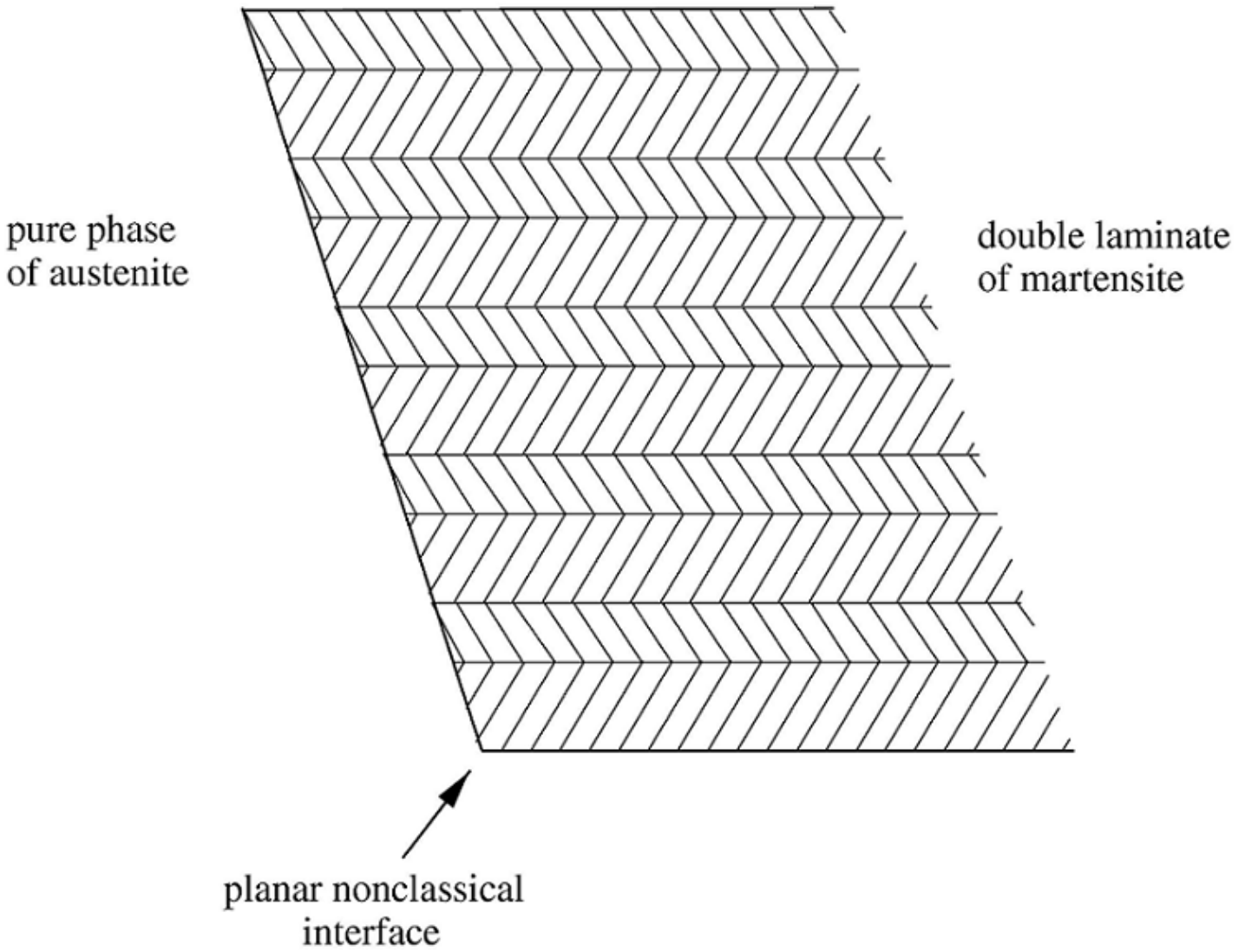
Nonclassical austenite-martensite interfaces (B/Carstensen 97)



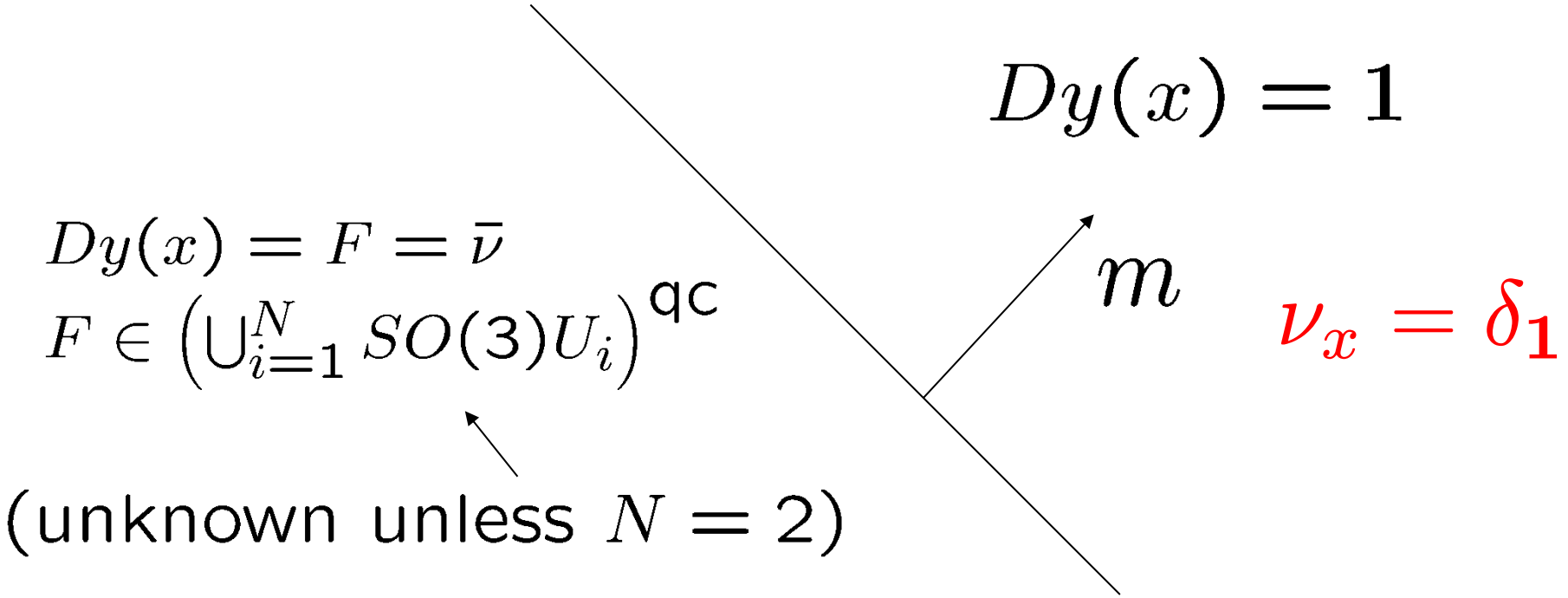
speculative nonhomogeneous martensitic microstructure with fractal refinement near interface

curved nonclassical interface

Nonclassical interface with double laminate



Nonclassical interface calculation



$\nu_x = \nu$

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

$$F = 1 + b \otimes m$$

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

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

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

Combining these inequalities we get that

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

For cubic to tetragonal we have that

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

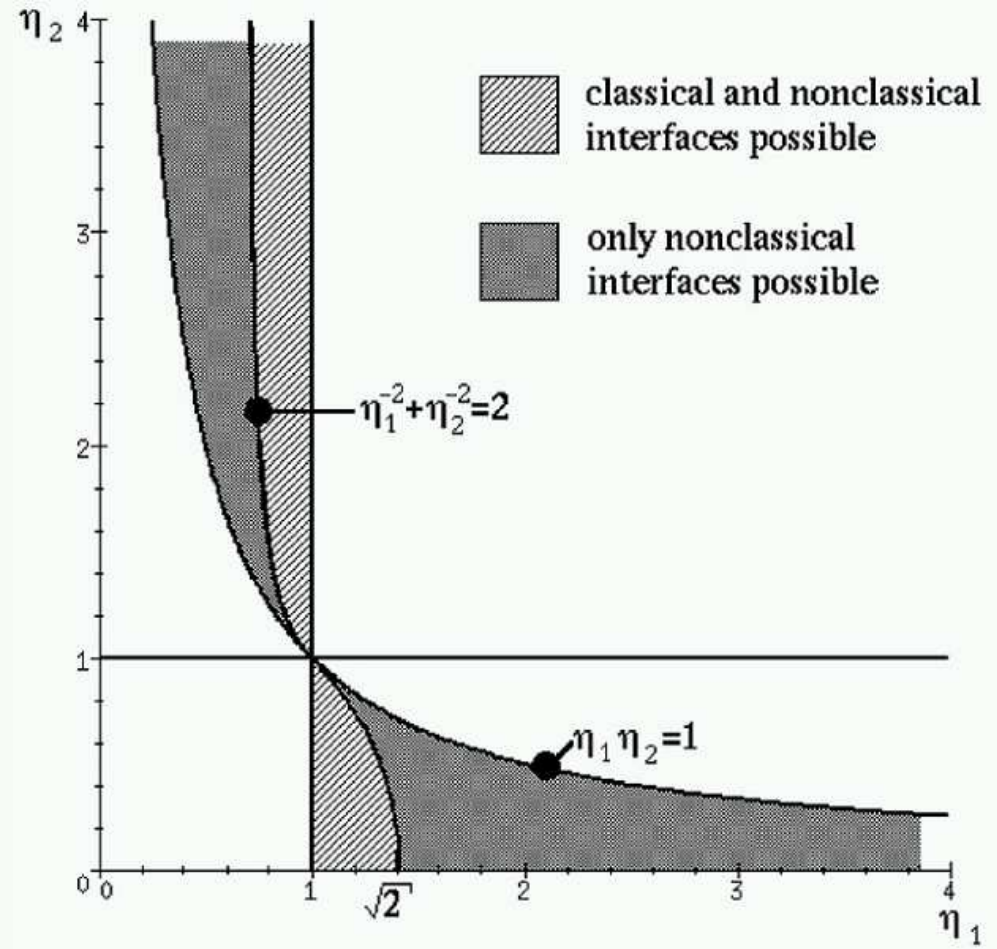
and the necessary conditions become

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

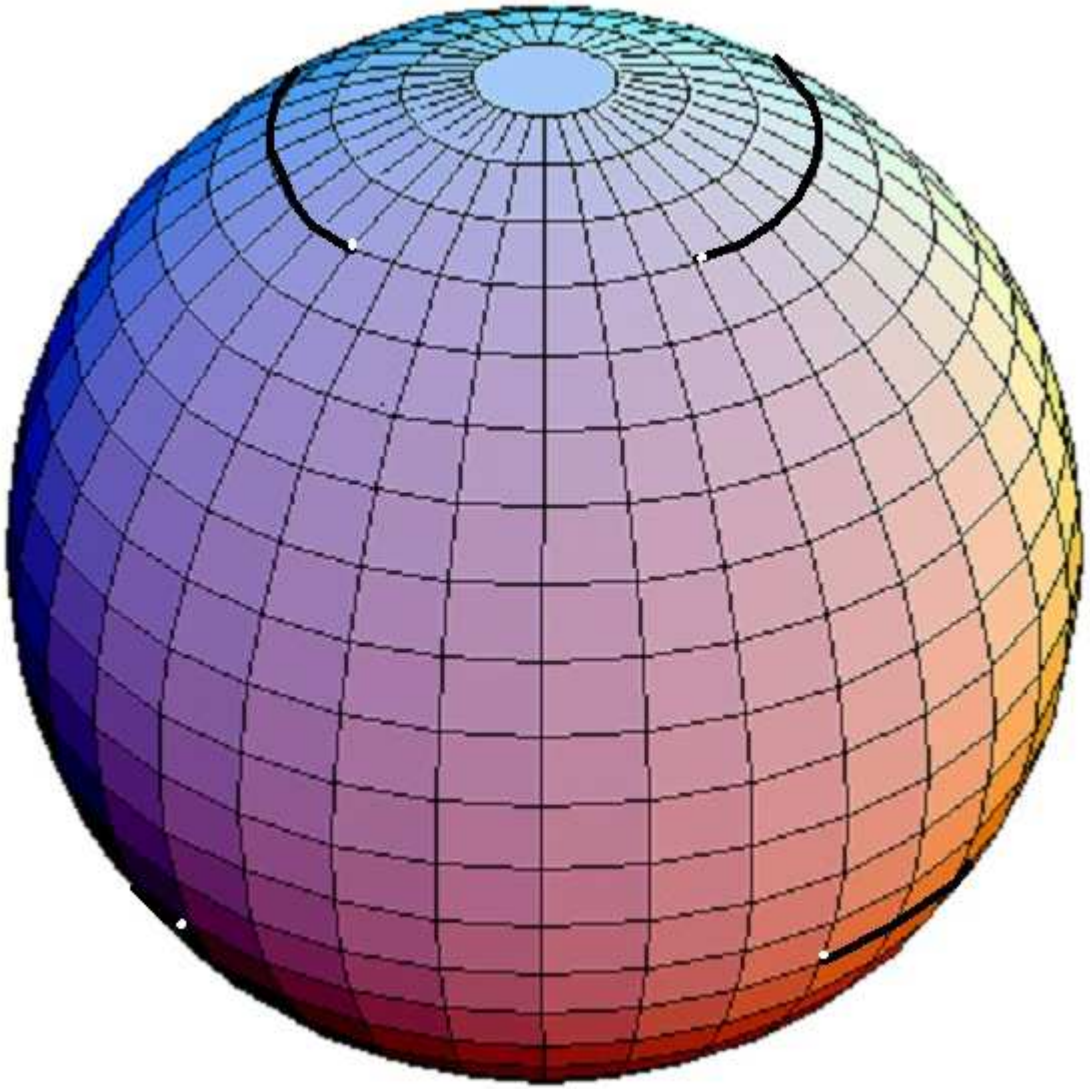
$$\eta_2 \leq \eta_1^{-1} \leq \eta_1 \text{ if } \eta_1 \geq \eta_2.$$

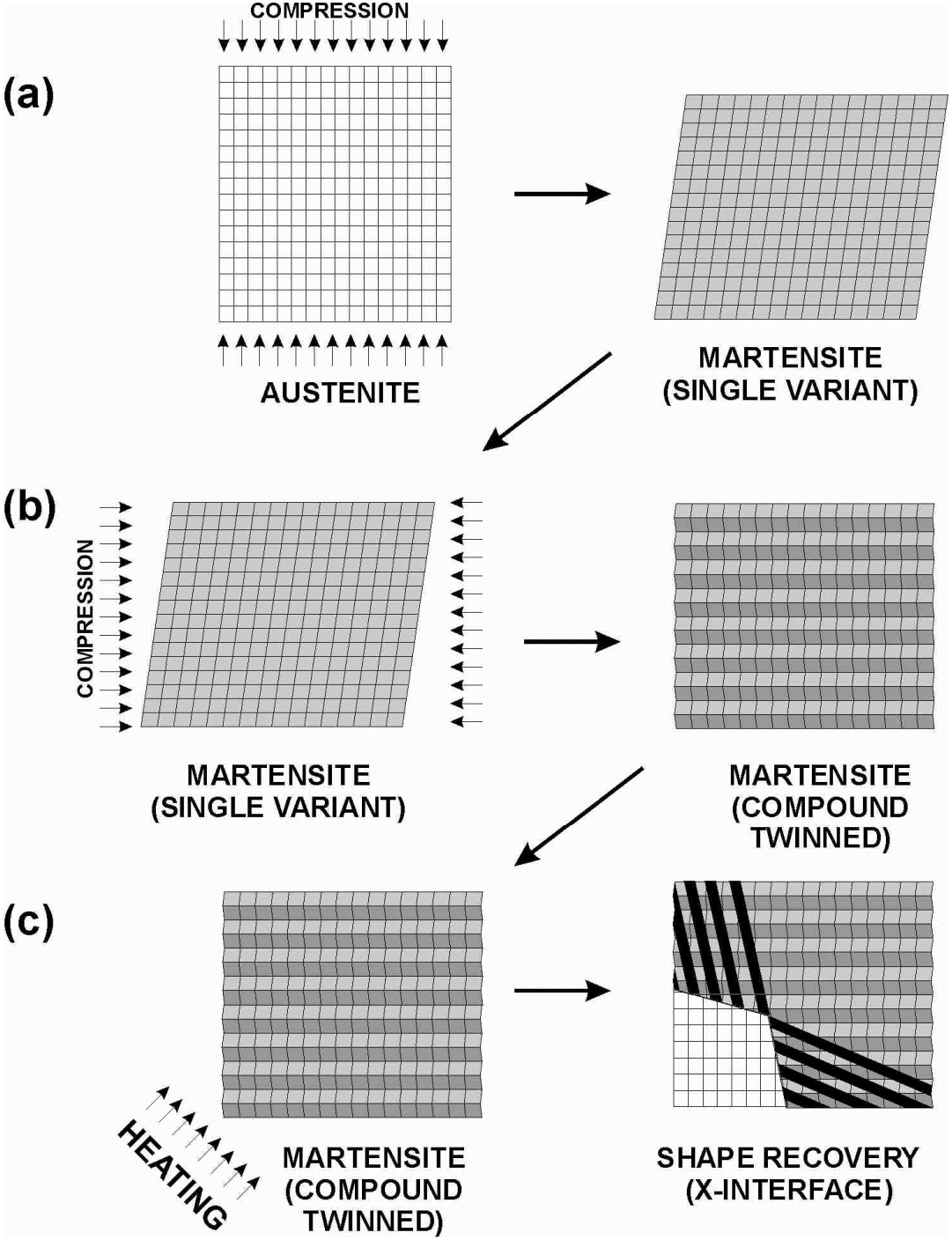
But these turn out to be exactly the conditions given by the two-well theorem to construct a rank-one connection from $(SO(3)U_1 \cup SO(3)U_2)^{qc}$ to the identity!
Hence the conditions are sufficient also.

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



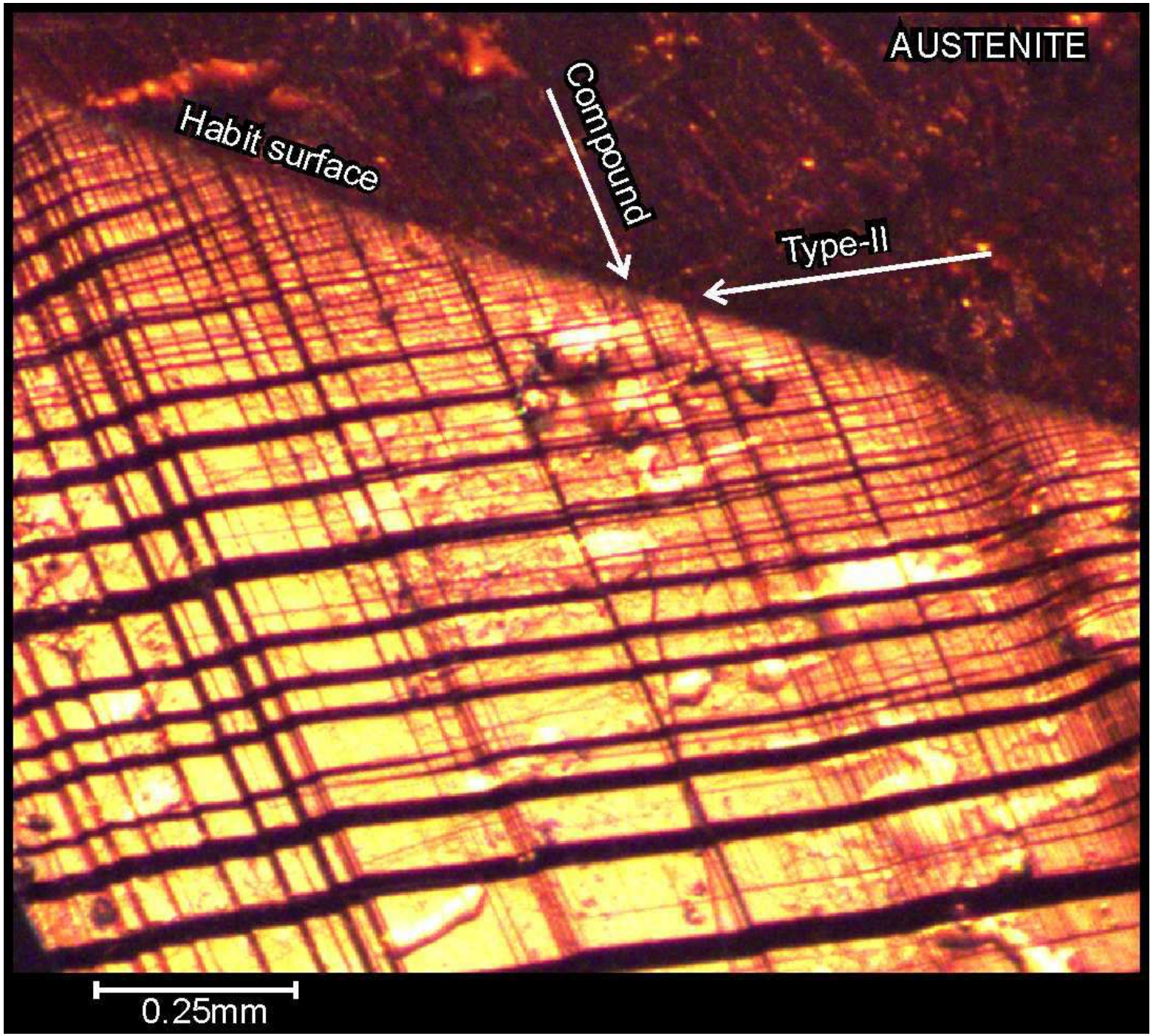
Interface normals



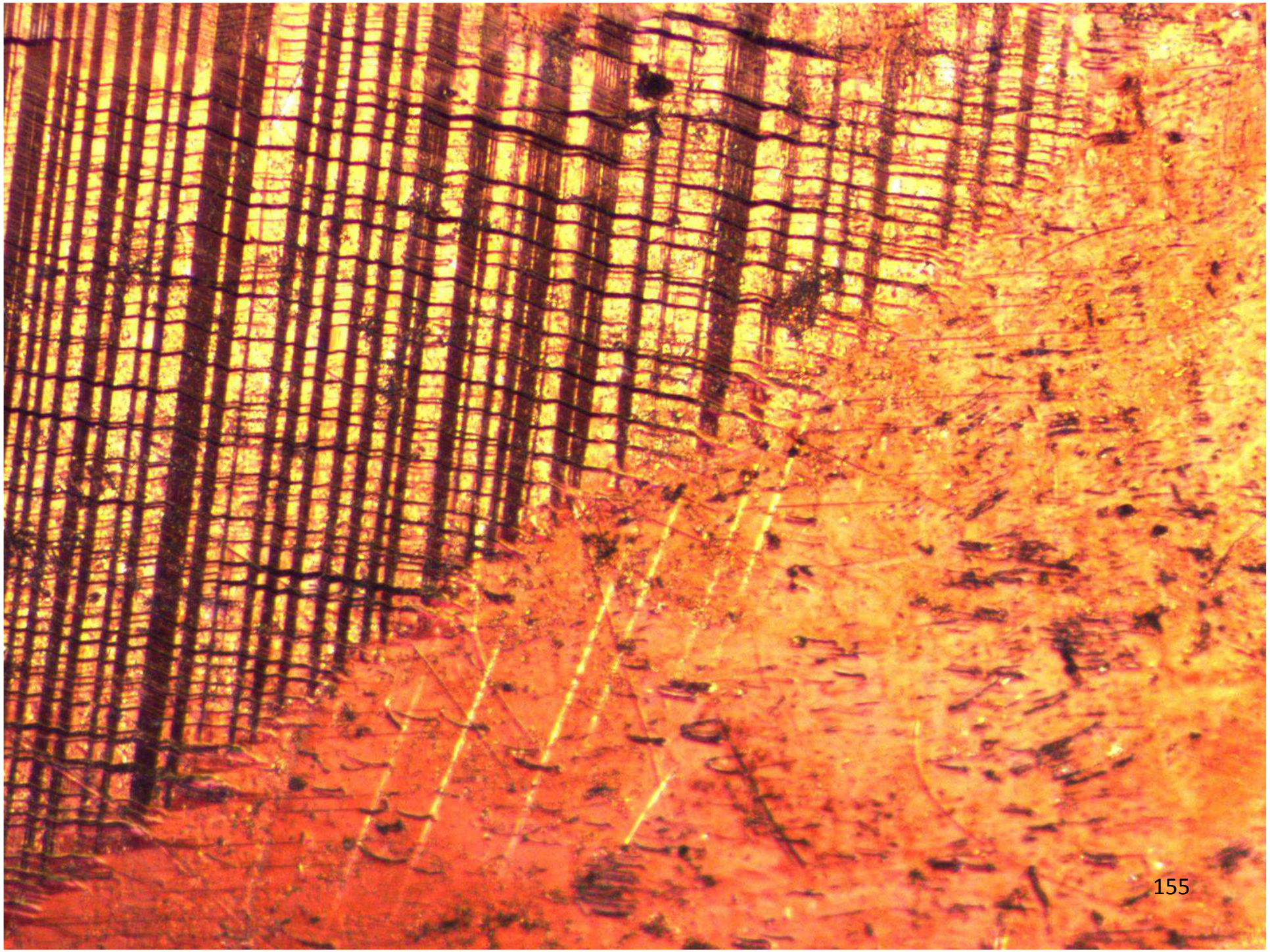


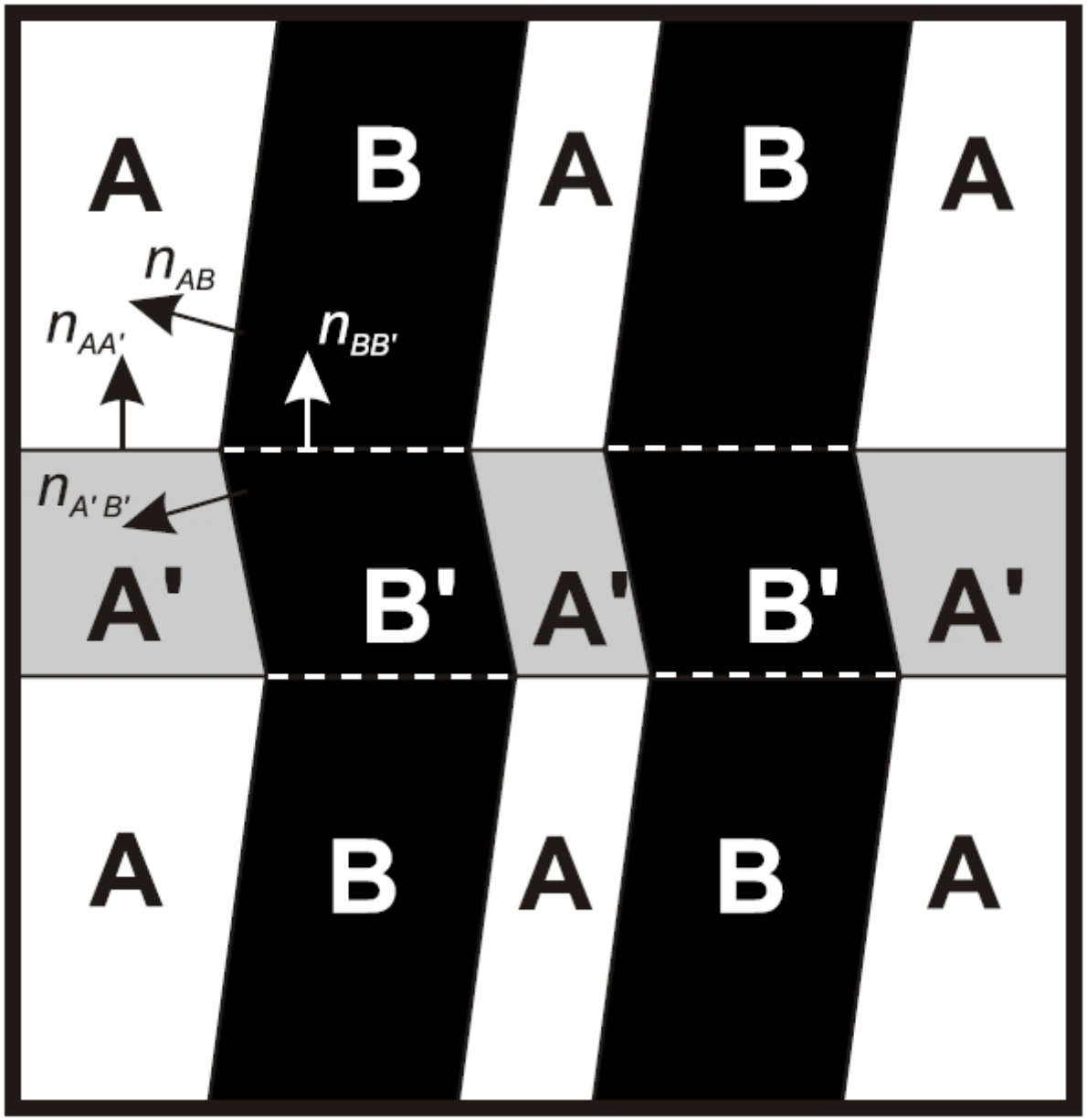
Experimental procedure (H. Seiner)

3.9×3.8×4.2mm CuAlNi single crystal



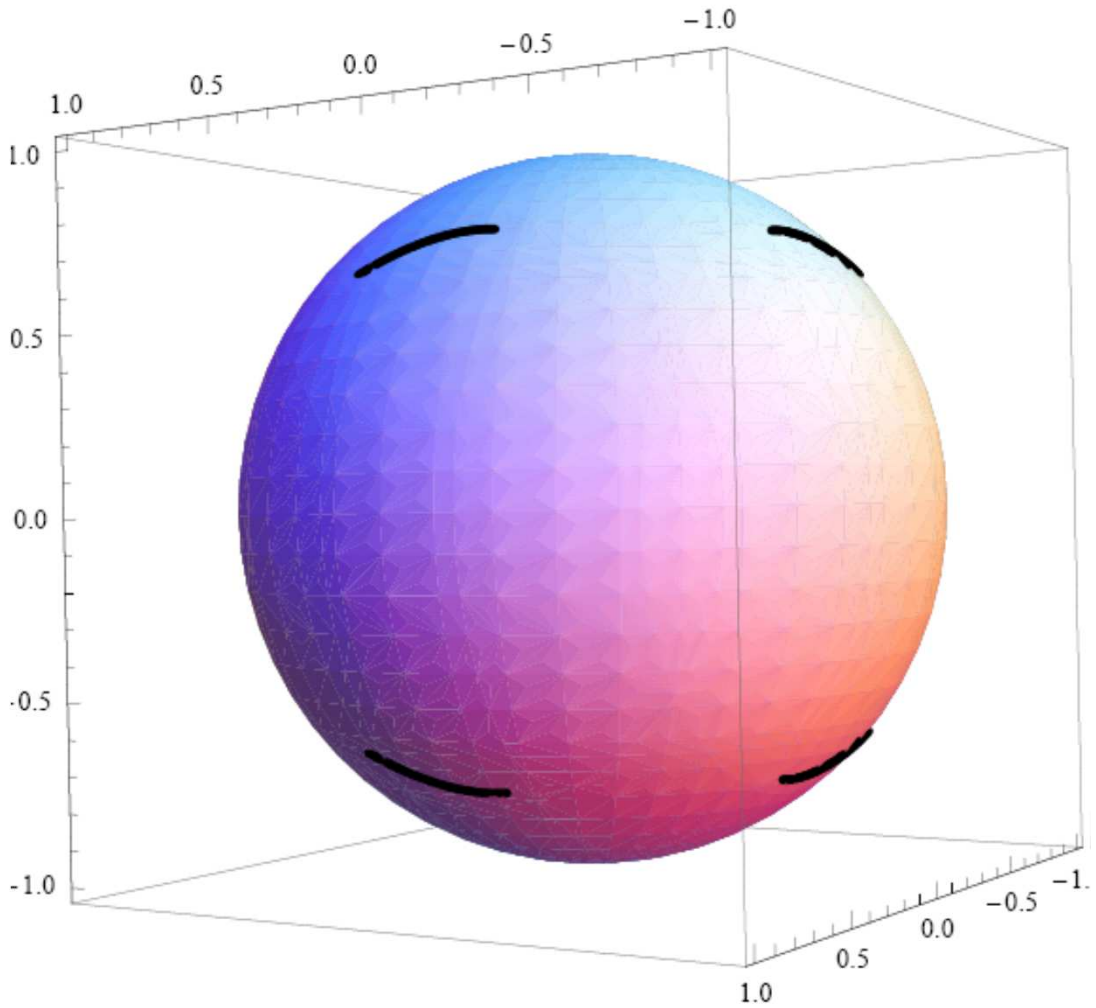
Optical micrograph (H. Seiner) of non-classical interface between austenite and a martensitic microstructure .
The arrows indicate the orientations of twinning planes of Type-II and compound twinning systems

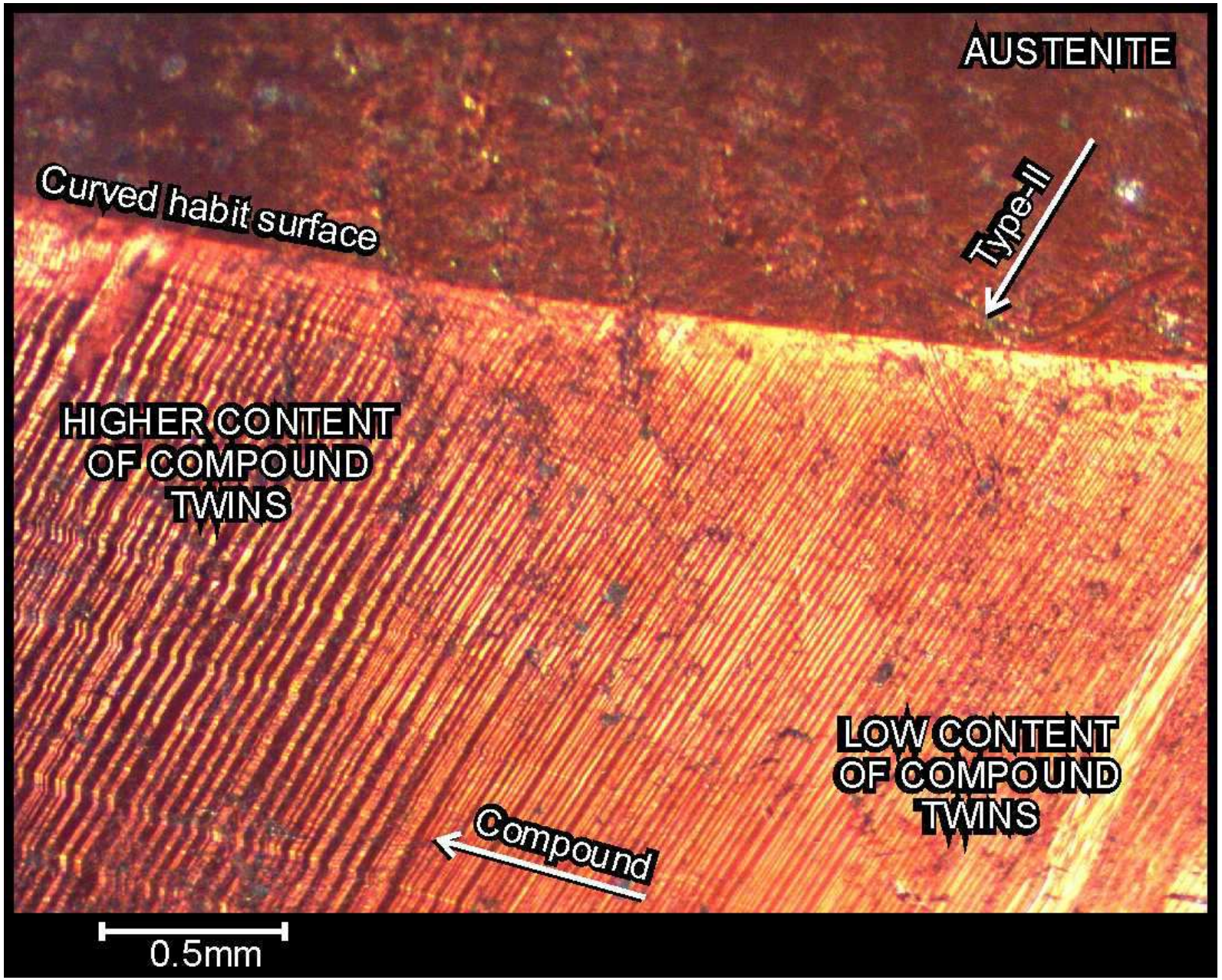




Twin crossing gradients

Possible nonclassical interface normals



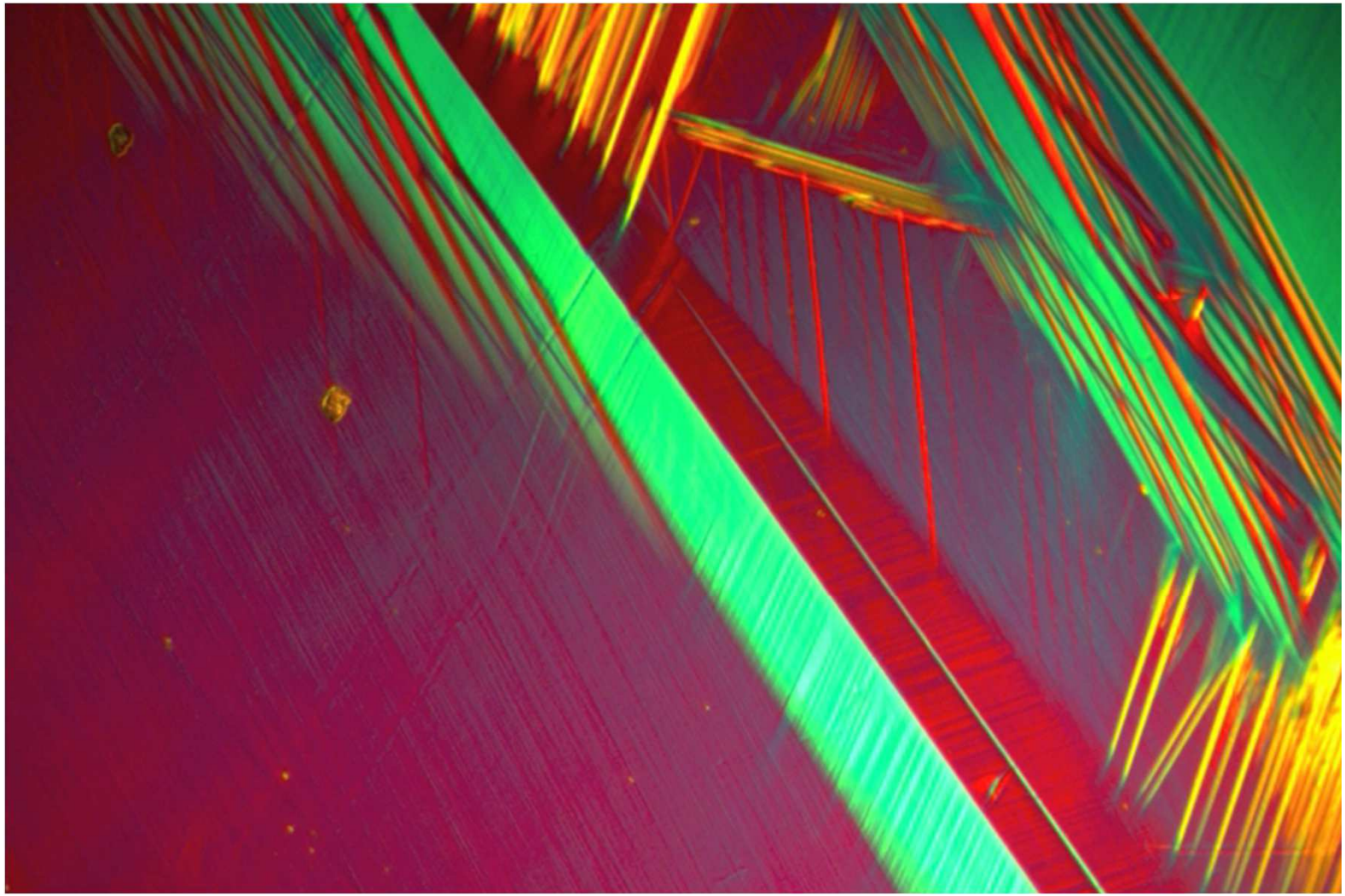


Curved interface between crossing twins and austenite resulting from the inhomogeneity of compound twinning. (Optical microscopy,H. Seiner)

Construction of curved interface

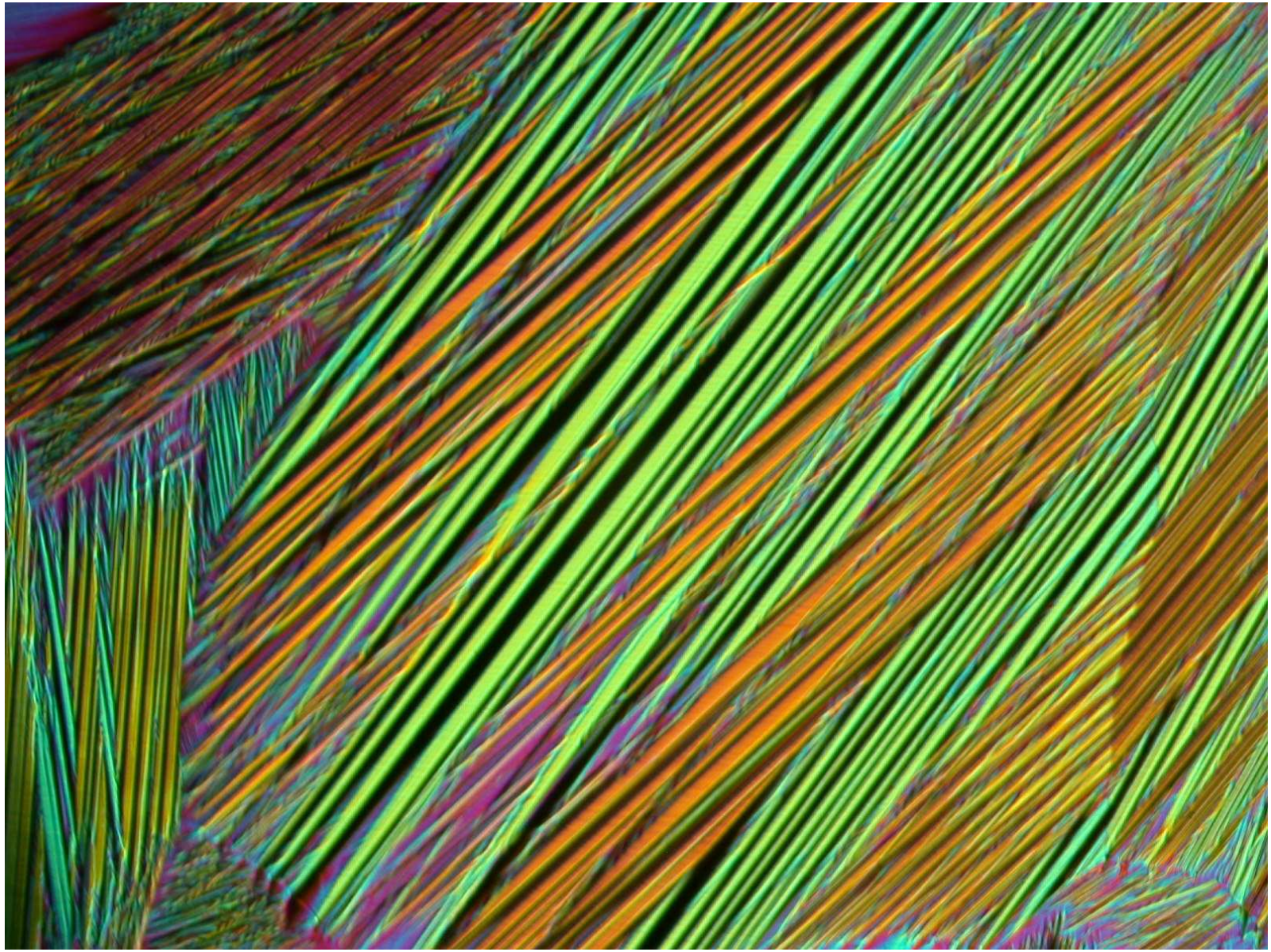
This is possible at zero stress provided $\mathbf{1}$ is rank-one connected to a relative interior point of the set $K = \cup_{i=1}^{N} SO(3)U_i$ of the martensitic wells, where relative is taken with respect to the set $D = \{A : \det A = \det U_i\}$. Such relative interior points are known to exist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

6. Complex microstructures. Nucleation of austenite.

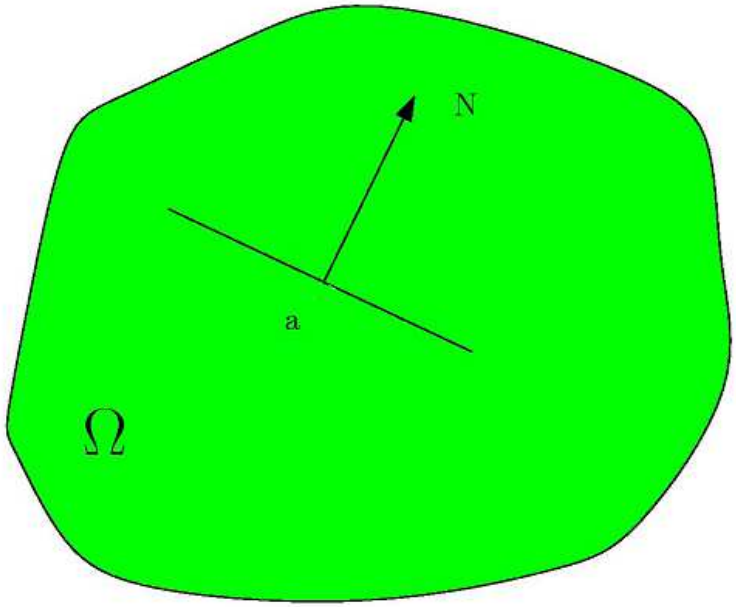


$Zn_{45}Au_{30}Cu_2$ ultra low hysteresis alloy

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



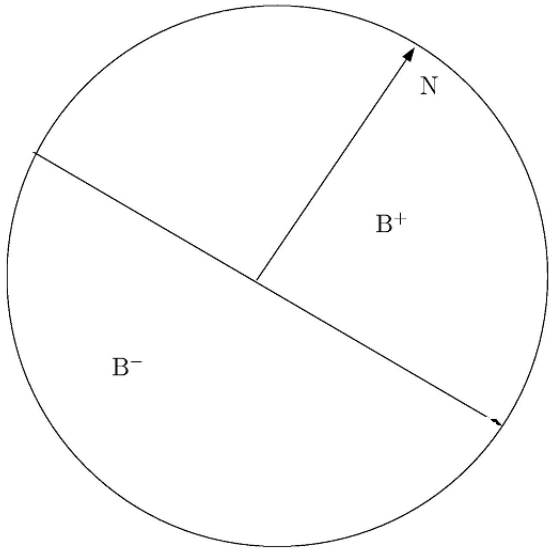
CuZnAl microstructure: Michel Morin (INSA de Lyon)



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



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

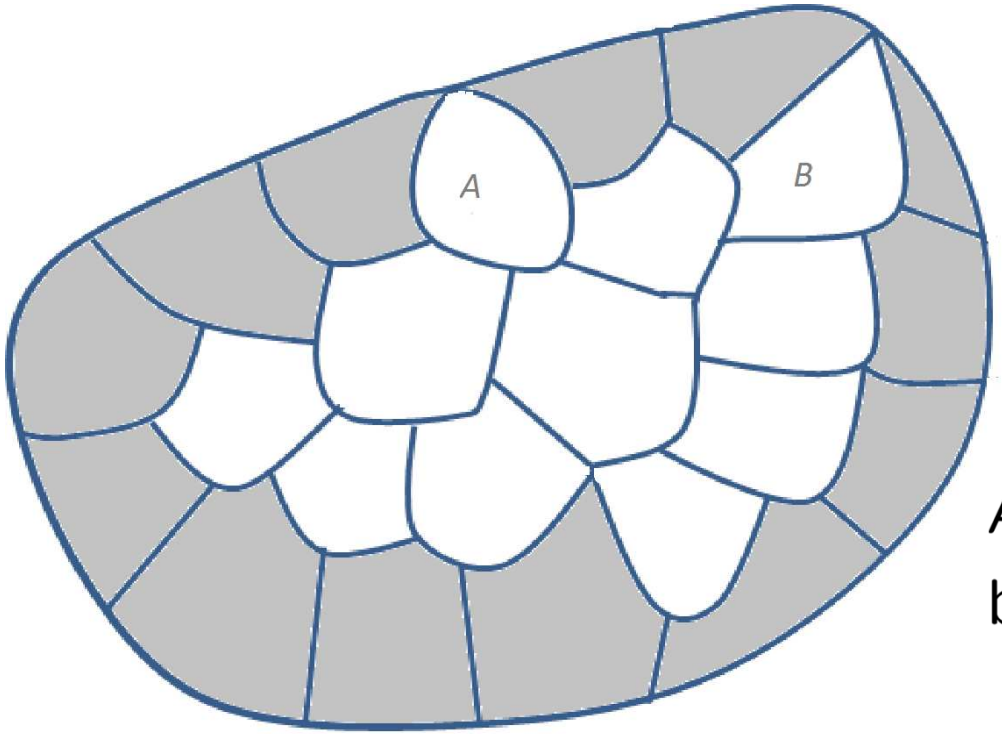
Proof of Theorem 2 uses quasiregular maps, which are useful also in constructing nonpolyconvex quasiconvex functions. False in higher dimensions (Iwaniec, Verhota, Vogel 2002)

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

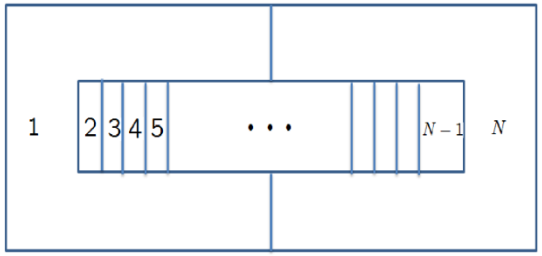
$$T = \bigcup_{1 \le i_1 < i_2 \le i_3} \partial\Omega_{i_1} \cap \partial\Omega_{i_2} \cap \partial\Omega_{i_3}.$$

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.

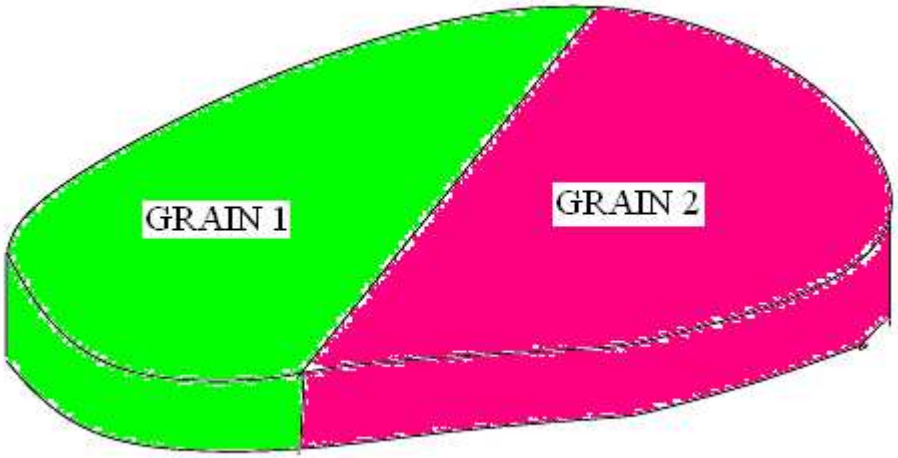
The bound is sharp.



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.

Application to a bicrystal

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



Grain 1

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

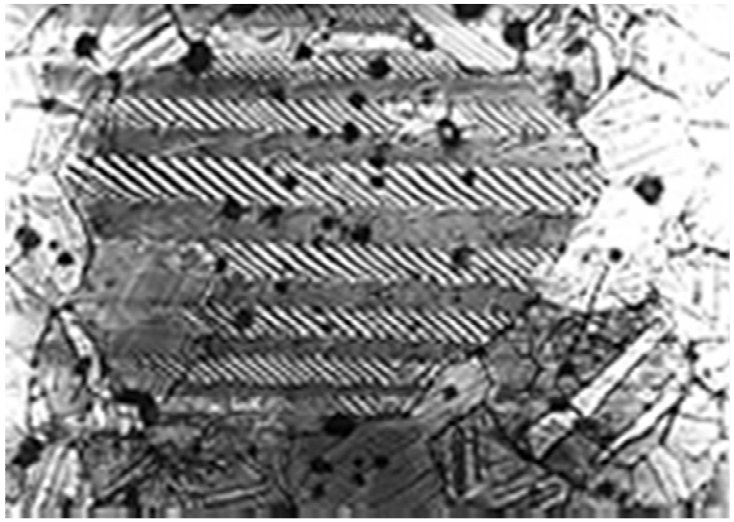
Grain 2

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

$$R_\alpha e_3 = e_3$$

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

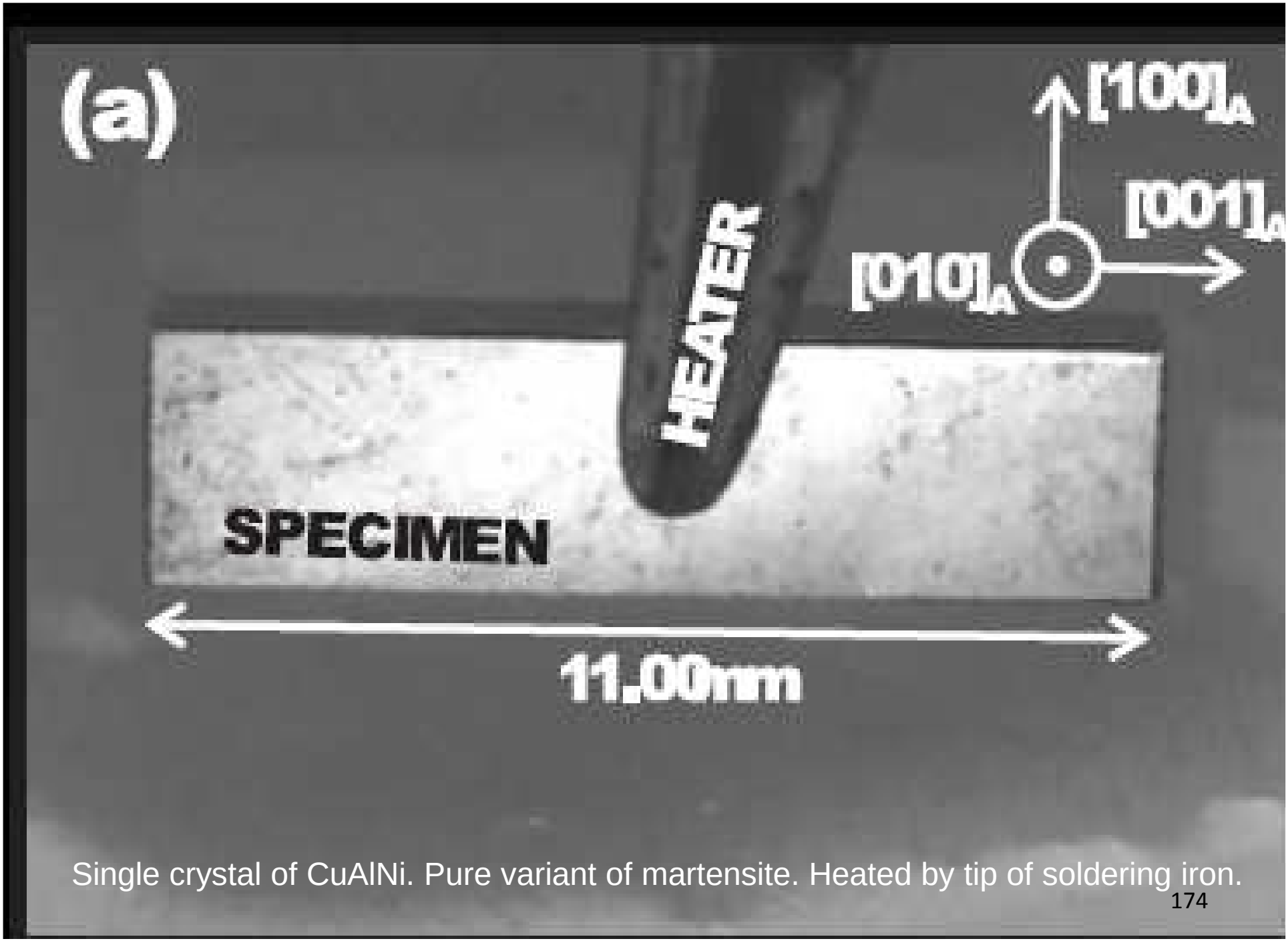
Localized heating experiment:

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.

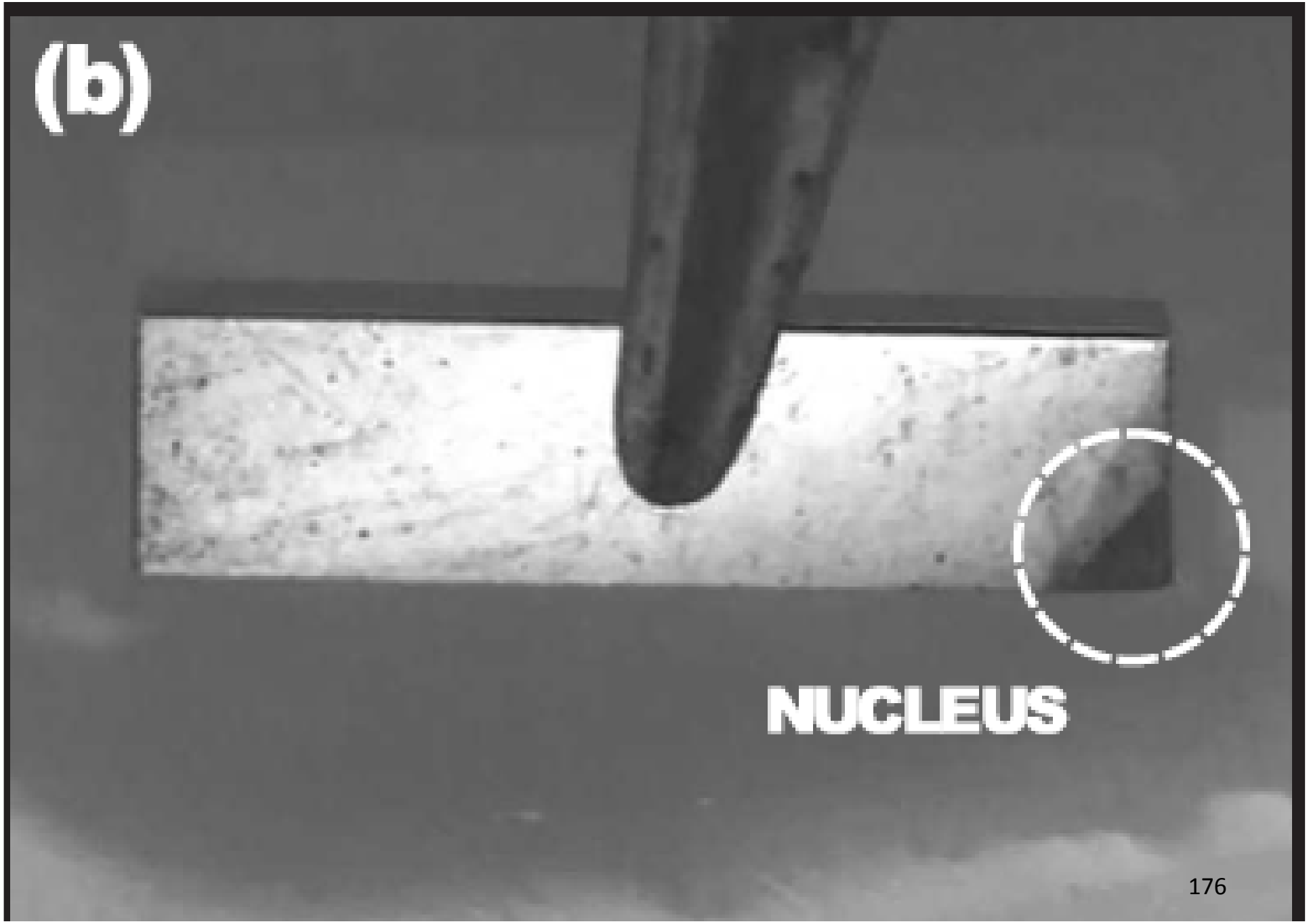
The martensite-to-austenite transition temperatures were $A_S = -6°$C and $A_F = 22°$C. The critical temperature T_C for the transition from the stabilized martensite induced by homogeneous heating for this specimen was $\sim$60°C. This was estimated from optical observations of the transition with one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

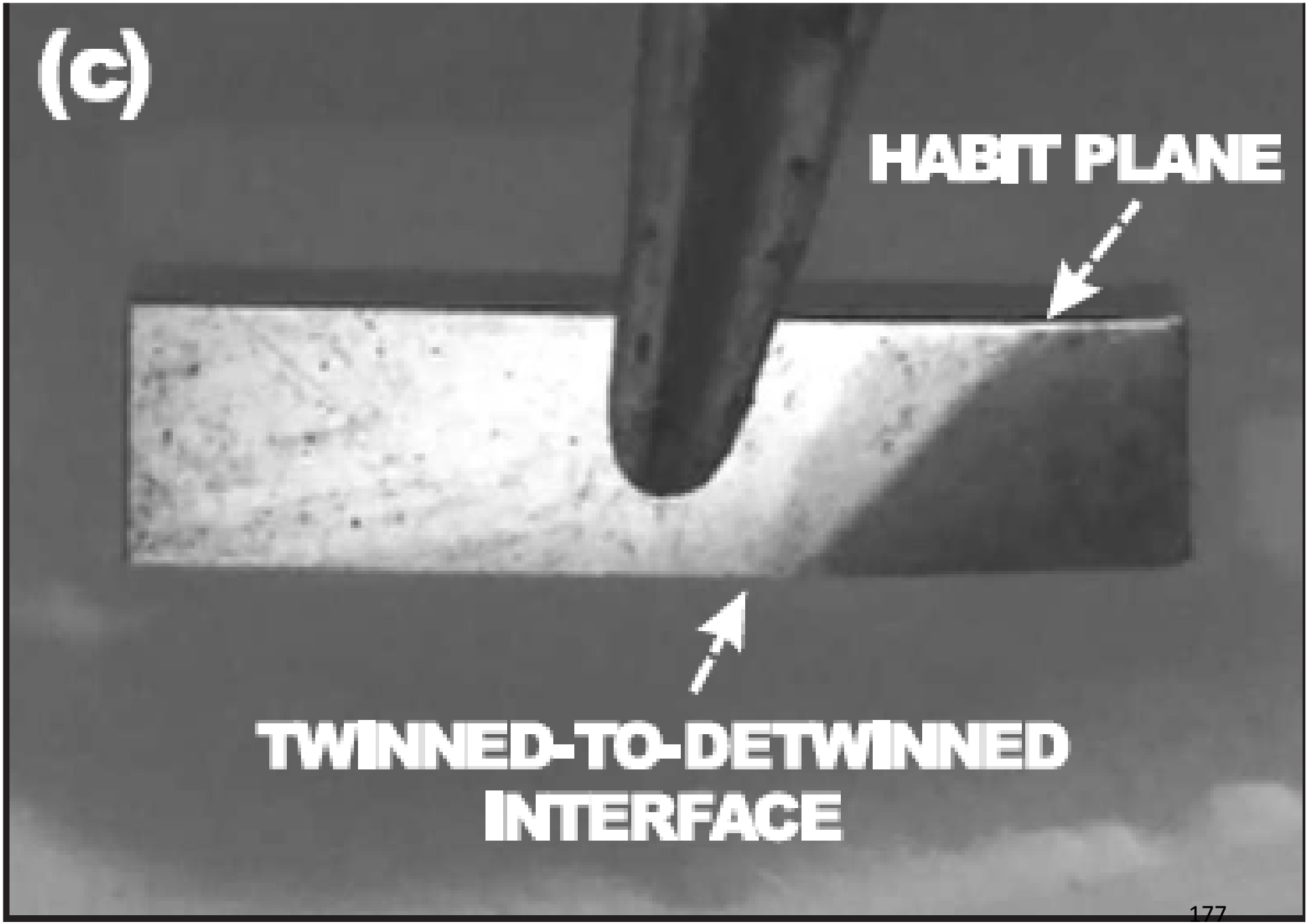
The specimen was freely laid on a slightly prestressed, free-standing polyethylene (PE) foil to ensure minimal mechanical constraints, then locally heated by touching its surface with an ohmically heated tip of a (digital) soldering iron with temperature electronically controlled to be 200°C, i.e. significantly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

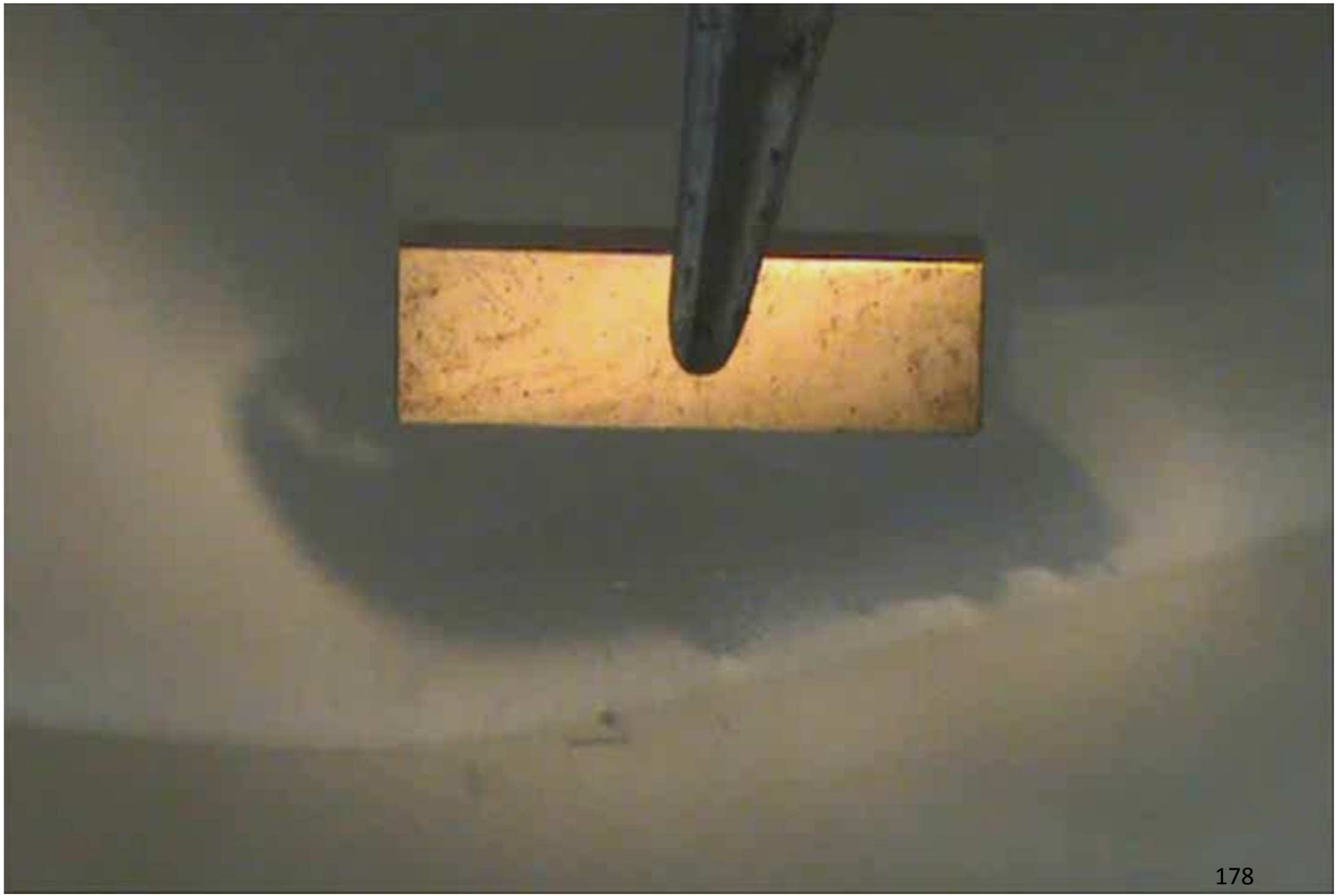


Single crystal of CuAlNi. Pure variant of martensite. Heated by tip of soldering iron.

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

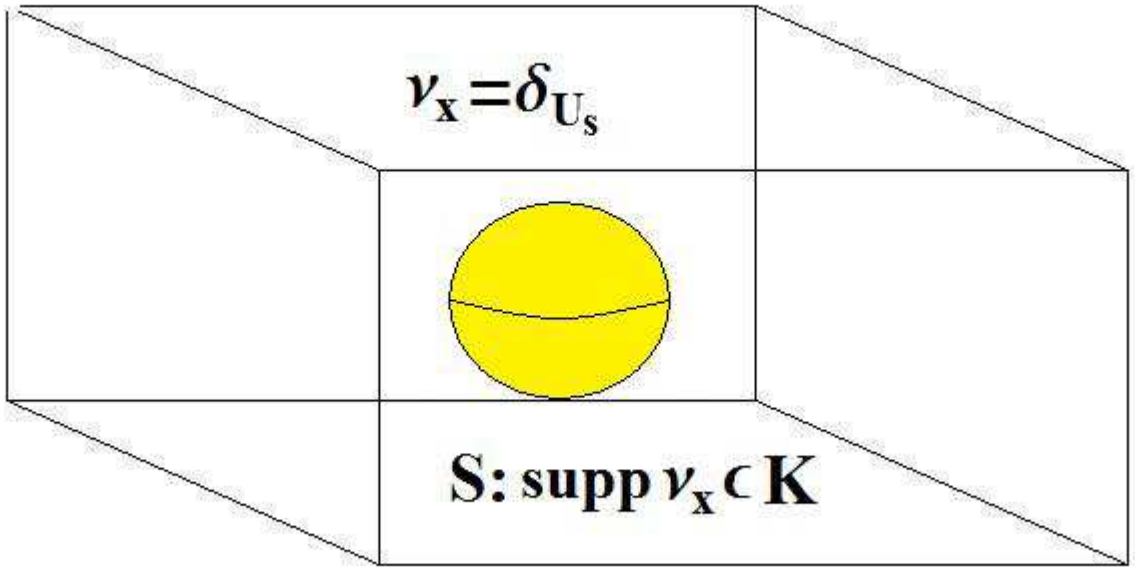
$$W(A) = \begin{cases} -\delta & A \in SO(3) \\ 0 & A \in \bigcup_{i=1}^{6} SO(3)U_i \\ +\infty & \text{otherwise} \end{cases},$$

and $\delta > 0$.

So $W(A) < \infty$ on

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

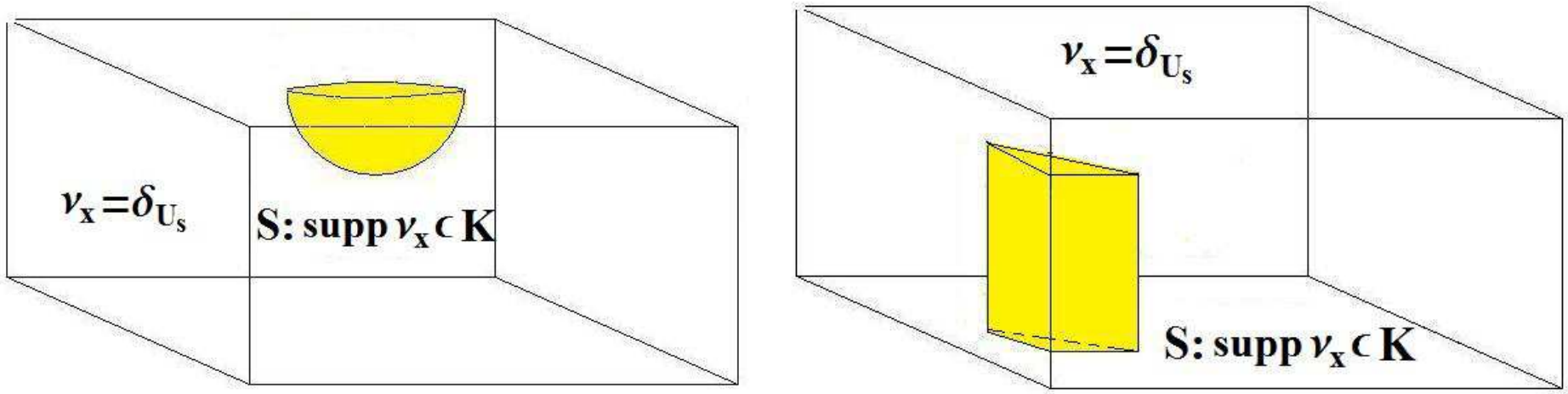
Nucleation impossible in the interior



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

(quasiconvexity at U_s)

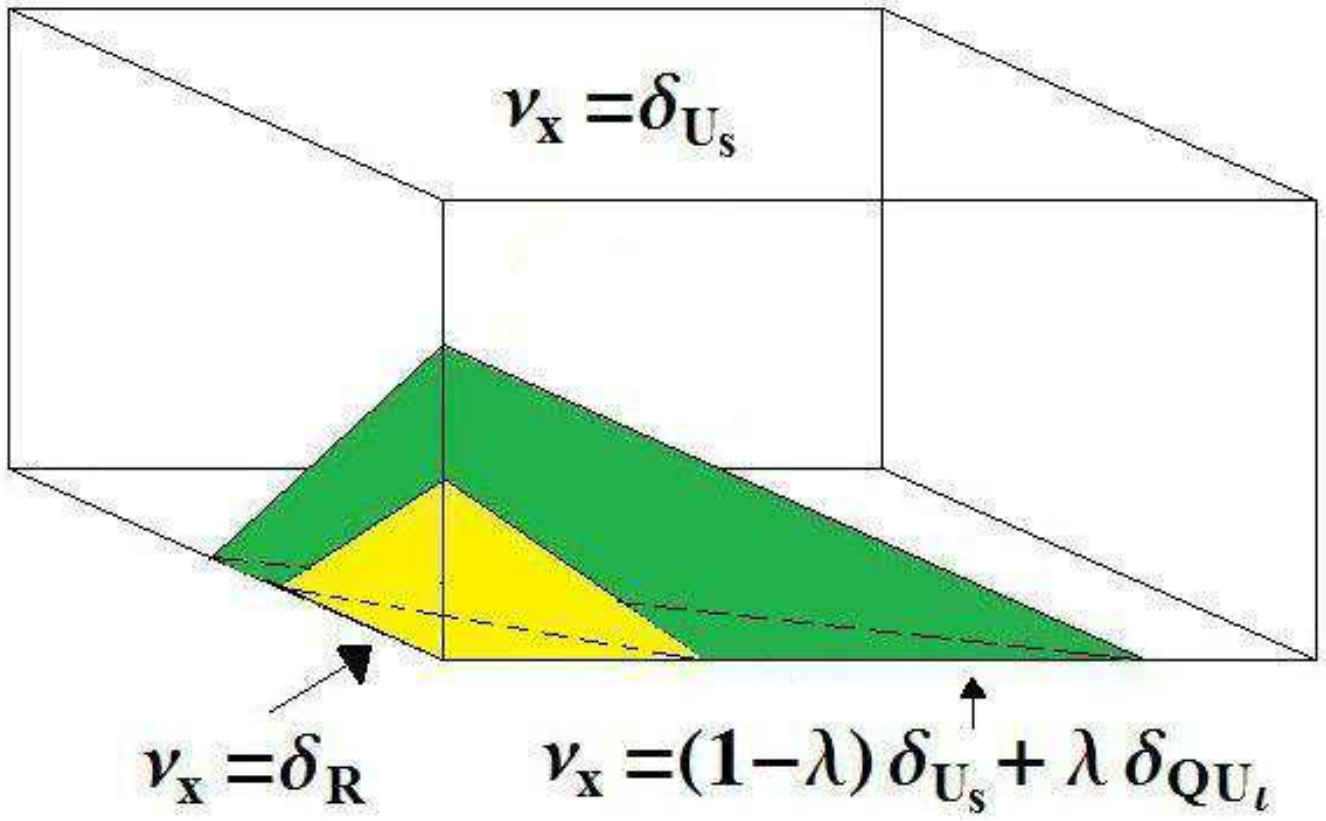
Nucleation impossible at faces or edges



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



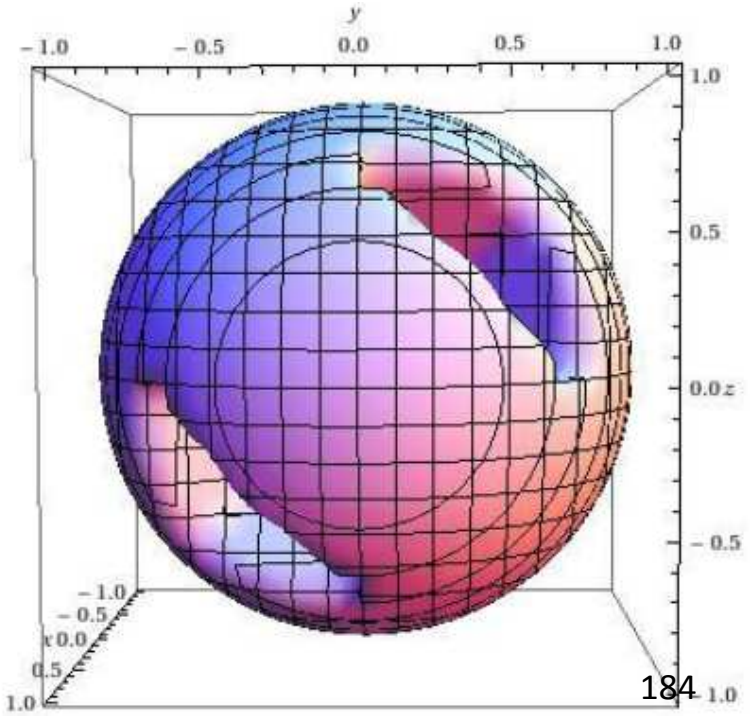
$I(\nu) < I(\delta_{U_s})$

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 $A_S = -6°\text{C}$ 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 $T_c \sim 60°\text{C}$? In other words, what is the explanation for the mechanical stabilization effect?

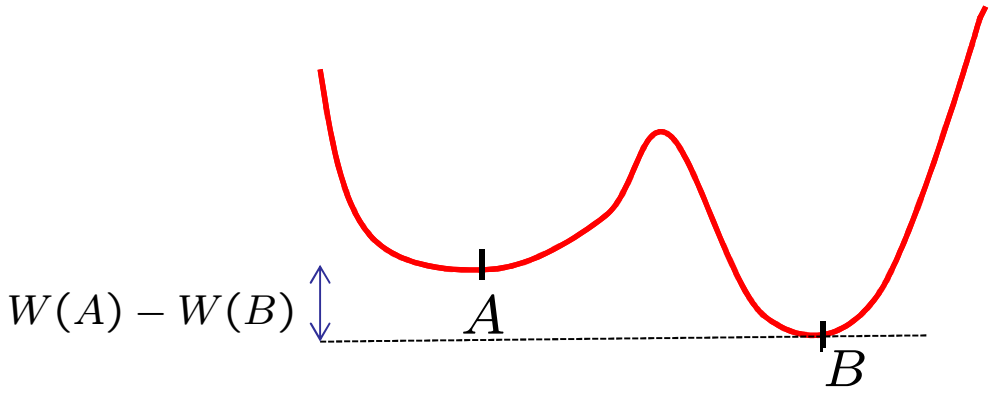
One piece of evidence is that under homogeneous heating the nucleation still takes place at a corner, suggesting the relevance of the quasiconvexity calculations.

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.

7. Local minimizers with and without interfacial energy

Incompatibility-induced hysteresis

JB/James 2014



Example.

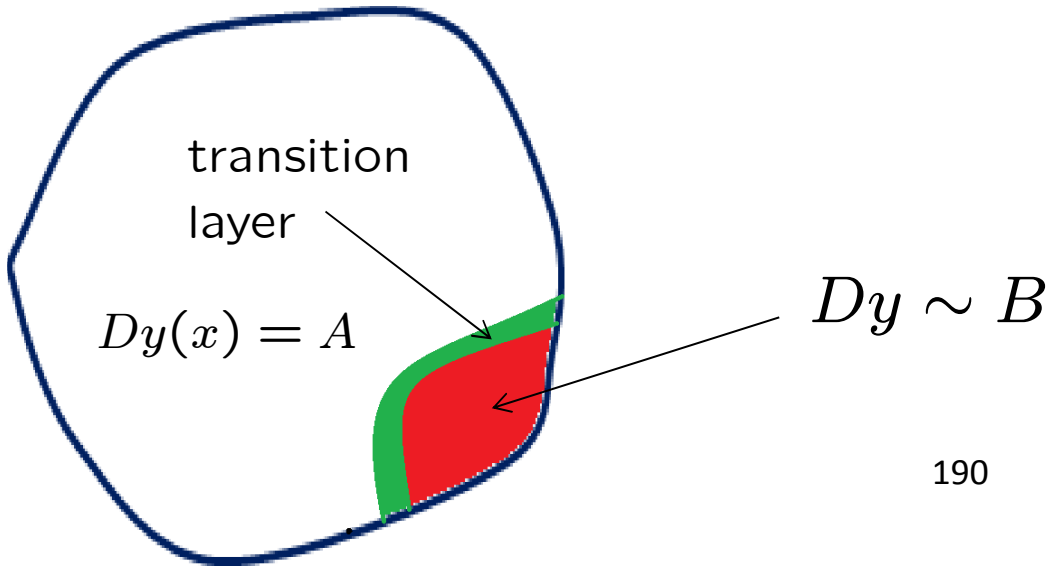
Consider the integral

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

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

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

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.

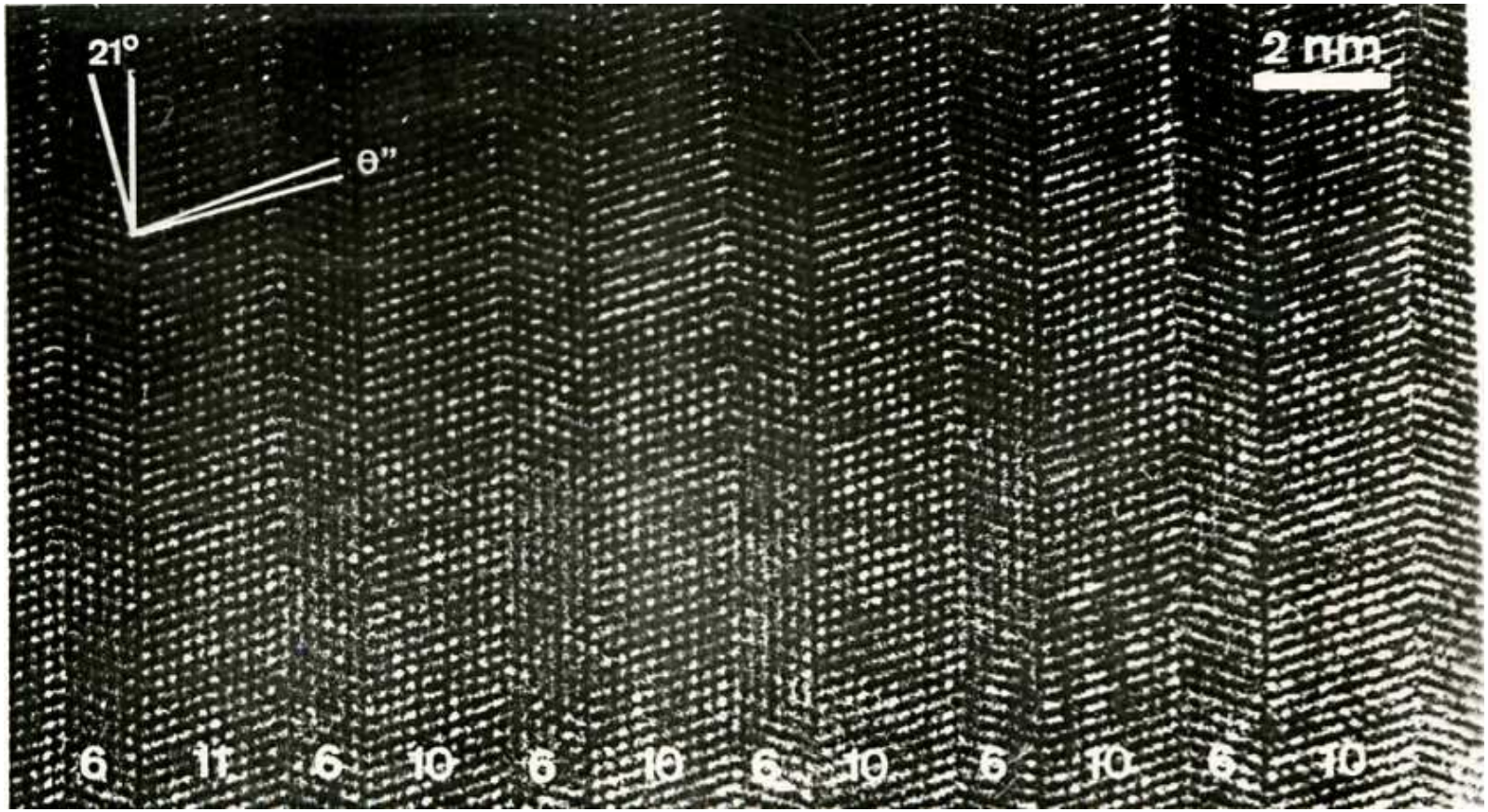
Applications:

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

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

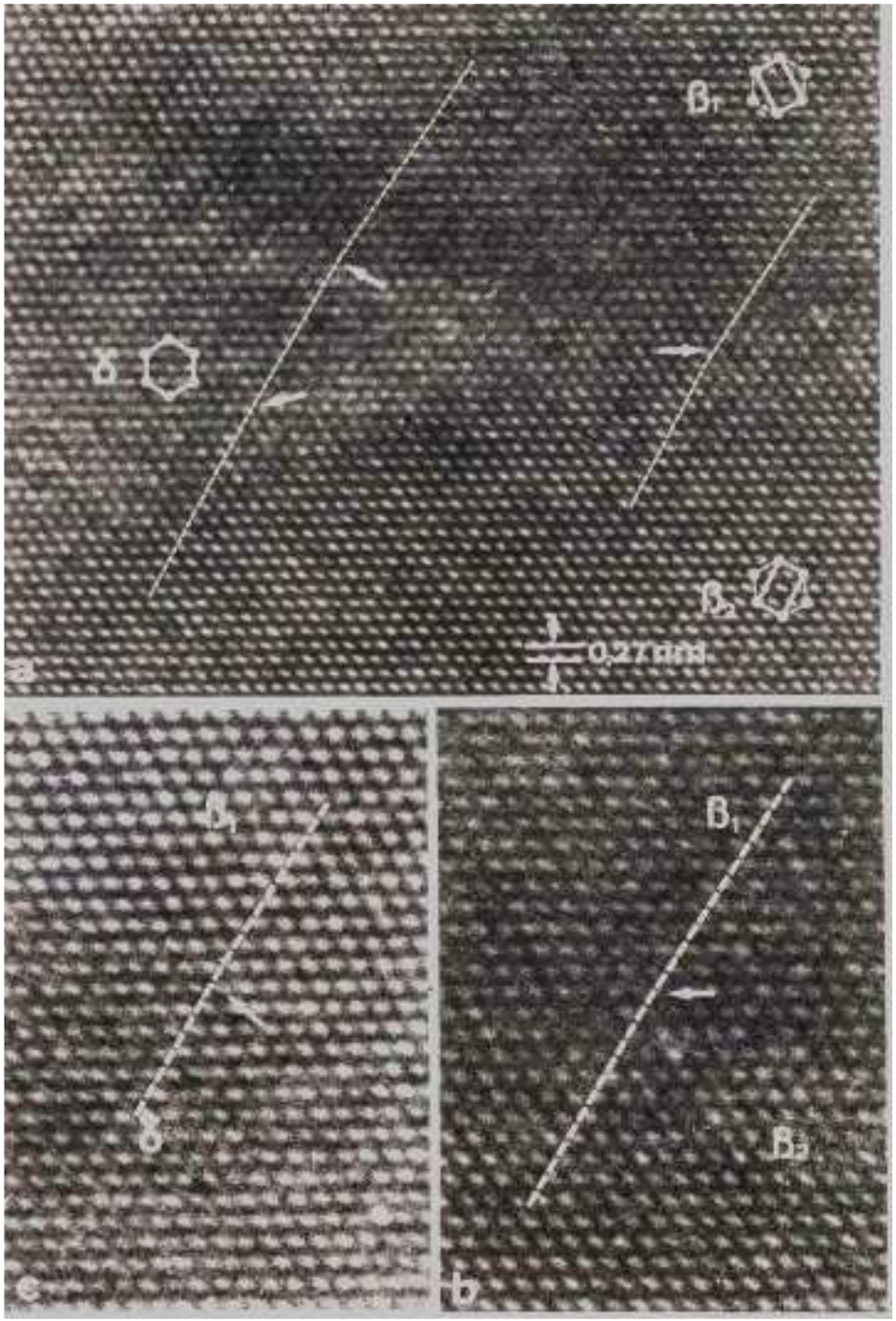
Interfacial energy

Some interfaces are atomistically sharp



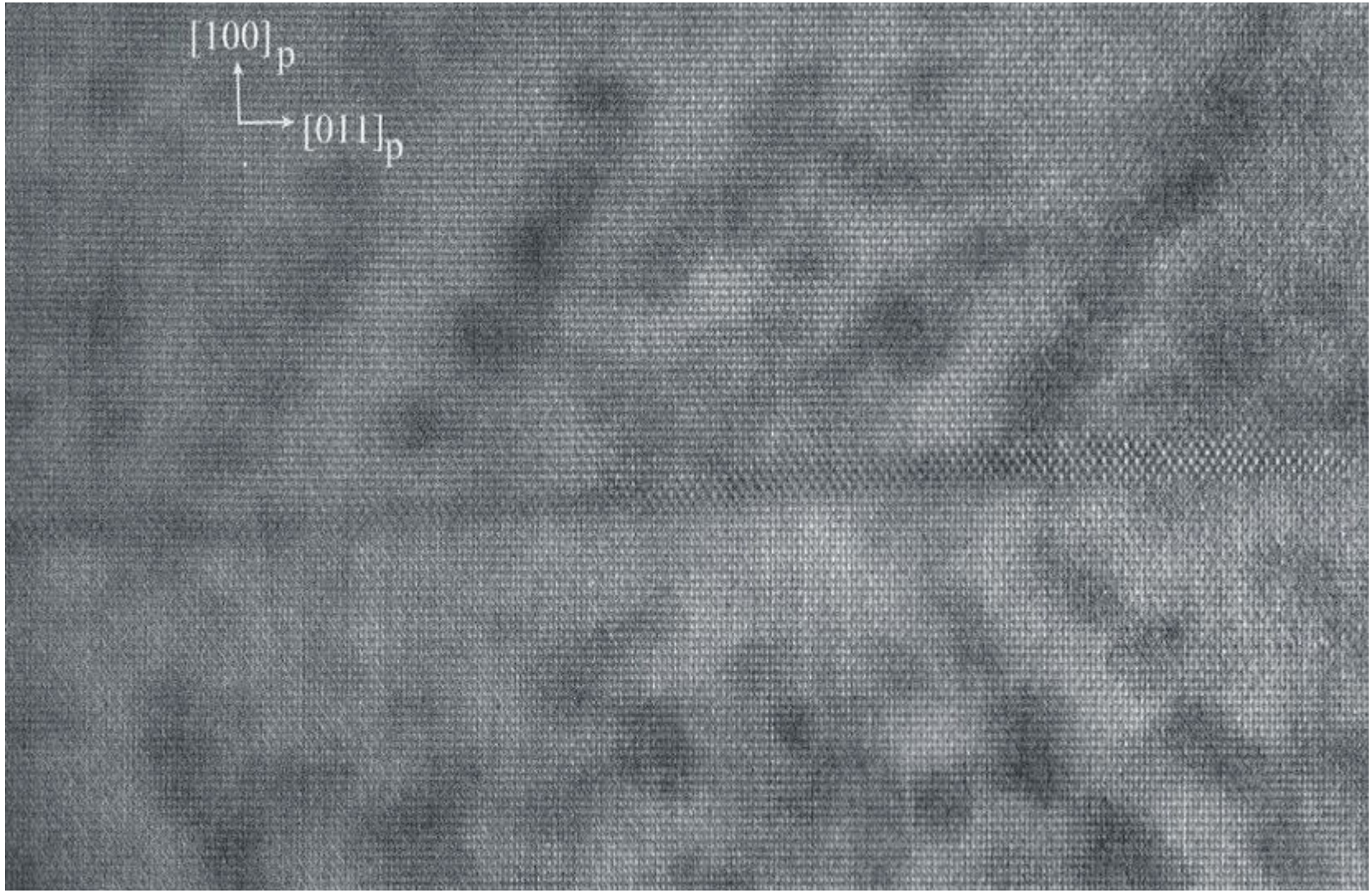
NiMn Baele, van Tenderloo, Amelinckx

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

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

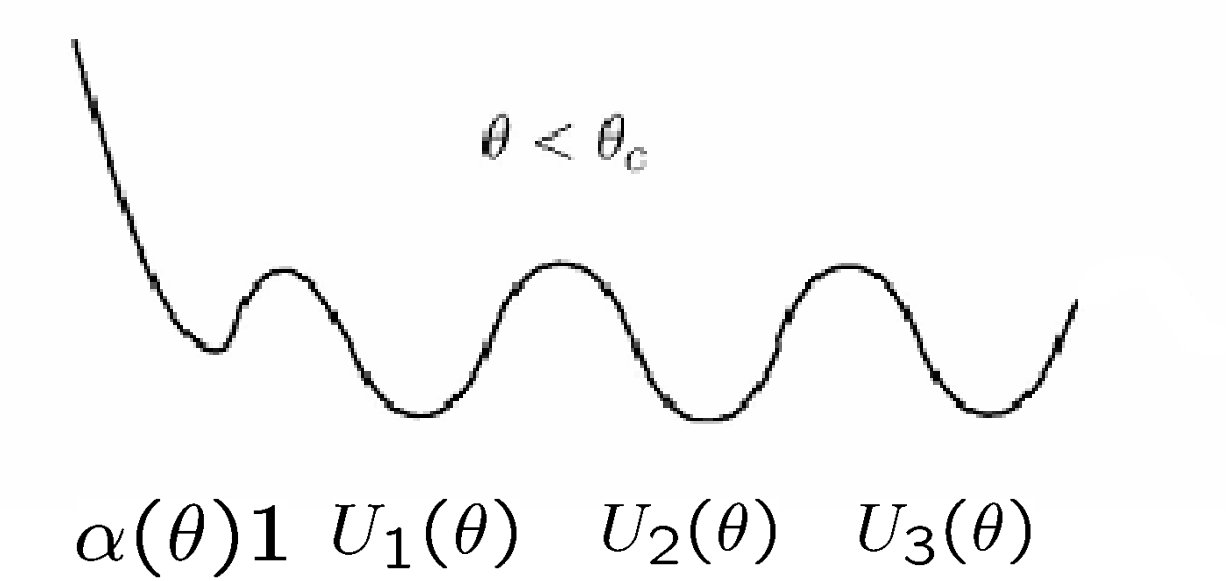
in $W^{1,\infty}(\Omega;\mathbf{R}^3)$.

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 $R \in \mathrm{SO}(3)$,
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. $\bar{y}(x) = \alpha Rx + a$, $R \in \mathsf{SO}(3), a \in \mathbf{R}^3$, *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* $\|y - \alpha Rx - a\|_1$ *is sufficiently small.*

Remark.

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

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

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.

Liquid crystals and the description of defects.

Topics

1. Liquid crystals, phase transitions and order parameters.
2. The Landau – de Gennes and Oseen – Frank theories.
3. Onsager theory.
4. The description of defects.

Some themes

- Function spaces as a part of models in physics
- Relation between different levels of description (e.g. molecular vs continuum, order parameters of different dimensions)
- Lessons from solid mechanics
- Constraints (equality and inequality) on unknowns in variational problems

1. Liquid crystals, phase transitions and order parameters

What are liquid crystals?

An intermediate state of matter between liquids and solids.

Liquid crystals flow like liquids, but the constituent molecules retain orientational order.

A multi-billion dollar industry.

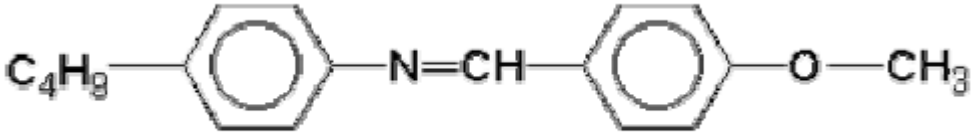
HP bistable display

Molecular structure

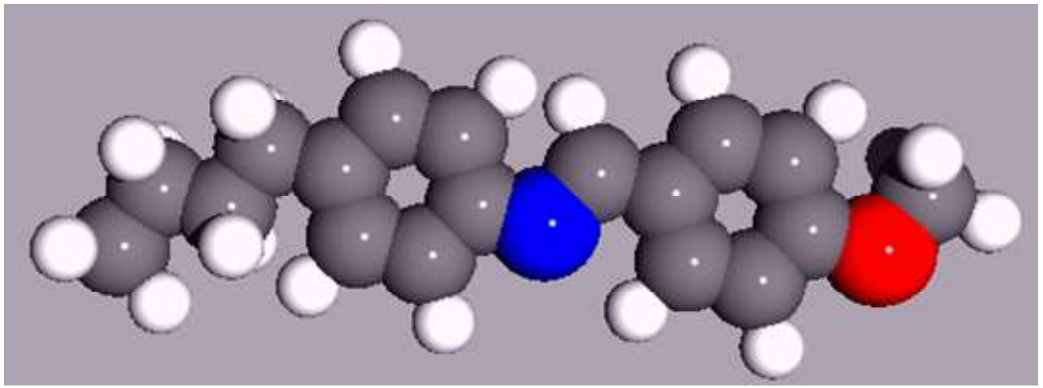
Liquid crystals are of many different types, the main classes being nematics, cholesterics and smectics

Nematics consist of rod-like molecules.

Length 2-3 nm



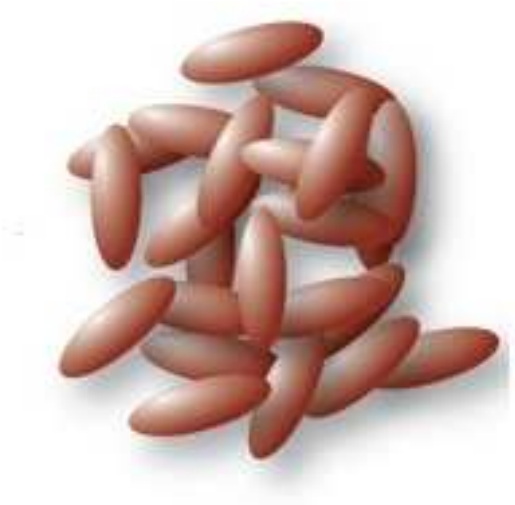
Methoxybenzilidene Butylanaline ("MBBA")



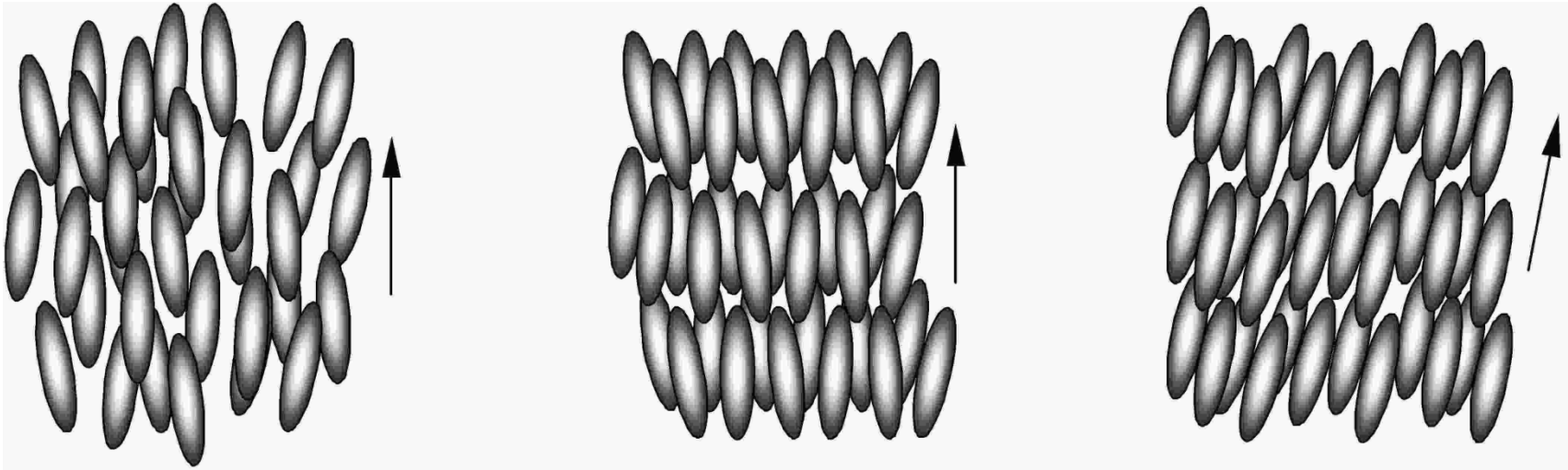
Prof. Dr. Wolfgang Muschik
TU Berlin
http://wwwitp.physik.tu-berlin.de/muschik/

Commercial liquid crystal displays use a mixture of several different fluids.

Depending on the nature of the molecules, the interactions between them and the temperature the molecules can arrange themselves in different phases.



Isotropic fluid – no orientational or positional order



Nematic phase orientational but no positional order

Smectic A phase

Smectic C phase

Orientational and some positional order

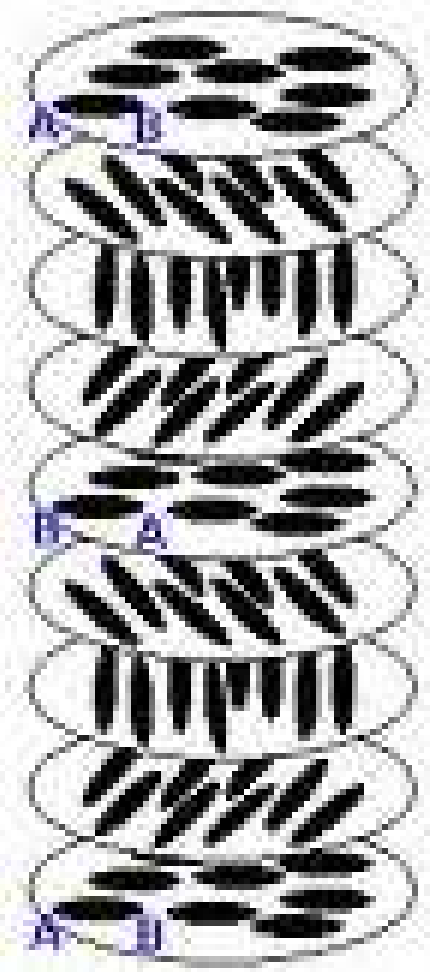
The molecules have time-varying orientations due to thermal motion.

Electron micrograph
of nematic phase

http://www.netwalk.com/~laserlab/lclinks.html

Cholesterics

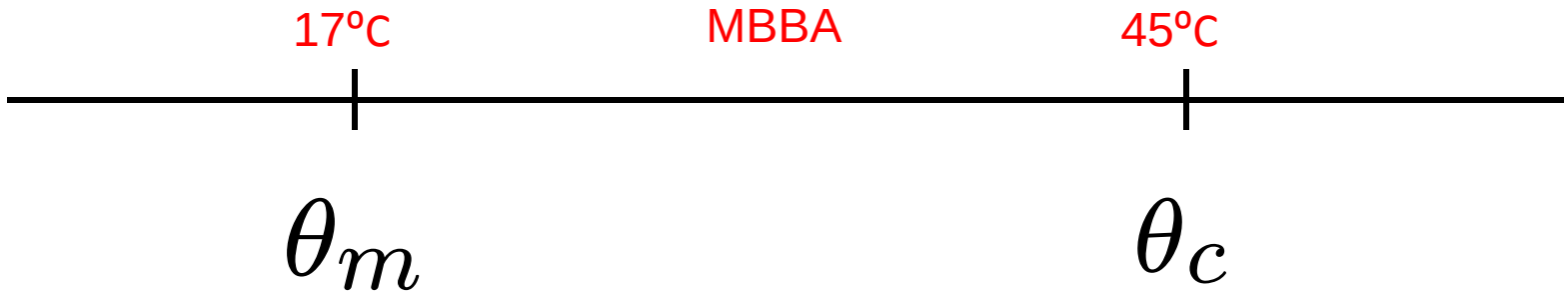
If a chiral dopant is added the molecules can form a cholesteric phase in which the mean orientation of the molecules rotates in a helical fashion.



DoITPoMS, Cambridge

Isotropic to nematic phase transition

The nematic phase typically forms on cooling through a critical temperature θ_c by a phase transformation from a high temperature isotropic phase.



$\theta < \theta_m$
other LC or solid phase

$\theta_m < \theta < \theta_c$
nematic

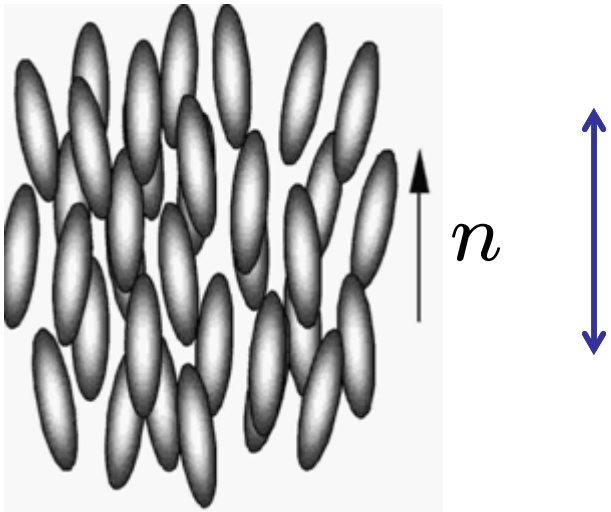
$\theta > \theta_c$
isotropic

MBBA

DoITPoMS, Cambridge

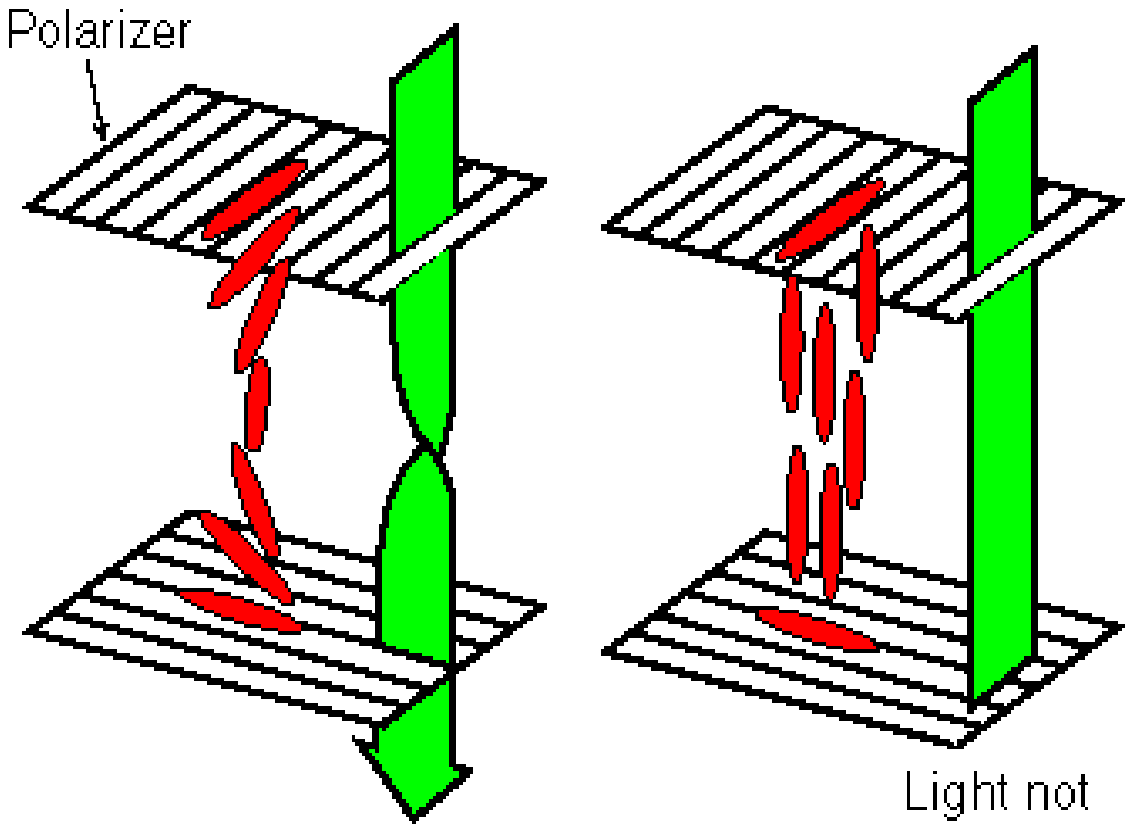
The director

A first mathematical description of the nematic phase is to represent the mean orientation of the molecules by a unit vector $n = n(x, t)$.



But note that for most liquid crystals n is equivalent to $-n$, so that a better description is via a *line field* in which we identify the mean orientation by the line through the origin parallel to it.

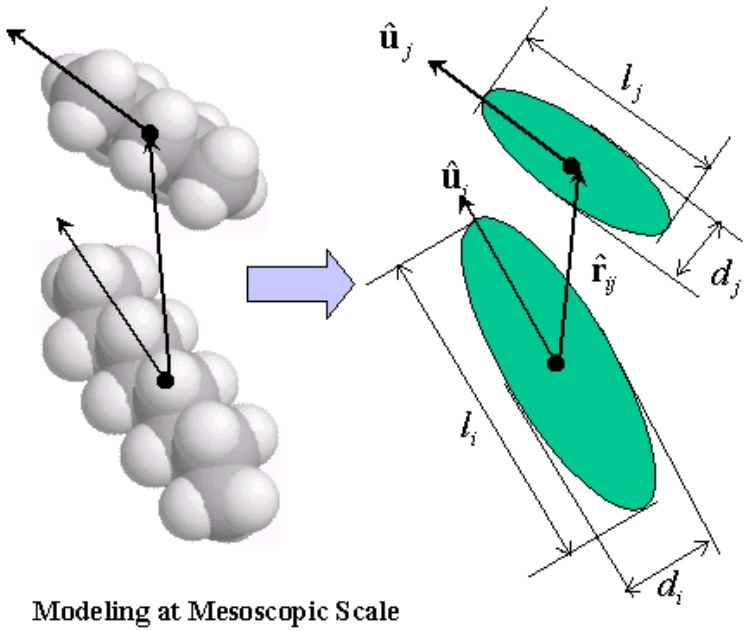
The twisted nematic display



(a) Voltage **OFF** (b) Voltage **ON**

Modelling via molecular dynamics

Monte-Carlo simulation using Gay-Berne potential to model the interaction between molecules, which are represented by ellipsoids.



Modeling at Mesoscopic Scale

This interaction potential is an anisotropic version of the Lennard-Jones potential between pairs of atoms or molecules.

http://mw.concord.org

$$U_{\mathrm{GB}} = 4\varepsilon_0\varepsilon(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)[u(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)^{12} - u(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)^{6}],$$

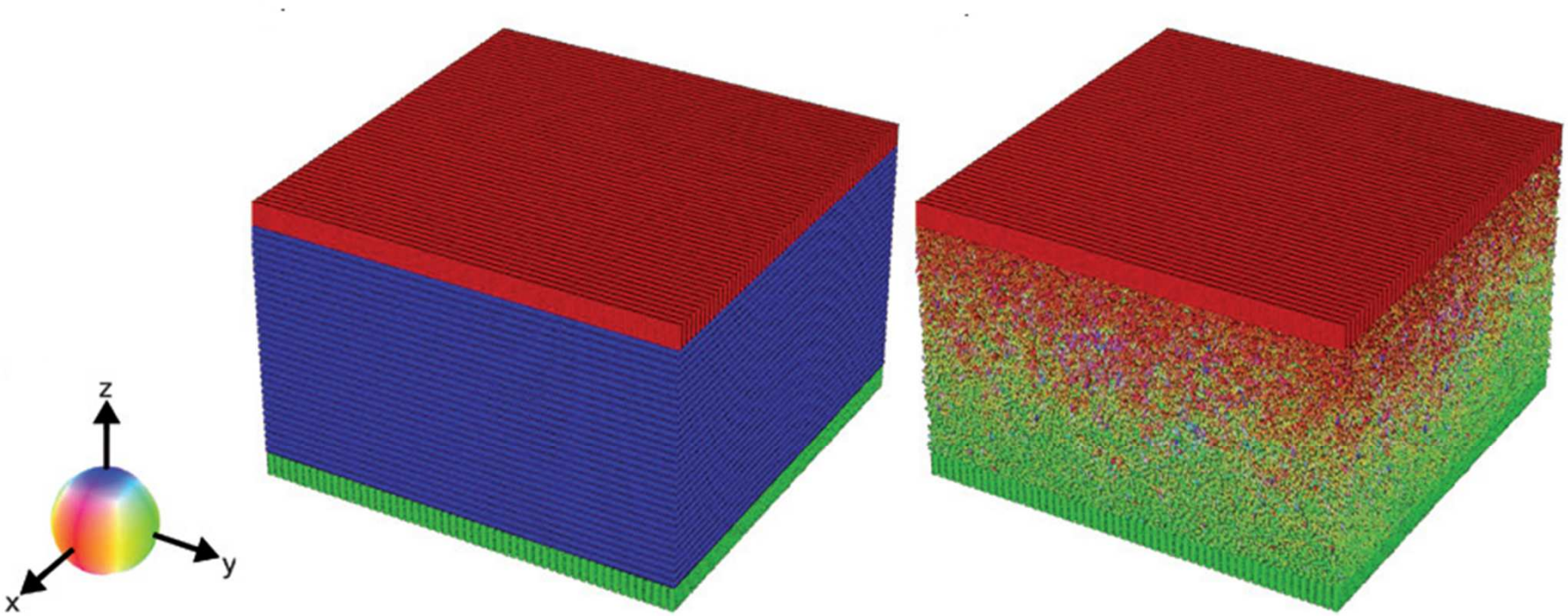
where

$$u(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j) = \frac{\sigma_c}{r_{ij} - \sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j) + \sigma_c},$$

$r_{ij} = |\hat{\mathbf{r}}_{ij}|$, and where the functions $\sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)$ and $\varepsilon(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)$ measure the contact distance between the ellipsoids and the attractive well depth respectively (depending in particular on the ellipsoid geometry) and ε_0, σ_c are empirical parameters.

Twisted nematic display simulation

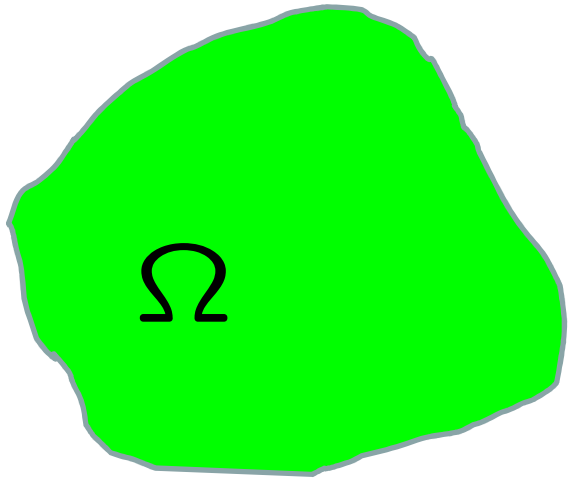
944,784 molecules, including 157,464 fixed in layers near the boundaries to prescribe the orientation there.



M. Ricci, M. Mazzeo, R. Berardi, P. Pasini, C. Zannoni, 2009
(courtesy Claudio Zannoni)

Continuum models

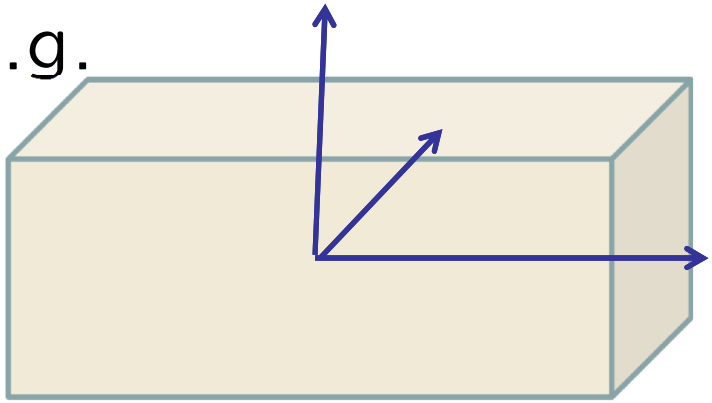
Consider a nematic liquid crystal filling a container $\Omega \subset \mathbb{R}^3$.



To keep things simple consider only static configurations, for which the fluid velocity is zero.

Microscopic state variables

We represent a typical liquid crystal molecule by a 3D region M (rod, ellipsoid, parallepiped ...) of approximately the same shape and symmetry. We place M in a standard position with centroid at the origin, e.g.



and define the isotropy groups

$$G_M = \{R \in O(3) : RM = M\}$$
$$G_M^+ = \{R \in SO(3) : RM = M\}$$

If $G_M = G_M^+$ then the molecule is said to be *chiral* (as in cholesterics).

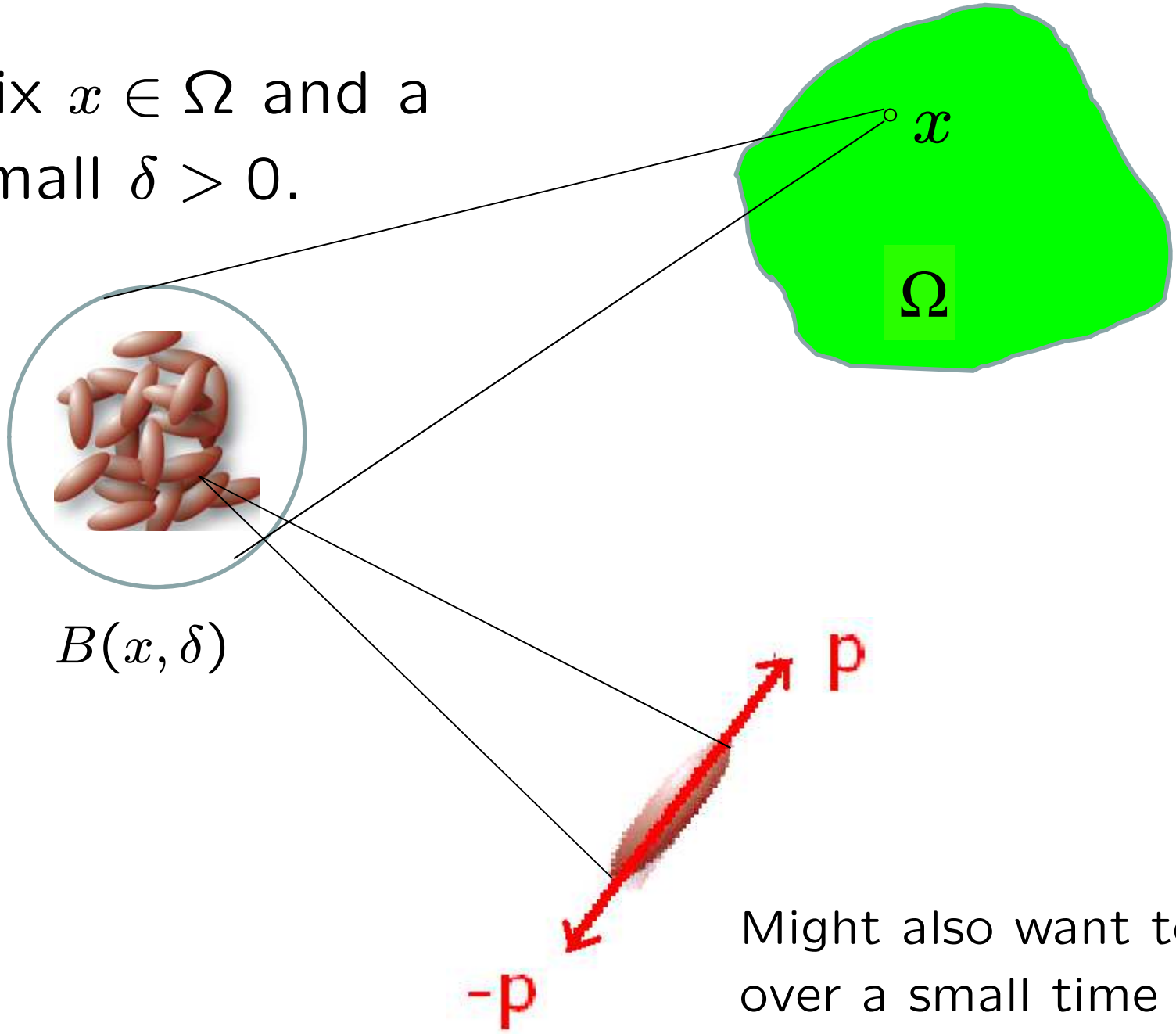
$RM = \tilde{R}M$ for $R, \tilde{R} \in SO(3)$ iff $\tilde{R}^T R \in G_M^+$. Hence the orientation of a molecule can be represented by an element of the space of cosets $SO(3)/G_M^+$ (cf Mermin 1979).

For M a cylindrical rod or ellipsoid of revolution

we can identify $SO(3)/G_M^+$ with $\mathbb{R}P^2$, that is with lines through the origin parallel to the long axis, or equivalently with matrices $p \otimes p, p \in S^2$.

Molecular orientations of nematics

Fix $x \in \Omega$ and a small $\delta > 0$.



Might also want to average over a small time interval.

The distribution of orientations of molecules in $B(x, \delta)$ can be represented by a probability measure on $\mathbb{R}P^2$, that is by a probability measure $\mu = \mu_x$ on the unit sphere S^2 satisfying $\mu(E) = \mu(-E)$ for $E \subset S^2$.

Example:
$\mu = \frac{1}{2}(\delta_e + \delta_{-e})$ represents a state of perfect alignment parallel to the unit vector e.

For a continuously distributed measure $d\mu(p) = \rho(p)dp$, where dp is the element of surface area on S^2 and $\rho \geq 0, \int_{S^2} \rho(p)dp = 1$, $\rho(p) = \rho(-p)$.

If the orientation of molecules is equally distributed in all directions, we say that the distribution is *isotropic*, and then $\mu = \mu_0$, where

$$d\mu_0(p) = \frac{1}{4\pi} dp,$$

for which $\rho(p) = \frac{1}{4\pi}$.

A natural idea would be to use as an order parameter the probability measure $\mu = \mu_x$. However this represents an infinite-dimensional state variable at each point x, and if we use as an approximation an order parameter consisting of a finite number of moments of μ then we have instead a finite-dimensional state variable.

Because $\mu(E) = \mu(-E)$ the first moment

$$\int_{S^2} p \, d\mu(p) = 0.$$

The second moment

$$M = \int_{S^2} p \otimes p \, d\mu(p)$$

is a symmetric non-negative 3×3 matrix satisfying $\mathrm{tr} M = 1$.

The second moment tensor of the isotropic distribution μ_0, $d\mu_0 = \frac{1}{4\pi} dp$, is

$$M_0 = \frac{1}{4\pi} \int_{S^2} p \otimes p \, dS = \frac{1}{3} \mathbf{1}$$

(since $\int_{S^2} p_1 p_2 \, dS = 0$, $\int_{S^2} p_1^2 \, dS = \int_{S^2} p_2^2 \, dS$ etc and $\operatorname{tr} M_0 = 1$.)

The *de Gennes Q-tensor*

$$Q = M - M_0 = \int_{S^2} \left(p \otimes p - \frac{1}{3} \mathbf{1} \right) d\mu(p)$$

thus measures the deviation of M from its isotropic value.

Note that $Q = Q^T$, $\operatorname{tr} Q = 0$, $Q \geq -\frac{1}{3} \mathbf{1}$.

Since Q is symmetric and $\operatorname{tr} Q = 0$,

$$Q = \lambda_1 n_1 \otimes n_1 + \lambda_2 n_2 \otimes n_2 + \lambda_3 n_3 \otimes n_3,$$

where $\{n_i\}$ is an orthonormal basis of eigenvectors of Q with corresponding eigenvalues $\lambda_i = \lambda_i(Q)$ satisfying $\lambda_1 + \lambda_2 + \lambda_3 = 0$.

Since $Q \geq -\frac{1}{3}\mathbf{1}$, each $\lambda_i \geq -\frac{1}{3}$ and hence $-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}$.

Conversely, if each $\lambda_i \geq -\frac{1}{3}$ then M is the second moment tensor for some μ, e.g. for

$$\mu = \sum_{i=1}^{3} (\lambda_i + \frac{1}{3}) \frac{1}{2} (\delta_{n_i} + \delta_{-n_i}).$$

If $\lambda_{\max}(Q) = \frac{2}{3}$ then for the corresponding eigenvector $e_{\max}$ we have

$$Me_{\max} \cdot e_{\max} = \int_{S^2} (p \cdot e_{\max})^2 dp = 1,$$

and hence

$$\int_{S^2} |p \otimes p - e_{\max} \otimes e_{\max}|^2 d\mu = 0,$$

and so $\mu = \frac{1}{2}(\delta_{e_{\max}} + \delta_{-e_{\max}})$.

If $\lambda_{\min}(Q) = -\frac{1}{3}$ then for the corresponding eigenvector $e_{\min}$ we have $Qe_{\min} \cdot e_{\min} = -\frac{1}{3}$, and hence

$$\int_{S^2} (p \cdot e_{\min})^2 d\mu(p) = 0,$$

and so μ is supported on the great circle of S^2 perpendicular to $e_{\min}$.

Remark. $Q = 0$ does not imply $\mu = \mu_0$.
For example we can take

$$\mu = \frac{1}{6} \sum_{i=1}^{3} (\delta_{e_i} + \delta_{-e_i}).$$

If two eigenvalues of Q are equal then Q is said to be *uniaxial* and has the form

$$Q = s\left(n \otimes n - \frac{1}{3}\mathbf{1}\right),$$

where $n \in S^2$ and the *scalar order parameter* $s \in [-\frac{1}{2}, 1]$. Otherwise Q is *biaxial*.

In fact it is extremely difficult to find Q that are not very close to uniaxial with a constant value of s (typically 0.6-0.7). We will see why this is to be expected later.

Note that

$$\begin{aligned} Qn \cdot n &= \frac{2s}{3} \\ &= \langle (p \cdot n)^2 - \frac{1}{3} \rangle \\ &= \langle \cos^2 \theta - \frac{1}{3} \rangle, \end{aligned}$$

where θ is the angle between p and n. Hence

$$s = \frac{3}{2} \langle \cos^2 \theta - \frac{1}{3} \rangle.$$

If Q is uniaxial and $s > 0$ then $\lambda_{\max}(Q) = \frac{2}{3}s$ and $n = n_{\max}(Q)$, the corresponding eigenvector of Q. For general biaxial Q the director is often identified with $n_{\max}(Q)$.

If $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$ is uniaxial then

$$|Q|^2 = \frac{2s^2}{3}, \det Q = \frac{2s^3}{27}.$$

Proposition.
Given $Q = Q^T$, $\operatorname{tr} Q = 0$, Q *is uniaxial iff*

$$|Q|^6 = 54(\det Q)^2.$$

Proof. The characteristic equation of Q is

$$\det(Q - \lambda 1) = \det Q - \lambda \operatorname{tr} \operatorname{cof} Q + 0\lambda^2 - \lambda^3.$$

But $2\operatorname{tr} \operatorname{cof} Q = 2(\lambda_2\lambda_3 + \lambda_3\lambda_1 + \lambda_1\lambda_2) = (\lambda_1 + \lambda_2 + \lambda_3)^2 - (\lambda_1^2 + \lambda_2^2 + \lambda_3^2) = -|Q|^2$. Hence the characteristic equation is

$$\lambda^3 - \frac{1}{2}|Q|^2\lambda - \det Q = 0,$$

and the condition that $\lambda^3 - p\lambda + q = 0$ has two equal roots is that $p \geq 0$ and $4p^3 = 27q^2$.

Thus for nematic liquid crystals we have various choices for the order parameter:

the probability density function ρ (∞-dimensional, Onsager-type theories)

Q (5-dimensional, Landau - de Gennes theory)

(s, n) (3-dimensional, Ericksen theory)

n (2-dimensional, Oseen-Frank theory)

The Landau – de Gennes and Oseen – Frank theories

Landau – de Gennes theory

For simplicity we work at a constant temperature θ. Let Ω be a bounded domain in $\mathbb{R}^3$. At each point $x \in \Omega$, we have a corresponding order parameter tensor $Q(x)$. We suppose that the material is described by a free-energy density $\psi(Q, \nabla Q, \theta)$, so that the total free energy is given by

$$I_\theta(Q) = \int_\Omega \psi(Q(x), \nabla Q(x), \theta)\, dx.$$

We write $\psi = \psi(Q, D, \theta)$, where D is a third order tensor.

Frame-indifference

We consider two observers, one using the Cartesian coordinates $x = (x_1, x_2, x_3)$ and the second using translated and rotated coordinates $z = \bar{x} + R(x - \bar{x})$, where $R \in SO(3)$, and we require that

$$\psi(Q^*(\bar{x}), \nabla_z Q^*(\bar{x}), \theta) = \psi(Q(\bar{x}), \nabla_x Q(\bar{x}), \theta),$$

where $Q^*(\bar{x})$ is the value of Q measured by the second observer.

Then

$$\begin{aligned} Q^*(\bar{x}) &= \int_{S^2}(q \otimes q - \frac{1}{3}\mathbf{1})d\mu_{\bar{x}}(R^T q) \\ &= \int_{S^2}(Rp \otimes Rp - \frac{1}{3}\mathbf{1})d\mu_{\bar{x}}(p) \\ &= R\int_{S^2}(p \otimes p - \frac{1}{3}\mathbf{1})d\mu_{\bar{x}}(p)R^T. \end{aligned}$$

Hence $Q^*(\bar{x}) = RQ(\bar{x})R^T$.

Therefore

$$\begin{aligned}\frac{\partial Q^*_{ij}}{\partial z_k}(\bar{x}) &= \frac{\partial}{\partial z_k}(R_{il}Q_{lm}(\bar{x})R_{jm}) \\ &= \frac{\partial}{\partial x_p}(R_{il}Q_{lm}R_{jm})\frac{\partial x_p}{\partial z_k} \\ &= R_{il}R_{jm}R_{kp}\frac{\partial Q_{lm}}{\partial x_p}.\end{aligned}$$

Thus, for every $R \in SO(3)$,

$$\psi(Q^*, D^*, \theta) = \psi(Q, D, \theta),$$

where $Q^* = RQR^T$, $D^*_{ijk} = R_{il}R_{jm}R_{kp}D_{lmp}$.
Such ψ are called *hemitropic*.

Material symmetry

The requirement that

$$\psi(Q^*(\bar{x}), \nabla_z Q^*(\bar{x}), \theta) = \psi(Q(\bar{x}), \nabla_x Q(\bar{x}), \theta)$$

when $z = \bar{x} + \hat{R}(x - \bar{x})$, where $\hat{R} = \mathbf{1} - 2e \otimes e$, $|e| = 1$, is a *reflection* is a condition of material symmetry satisfied by nematics, but not cholesterics, whose molecules have a chiral nature.

Since any $R \in O(3)$ can be written as $\hat{R}\tilde{R}$, where $\tilde{R} \in SO(3)$ and $\hat{R}$ is a reflection, for a nematic

$$\psi(Q^*, D^*, \theta) = \psi(Q, D, \theta)$$

where $Q^* = RQR^T$, $D^*_{ijk} = R_{il}R_{jm}R_{kp}D_{lmp}$ and $R \in O(3)$. Such ψ are called *isotropic*.

Bulk and elastic energies

We can decompose ψ as

$$\begin{aligned}\psi(Q,\nabla Q,\theta) &= \psi(Q,0,\theta)+(\psi(Q,\nabla Q,\theta)-\psi(Q,0,\theta))\\ &= \psi_B(Q,\theta)+\psi_E(Q,\nabla Q,\theta)\\ &= \text{ bulk } + \text{ elastic},\end{aligned}$$

so that $\psi_B(Q,\theta)=\psi(Q,0,\theta)$.

By frame-indifference we have that

$$\psi_B(RQR^T,\theta)=\psi_B(Q,\theta) \text{ for all } R\in SO(3).$$

Hence $\psi_B(Q,\theta)$ depends only on the invariants of Q, and one of these, $\operatorname{tr} Q$, is zero. Hence $\psi_B(Q,\theta)=\widehat{\psi}_B(|Q|^2,\det Q,\theta)$ for some function $\widehat{\psi}_B$.

The domain of ψ

For what Q, D should $\psi(Q, D, \theta)$ be defined?
Let $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$
$\mathcal{D} = \{D = (D_{ijk}) : D_{ijk} = D_{jik}, D_{kki} = 0\}$.
We suppose that $\psi(\cdot, \theta) : \operatorname{dom} \psi \to \mathbb{R}$, where

$$\operatorname{dom} \psi = \{(Q, D) \in \mathcal{E} \times \mathcal{D}, \lambda_i(Q) > -\frac{1}{3}\}.$$

But in order to differentiate ψ easily with respect to its arguments, it is convenient to extend $\psi(\cdot, \theta)$ to all of $M^{3\times 3}\times$(3rd order tensors). To do this first set $\psi(Q, D, \theta) = \infty$ if $(Q, D) \in \mathcal{E} \times \mathcal{D}$ with some $\lambda_i(Q) \leq -\frac{1}{3}$.

Then note that

$$PA = \frac{1}{2}(A + A^T) - \frac{1}{3}(\mathrm{tr}\, A)\mathbf{1}$$

is the orthogonal projection of $M^{3\times 3}$ onto $\mathcal{E}$. So for any Q, D we can set

$$\psi(Q, D, \theta) = \psi(PQ, PD, \theta),$$

where $(PD)_{ijk} = \frac{1}{2}(D_{ijk} + D_{jik}) - \frac{1}{3}D_{llk}\delta_{ij}$.

Thus we can assume that ψ satisfies

$$\frac{\partial \psi}{\partial Q_{ij}} = \frac{\partial \psi}{\partial Q_{ji}}, \ \frac{\partial \psi}{\partial Q_{ii}} = 0,$$

$$\frac{\partial \psi}{\partial D_{ijk}} = \frac{\partial \psi}{\partial D_{jik}}, \ \frac{\partial \psi}{\partial D_{iik}} = 0.$$

Q-tensor description of the isotropic to nematic phase transformation

Following de Gennes, Schophol & Sluckin PRL 59(1987), Mottram & Newton, *Introduction to Q-tensor theory* arXiv:1409.3542, we consider the special quartic bulk energy

$$\psi_B(Q,\theta) = a(\theta)\mathrm{tr}\,Q^2 - \frac{2b}{3}\mathrm{tr}\,Q^3 + \frac{c}{2}\mathrm{tr}\,Q^4,$$

where $b > 0, c > 0, a = \alpha(\theta - \theta^*), \alpha > 0$.

Then

$$\psi_B = a\sum_{i=1}^{3}\lambda_i^2 - \frac{2b}{3}\sum_{i=1}^{3}\lambda_i^3 + \frac{c}{2}\sum_{i=1}^{3}\lambda_i^4.$$

ψ_B attains a minimum subject to $\sum_{i=1}^{3}\lambda_i = 0$. A calculation shows that the critical points have two λ_i equal, so that $\lambda_1 = \lambda_2 = \lambda, \lambda_3 = -2\lambda$ say, and that

$$\lambda(a + b\lambda + 3c\lambda^2) = 0.$$

Hence $\lambda = 0$ or $\lambda = \lambda_\pm$, and

$$\lambda_\pm = \frac{-b \pm \sqrt{b^2 - 12ac}}{6c}.$$

For such a critical point we have that

$$\psi_B = 4a\lambda^2 + 4b\lambda^3 + 9c\lambda^4,$$

which is negative when

$$4a + 4b\lambda + 9c\lambda^2 = a + b\lambda < 0.$$

A short calculation then shows that $a + b\lambda_- < 0$ if and only if $a < \frac{2b^2}{27c}$.

Hence we find that there is a phase transformation from an isotropic fluid to a uniaxial nematic phase at the critical temperature $\theta_{\mathrm{NI}} = \theta^* + \frac{2b^2}{27\alpha c}$. If $\theta > \theta_{\mathrm{NI}}$ then the unique minimizer of ψ_B is $Q = 0$.

If $\theta < \theta_{\mathrm{NI}}$ then the minimizers are

$$Q = s_{\mathrm{min}}(n \otimes n - \frac{1}{3}\mathbf{1}) \text{ for } n \in S^2,$$

where $s_{\mathrm{min}} = \frac{b+\sqrt{b^2-12ac}}{2c} > 0$.

Form of the elastic energy.

Usually it is assumed that $\psi_E(Q, \nabla Q, \theta)$ is quadratic in ∇Q. Examples of isotropic functions quadratic in ∇Q are:

$$I_1 = Q_{ij,j}Q_{ik,k}, \quad I_2 = Q_{ik,j}Q_{ij,k}$$
$$I_3 = Q_{ij,k}Q_{ij,k}, \quad I_4 = Q_{lk}Q_{ij,l}Q_{ij,k}$$

Note that

$I_1 - I_2 = (Q_{ij}Q_{ik,k})_{,j} - (Q_{ij}Q_{ik,j})_{,k}$

is a null Lagrangian.

An example of a hemitropic, but not isotropic, function is

$$I_5 = \varepsilon_{ijk}Q_{il}Q_{jl,k}.$$

For the elastic energy we take

$$\psi_E(Q, \nabla Q, \theta) = \sum_{i=1}^{4 \text{ or } 5} L_i I_i,$$

where the $L_i = L_i(\theta)$ are material constants, with $L_5 = 0$ for nematics.

To summarize, we assume that for nematics and cholesterics

$$\psi(Q, \nabla Q, \theta) = \psi_B(Q, \theta) + \sum_{i=1}^{4 \text{ or } 5} L_i I_i,$$

where $\psi_B(Q, \theta) = \widehat{\psi}_B(|Q|^2, \det Q, \theta)$, and $L_i = L_i(\theta)$, with $L_5 = 0$ for nematics.

The constrained theory

For small L_i it is reasonable to consider a constrained theory in which we require Q to be uniaxial with a constant scalar order parameter $s = s(\theta) > 0$, so that

$$Q = s\left(n \otimes n - \frac{1}{3}\mathbf{1}\right), \quad n \in S^2.$$

(For recent rigorous work studying whether and when this is justified see Majumdar & Zarnescu, Nguyen & Zarnescu, Bauman, Phillips & Park.)

Then the bulk energy just depends on θ, so we only have to consider the elastic energy

$$I_\theta(Q) = \int_\Omega \psi_E(Q, \nabla Q, \theta)\, dx.$$

Oseen-Frank energy

Formally calculating ψ_E in terms of $n, \nabla n$ we obtain the Oseen-Frank energy functional

$$I_\theta(n) = \int_\Omega [K_1(\operatorname{div} n)^2 + K_2(n \cdot \operatorname{curl} n + q_0)^2 + K_3|n \times \operatorname{curl} n|^2 + (K_2 + K_4)(\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2)]\, dx,$$

where

$K_1 = L_1 s^2 + L_2 s^2 + 2L_3 s^2 - \frac{2}{3} L_4 s^3,$

$K_2 = 2L_3 s^2 - \frac{2}{3} L_4 s^3,$

$K_3 = L_1 s^2 + L_2 s^2 + 2L_3 s^2 + \frac{4}{3} L_4 s^3,$

$K_4 = L_2 s^2$, $q_0 = -\frac{L_5 s^2}{2K_2}$ and

$q_0 = 0$ for nematics, $q_0 \neq 0$ for cholesterics.

Boundary conditions

(a) Constrained LdG/Oseen-Frank theory.

(i) Strong anchoring

$$n(x) = \pm\bar{n}(x),\ x \in \partial\Omega.$$

Special cases:

1. (*Homeotropic*) $\bar{n}(x) = \nu(x)$,

$\nu(x) =$ unit outward normal

2. (*Planar*) $\bar{n}(x) \cdot \nu(x) = 0$.

(ii) Conical anchoring:

$$|n(x) \cdot \nu(x)| = \alpha(x) \in [0, 1],\ x \in \partial\Omega,$$

where $\nu(x)$ is the unit outward normal.

Special cases:

1. $\alpha(x) = 1$ homeotropic .

2. $\alpha(x) = 0$ *planar degenerate* (or *tangent*), director parallel to boundary but preferred direction not prescribed.

(iii) No anchoring: no condition on n on $\partial\Omega$. This is natural mathematically but seems difficult to realize in practice.

(iv) Weak anchoring. No boundary condition is explicitly imposed, but a surface energy term is added, of the form

$$\int_{\partial\Omega} w(x,n)\,dS$$

where $w(x,n) = w(x,-n)$.

For example, corresponding to strong anchoring we can choose

$$w(x,n) = -K(n(x)\cdot\bar{n}(x))^2,$$

formally recovering the strong anchoring condition in the limit $K \to \infty$.

(b) Landau - de Gennes

(i) Strong anchoring:

$$Q(x) = \bar{Q}(x),\ x \in \partial\Omega.$$

(ii) Weak anchoring: add surface energy term

$$\int_{\partial\Omega} w(x, Q)\, dS.$$

But is the derivation of the Oseen-Frank theory from Landau - de Gennes correct? The constrained Landau - de Gennes theory is invariant to changing n to $-n$, but is Oseen-Frank?

The issue here is whether a line field can be oriented, i.e. turned into a vector field by assigning an orientation at each point. If we don't care about the regularity of the vector field this can always be done by choosing an arbitrary orientation at each point.

For s a nonzero constant and $n \in S^2$ let

$$\Pi(n) = s\left(n \otimes n - \frac{1}{3}\mathbf{1}\right),$$

and set

$$\mathcal{Q} = \left\{Q \in M^{3\times 3} : Q = \Pi(n) \text{ for some } n \in S^2\right\}.$$

Thus $\Pi : S^2 \to \mathcal{Q}$. The operator Π provides us with a way of 'unorienting' an S^2-valued vector field.

Given $Q \in W^{1,p}(\Omega, \mathcal{Q})$ we say Q is *orientable* if we can write

$$Q(x) = \Pi(n(x)),$$

where $n \in W^{1,p}(\Omega, S^2)$. In topological language this means that Q has a *lifting* to $W^{1,p}(\Omega, S^2)$.

Relating the Q and n descriptions

Proposition

Let $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$, s a nonzero constant, $|n| = 1$ a.e., belong to $W^{1,p}(\Omega; \mathbb{R}P^2)$ for some p, $1 \leq p < \infty$. If n is continuous along almost every line parallel to the coordinate axes, then $n \in W^{1,p}(\Omega, S^2)$ (in particular n is orientable), and

$$n_{i,k} = Q_{ij,k} n_j.$$

Theorem. *An orientable Q has exactly two orientations.*

Proof

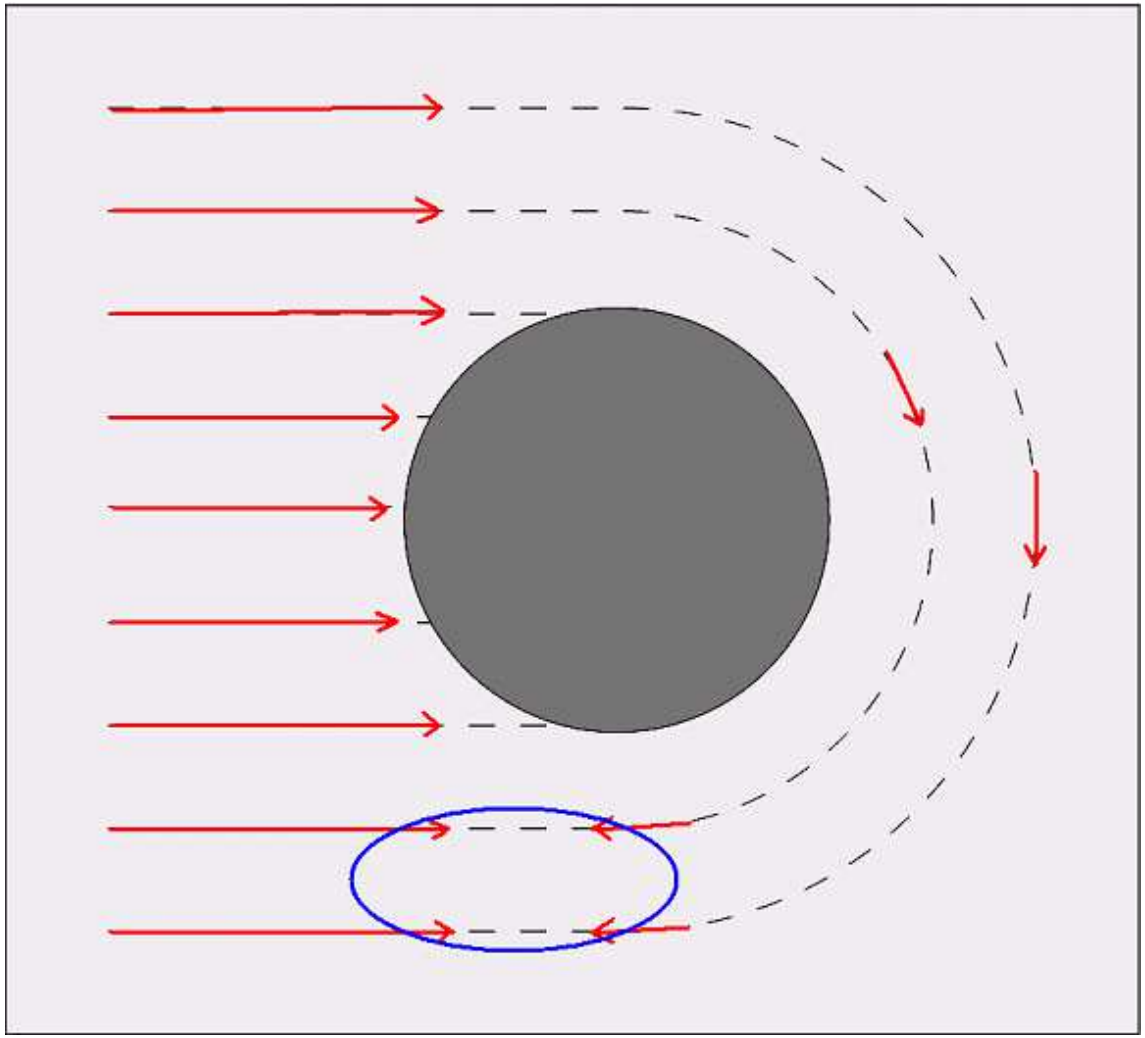
Suppose that n and τn both generate Q and belong to $W^{1,1}(\Omega, S^2)$, where $\tau^2(x) = 1$ a.e.. Let $C \subset \Omega$ be a cube with sides parallel to the coordinate axes. Let x_2, x_3 be such that the line $x_1 \mapsto (x_1, x_2, x_3)$ intersects C. Let $L(x_2, x_3)$ denote the intersection. For a.e. such x_2, x_3 we have that $n(x)$ and $\tau(x)n(x)$ are absolutely continuous in x_1 on $L(x_2, x_3)$. Hence $n(x) \cdot \tau(x)n(x) = \tau(x)$ is continuous in x_1, so that $\tau(x)$ is constant on $L(x_2, x_3)$.

Let $\varphi \in C_0^\infty(C)$. Then by Fubini's theorem

$$\int_C \tau\varphi_{,1} dx = \int_C (\tau\varphi)_{,1} dx = 0,$$

so that the weak derivative $\tau_{,1}$ exists in C and is zero. Similarly the weak derivatives $\tau_{,2}, \tau_{,3}$ exist in C and are zero. Thus $\nabla\tau = 0$ in C and hence τ is constant in C. Since Ω is connected, τ is constant in Ω, and thus $\tau \equiv 1$ or $\tau \equiv -1$ in Ω.

A smooth nonorientable line field in a non simply connected region.



Theorem (JB/Zarnescu 2011) *If Ω is simply-connected and $Q \in W^{1,p}$, $p \geq 2$, then Q is orientable.*

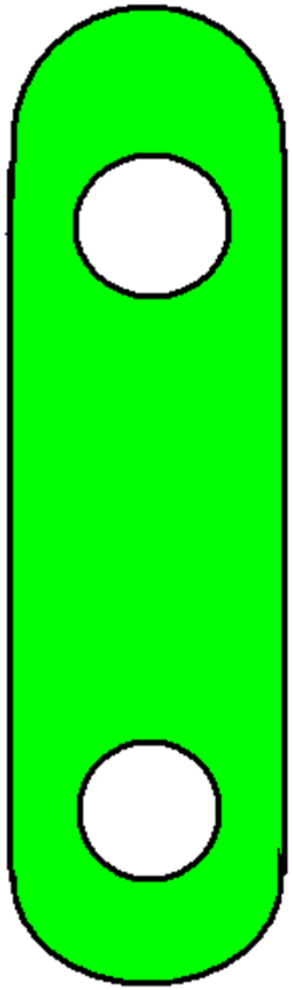
(There is a related topologically more general lifting result of Bethuel and Chiron 2007.)

Thus in a simply-connected region the uniaxial de Gennes and Oseen-Frank theories are equivalent.

Ingredients of proof

- Lifting possible if Q is smooth and Ω is simply connected
- Pakzad-Rivière theorem (2003) implies that if $\partial\Omega$ is smooth, then there is a sequence of smooth $Q^{(j)} : \Omega \to \mathbb{R}P^2$ converging weakly to Q in $W^{1,2}$.
- We can approximate a simply-connected domain with boundary of class C^0 by ones that are simply-connected with smooth boundary. (This can be avoided using an argument of Bedford (2015))
- Orientability is preserved under weak convergence

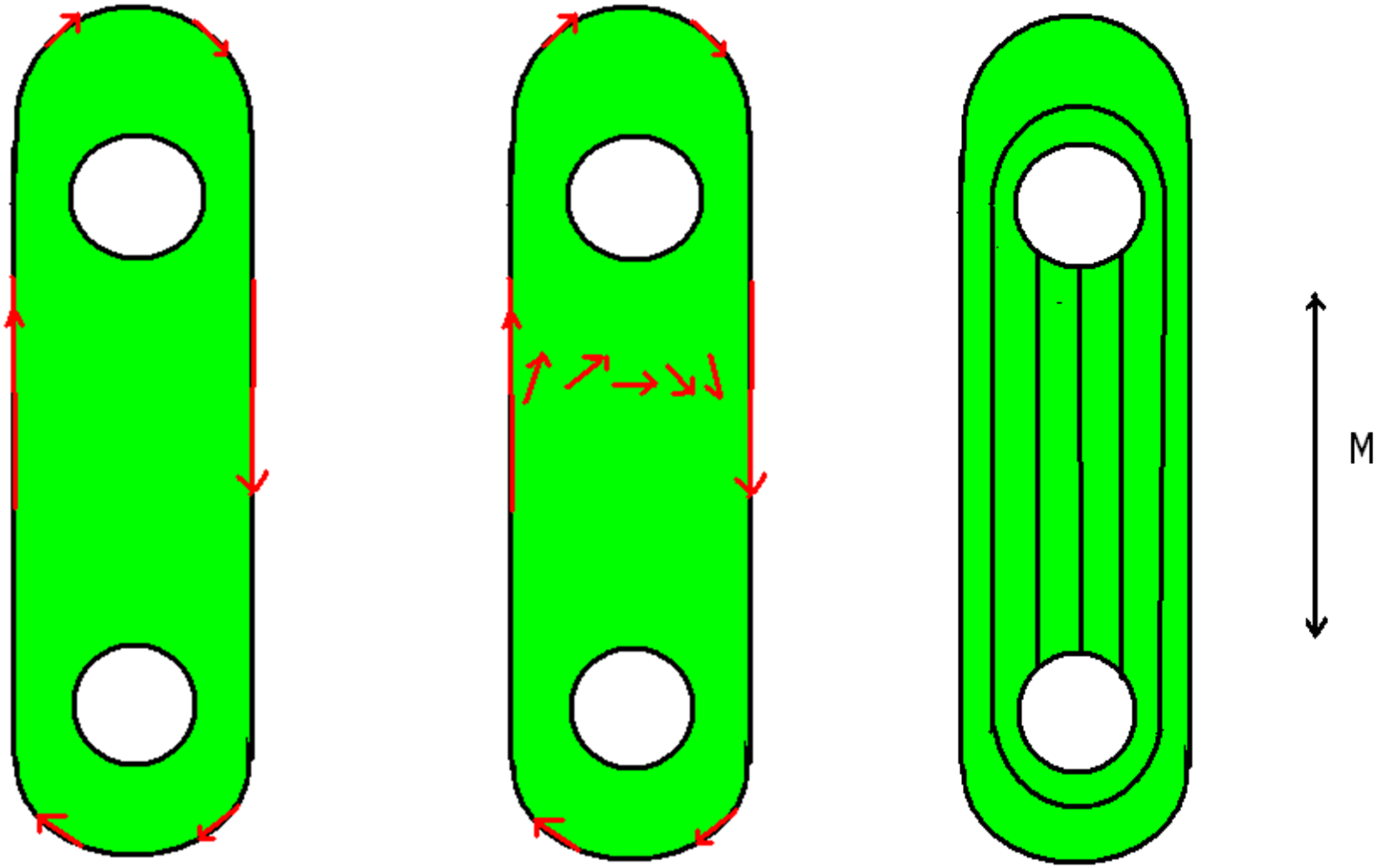
Non-equivalence of Oseen-Frank and constrained LdG in non simply-connected 2D domain

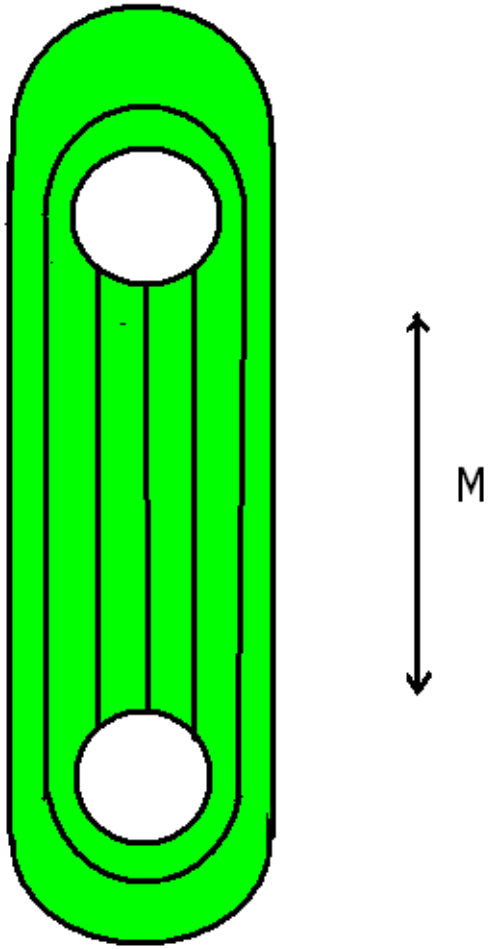


Tangent boundary conditions on outer boundary. No (free) boundary conditions on inner circles.

$$I(Q) = \int_\Omega |\nabla Q|^2 dx$$

$$I(n) = 2s^2 \int_\Omega |\nabla n|^2 dx$$


M



For M large enough the minimum energy configuration is unoriented, even though there is a minimizer among oriented maps. (In fact this is true whatever M is.)

If the boundary conditions correspond to the Q-field shown, then there is no orientable Q that satisfies them.

Existence in Landau – de Gennes theory

Let $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$.

Theorem (Davis & Gartland 1998)
Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with smooth boundary $\partial\Omega$. Let $\psi_B(\cdot,\theta)$ be continuous and bounded below, $L_4 = L_5 = 0$ and

$$L_3 > 0, -L_3 < L_2 < 2L_3, -\frac{3}{5}L_3 - \frac{1}{10}L_2 < L_1.$$

Let $\bar{Q} : \partial\Omega \to \mathcal{E}$ be smooth. Then

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + \sum_{i=1}^{3} L_i I_i(\nabla Q)]\, dx$$

attains a minimum on

$$\mathcal{A} = \{Q \in W^{1,2}(\Omega;\mathcal{E}) : Q|_{\partial\Omega} = \bar{Q}\}.$$

Proof

By the direct method of the calculus of variations. Let $Q^{(j)}$ be a minimizing sequence in $\mathcal{A}$. the inequalities on the L_i imply that

$$\sum_{i=1}^{3} L_i I_i(\nabla Q) \geq \mu |\nabla Q|^2$$

for all Q (in particular $\sum_{i=1}^{3} I_i(\nabla Q)$ is convex in ∇Q). By the Poincaré inequality we have that

$$Q^{(j)} \text{ is bounded in } W^{1,2}$$

so that for a subsequence (not relabelled)

$$Q^{(j)} \rightharpoonup Q^* \text{ in } W^{1,2}$$

for some $Q^* \in \mathcal{A}$.

We may also assume, by the compactness of the embedding of $W^{1,2}$ in L^2, that $Q^{(j)} \to Q$ a.e. in Ω. But

$$I(Q^*) \leq \liminf_{j \to \infty} I(Q^{(j)})$$

by Fatou's lemma and the convexity in ∇Q. Hence Q^* is a minimizer.

In the quartic case we can use elliptic regularity (Davis & Gartland) to show that any minimizer Q^* is smooth.

But what if $L_4 \neq 0$?

Proposition (JB/Majumdar) *For any boundary conditions, if* $L_4 \neq 0$ *then*

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + \sum_{i=1}^{4} L_i I_i]\, dx$$

is unbounded below.

Proof. Choose any Q satisfying the boundary conditions, and multiply it by a smooth function $\varphi(x)$ which equals one in a neighbourhood of $\partial\Omega$ and is zero in some ball $B \subset \Omega$, which we can take to be $B(0,1)$. We will alter Q in B so that

$$J(Q) = \int_B [\psi_B(Q,\theta) + \sum_{i=1}^{4} L_i I_i]\, dx$$

is unbounded below subject to $Q|_{\partial B} = 0$.

Choose

$$Q(x) = h(r)\left[\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathbf{1}\right],\ h(1) = 0,$$

where $r = |x|$. Then

$$|\nabla Q|^2 = \frac{2}{3}h'^2 + \frac{4}{r^2}h^2,$$

and

$$I_4 = Q_{kl}Q_{ij,k}Q_{ij,l} = \frac{4}{9}h(h'^2 - \frac{3}{r^2}h^2).$$

Hence

$$J(Q) \leq 4\pi \int_0^1 r^2 \left[\psi_B(Q) + C \left(\frac{2}{3} h'^2 + \frac{4}{r^2} h^2 \right) + L_4 \frac{4}{9} h \left(h'^2 - \frac{3}{r^2} h^2 \right) \right] dr,$$

where C is a constant.

Provided h is bounded, all the terms are bounded except

$$4\pi \int_0^1 r^2 \left(\frac{2}{3} C + \frac{4}{9} L_4 h \right) h'^2 \, dr.$$

Choose

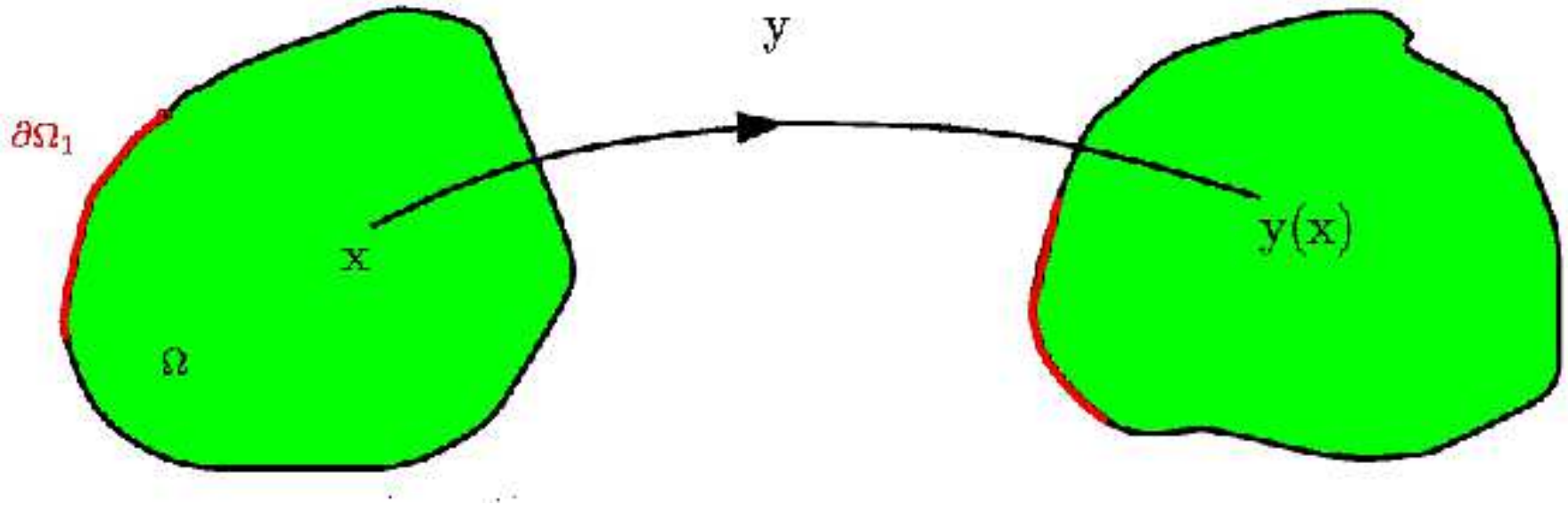
$$h(r) = \begin{cases} h_0(2 + \sin kr) & 0 < r < \frac{1}{2} \\ 2h_0(2 + \sin \frac{k}{2})(1 - r) & \frac{1}{2} < r < 1 \end{cases}$$

The integrand is then bounded on $(\frac{1}{2}, 1)$ and we need to look at

$$4\pi \int_0^{\frac{1}{2}} r^2 \left(\frac{2}{3} C + \frac{4}{9} L_4 h_0 (2 + \sin kr) \right) h_0^2 k^2 \cos^2 kr \, dr,$$

which tends to $-\infty$ if $L_4 h_0$ is sufficiently negative.

Analogy with nonlinear elasticity



Minimize

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

subject to suitable boundary conditions,

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

To prevent interpenetration of matter we required that y is invertible, and in particular that

$$\det Dy(x) > 0 \text{ a.e. } x \in \Omega.$$

To help ensure this we assumed that

$$W(A) \to \infty \text{ as } \det A \to 0+$$

Correspondingly, it is natural to suppose that

$$\psi_B(Q,\theta) \to \infty \text{ as } \lambda_{\min}(Q) \to -\frac{1}{3}+ .$$

Such a suggestion was made by Ericksen in the context of his model of nematic liquid crystals.

We show how such an ψ_B can be constructed on the basis of a microscopic model, the interpretation being that perfectly aligned states have entropy $-\infty$.

This will also allow us to get existence of a minimizer when $L_4 \neq 0$.

3. Onsager theory.

In the Onsager model the probability measure μ is assumed to be continuous with density $\rho = \rho(p)$, and the bulk free-energy at temperature $\theta > 0$ has the form

$$I_\theta(\rho) = U(\rho) - \theta\eta(\rho),$$

where the entropy is given by

$$\eta(\rho) = -k_B \int_{S^2} \rho(p) \ln \rho(p)\, dp,$$

where k_B is Boltzmann's constant.

We suppose that U is given by

$$U(\rho) = \int_{S^2} \int_{S^2} K(p,q)\rho(p)\rho(q)\,dp\,dq.$$

We assume that K is frame-indifferent, so that

$$K(Rp, Rq) = K(p,q) \text{ for all } R \in SO(3),$$

which holds iff

$$K(p,q) = k(p \cdot q)$$

for some $k : [-1,1] \to \mathbb{R}$.

Two important examples of the potential k are:

(i) $k(p \cdot q) = \kappa(\frac{1}{3} - (p \cdot q)^2)$ (Maier-Saupe)

(ii) $k(p \cdot q) = \kappa\sqrt{1 - (p \cdot q)^2}$ (Onsager),

where $\kappa > 0$ is a coupling constant.

We will assume that κ is independent of θ. If κ depends on θ (due to steric effects) then the analysis is similar.

Denoting by

$$Q(\rho) = \int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1})\rho(p)\, dp$$

the corresponding Q-tensor, we have that

$$\begin{aligned} |Q(\rho)|^2 &= \int_{S^2}\int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1}) \cdot (q \otimes q - \frac{1}{3}\mathbf{1})\rho(p)\rho(q) dp\, dq \\ &= \int_{S^2}\int_{S^2} [(p \cdot q)^2 - \frac{1}{3}]\rho(p)\rho(q)\, dp\, dq. \end{aligned}$$

Hence for the Maier-Saupe potential $U(\rho) = -\kappa|Q(\rho)|^2$ and

$$I_\theta(\rho) = k_B\theta \int_{S^2} \rho(p) \ln \rho(p)\, dp - \kappa|Q(\rho)|^2.$$

Theorem (Fatkullin & Slastikov 2005, Liu, Zhang & Zhang 2005)
For the Maier-Saupe potential all critical points of ρ can be explicitly determined and are uniaxial. The isotropic state $\bar{\rho} = \frac{1}{4\pi}$ is a critical point for all θ. At the largest bifurcation point θ_c there is a transcritical bifurcation, so that $\bar{\rho}$ is stable for $\theta > \theta_c$, and unstable for $\theta < \theta_c$.

Using equivariant bifurcation theory and an analysis involving spherical harmonics, Michaela Vollmer (2015) has established a similar bifurcation picture for a class of potentials k including the Onsager potential.

For the Maier-Saupe potential, given Q we define (here and below we follow JB/Majumdar 2012)

$$\begin{aligned}\psi_B(Q,\theta) &= \inf_{\{\rho:Q(\rho)=Q\}} U(\rho) - \theta\eta(\rho) \\ &= k_B\theta \inf_{\{\rho:Q(\rho)=Q\}} \int_{S^2} \rho \ln \rho \, dp - \kappa|Q|^2.\end{aligned}$$

(cf. Katriel, J., Kventsel, G. F., Luckhurst, G. R. and Sluckin, T. J.(1986))

Thus we just need to understand how to minimize

$$I(\rho) = \int_{S^2} \rho(p) \ln \rho(p) \, dp$$

subject to $Q(\rho) = Q$.

Given Q with $Q = Q^T, \operatorname{tr} Q = 0$ and satisfying $\lambda_i(Q) > -1/3$ we seek to minimize $I(\rho) = \int_{S^2} \rho(p) \ln \rho(p)\, dp$ on

$$\mathcal{A}_Q = \{\rho \in L^1(S^2) : \rho \geq 0, Q(\rho) = Q\}.$$

Remarks: Note that for $\rho \in \mathcal{A}_Q$ the constraint

$$\int_{S^2} \rho(p)\, dp = 1$$

follows from $\operatorname{tr} Q(\rho) = 0$. Also we do not impose the condition $\rho(p) = \rho(-p)$, since it turns out that the minimizer in $\mathcal{A}_Q$ satisfies this condition automatically.

Lemma. $\mathcal{A}_Q$ is nonempty.

Sketch of proof. We can suppose that $Q = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$. The singular measure

$$\mu(p) = \frac{1}{2} \sum_{i=1}^{3} \left(\lambda_i + \frac{1}{3} \right) (\delta_{e_i} + \delta_{-e_i})$$

satisfies $\int_{S^2} \left(p \otimes p - \frac{1}{3}\mathbf{1} \right) d\mu(p) = Q$ and can be approximated by an L^1 function ρ satisfying $Q(\rho) = Q$.

Theorem. I attains a minimum at a unique $\rho_Q \in \mathcal{A}_Q$.

Proof. Let $\rho^{(j)}$ be a minimizing sequence for I in $\mathcal{A}_Q$. By the de la Vallée Poussin criterion and the superlinear growth of $\rho \ln \rho$, we may assume that $\rho^{(j)} \rightharpoonup \rho_Q$ in $L^1(S^2)$ for some ρ_Q, and $\rho_Q \geq 0$, $Q(\rho_Q) = Q$.

Since $\rho \ln \rho$ is convex,
$I(\rho_Q) \leq \liminf_{j\to\infty} I(\rho^{(j)})$,
so that ρ_Q is a minimizer, which is unique since $\rho \ln \rho$ is strictly convex.

The Euler-Lagrange equation for I

Theorem. Let $Q = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$. Then

$$\rho_Q(p) = \frac{\exp(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2)}{Z(\mu_1, \mu_2, \mu_3)},$$

where

$$Z(\mu_1, \mu_2, \mu_3) = \int_{S^2} \exp(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2)\, dp.$$

The μ_i (unique up to adding a constant to each) solve the equations

$$\frac{\partial \ln Z}{\partial \mu_i} = \lambda_i + \frac{1}{3}, \quad i = 1, 2, 3.$$

To show that ρ_Q satisfies the corresponding Euler-Lagrange equation, the μ_i appearing as Lagrange multipliers, is a bit tricky because of the possibility that ρ_Q is not bounded away from zero. A quicker proof is to use a 'dual' variational principle for $\mu = (\mu_1, \mu_2, \mu_3)$ (cf Mead & Papanicolaou 1984), from which the existence of a minimizer ρ_Q also follows.

Write $\gamma_i = \lambda_i + \frac{1}{3}$, so that $\gamma_i > 0, \sum_{j=1}^{3} \gamma_j = 1$, and $\gamma = (\gamma_1, \gamma_2, \gamma_3)$. For $\nu \in \mathbb{R}^3$ let

$$J(\nu) = \gamma \cdot \nu - \ln Z(\nu).$$

Note that if $m = (1, 1, 1)$ then for any $\tau \in \mathbb{R}$

$$\begin{aligned} J(\nu + \tau m) &= \gamma \cdot \nu + \tau - \ln \int_{S^2} \exp\left(\sum_{i=1}^{3} \nu_i p_i^2 + \tau \right) dp \\ &= \gamma \cdot \nu - \ln Z(\nu) = J(\nu), \end{aligned}$$

so that it is sufficient to consider $J(\nu)$ for ν with $\nu \cdot m = 0$.

Consider the problem

$$\max_{\mu \in \mathbb{R}^3} J(\mu),$$

or equivalently

$$\max_{\nu \in m^\perp} J(\nu),$$

where $m^\perp = \{\nu \in \mathbb{R}^3 : \nu \cdot m = 0\}$.

Lemma. $J(\nu)$ is a strictly concave function on $m^\perp$ with $J(\nu) \to -\infty$ as $|\nu| \to \infty$, and hence attains a unique maximum on $m^\perp$.

Proof. If $a \cdot m = 0$ then a calculation shows that

$$\frac{\partial^2 \ln Z(\mu)}{\partial \mu_i \partial \mu_j} a_i a_j \;=\; \frac{1}{2Z(\mu)^2} \int_{S^2} \int_{S^2} \left(\sum_{i=1}^{3} a_i (p_i^2 - q_i^2) \right)^2 \exp\left(\sum_{k=1}^{3} \mu_k (p_k^2 + q_k^2) \right) \, dp \, dq.$$

To prove that $J(\nu) \to -\infty$ as $|\nu| \to \infty$ it suffices to prove that $\exp(-J(\nu)) \to \infty$. But

$$\exp(-J(\nu)) = \int_{S^2} \exp\left(\sum_{i=1}^{3} \nu_i(p_i^2 - \gamma_i)\right) dp$$

and

$$\begin{aligned}\sum_{i=1}^{3} \nu_i(p_i^2 - \gamma_i) \;\; &= \;\; \nu_1(2p_1^2 + p_2^2 - 2\gamma_1 - \gamma_2) \\ &\quad + \nu_2(2p_2^2 + p_1^2 - 2\gamma_2 - \gamma_1).\end{aligned}$$

The result follows by examining the sets of $p \in S^2$ where the two quantities in brackets are positive and negative.

Given a maximizer μ of J we have that $\nabla_\mu J(\mu) = 0$, that is

$$\frac{\nabla_\mu Z(\mu)}{Z(\mu)} = \gamma,$$

expressing the fact that

$$\rho_Q(p) = \frac{\exp\left(\sum_{i=1}^3 \mu_i p_i^2\right)}{Z(\mu)}$$

satisfies $Q(\rho_Q) = Q$.

Now let $\rho \in \mathcal{A}_Q$, $\rho \neq \rho_Q$. Then by the strict convexity of $\rho \ln \rho$ we have that

$$\begin{aligned} I(\rho) &= \int_{S^2} \rho \ln \rho \, dp \\ &> \int_{S^2} [\rho_Q \ln \rho_Q + \\ &\qquad (\rho - \rho_Q)(1 + \sum_{i=1}^{3} \mu_i p_i^2 - \ln Z(\mu))] \, dp \\ &= I(\rho_Q), \end{aligned}$$

so that ρ_Q is the unique global minimizer.

Note that we have the dual extremum result

$$\min_{\rho \in \mathcal{A}_Q} I(\rho) = \max_{\mathbb{R}^3} J(\mu),$$

whereas the usual Lagrange duality principle (cf Borwein & Lewis 1991) is

$$\min_{\rho \in \mathcal{A}_Q} I(\rho) = \max_{\mathbb{R}^3} \hat{J}(\mu),$$

where

$$\hat{J}(\mu) = \gamma \cdot \mu - \int_{S^2} \exp(\sum_{i=1}^{3} \mu_i p_i^2 - 1)\, dp \leq J(\mu).$$

Let $f(Q) = I(\rho_Q) = \inf_{\rho \in \mathcal{A}_Q} I(\rho)$, so that

$$\psi_B(Q, \theta) = \theta k_B f(Q) - \kappa |Q|^2.$$

Hence the bulk free energy has the form

$$\psi_B(Q, \theta) = k_B \theta \left(\sum_{i=1}^{3} \mu_i (\lambda_i + \frac{1}{3}) - \ln Z(\mu) \right) - \kappa \sum_{i=1}^{3} \lambda_i^2.$$

Theorem

f is strictly convex in Q and

$$\lim_{\lambda_{\min}(Q)\to -\frac{1}{3}+} f(Q) = \infty.$$

Proof

The strict convexity of f follows from that of $\rho \ln \rho$. Suppose that $\lambda_{\min}(Q^{(j)}) \to -\frac{1}{3}$ but $f(Q^{(j)})$ remains bounded. Then

$$Q^{(j)}e^{(j)}.e^{(j)} + \frac{1}{3}|e^{(j)}|^2 = \int_{S^2} \rho_{Q^{(j)}}(p)(p \cdot e^{(j)})^2 dp \to 0,$$

where $e^{(j)}$ is the eigenvector of $Q^{(j)}$ corresponding to $\lambda_{\min}(Q^{(j)})$.

But we can assume that $\rho_{Q^{(j)}} \rightharpoonup \rho$ in $L^1(S^2)$, where $\int_{S^2} \rho(p)\, dp = 1$ and that $e^{(j)} \to e$, $|e| = 1$. Passing to the limit we deduce that

$$\int_{S^2} \rho(p)(p \cdot e)^2 dp = 0.$$

But this means that $\rho(p) = 0$ except when $p \cdot e = 0$, contradicting $\int_{S^2} \rho(p)\, dp = 1$. $\square$

Asymptotics

Theorem

$$C_1 - \frac{1}{2}\ln(\lambda_{\min}(Q) + \frac{1}{3}) \leq f(Q) \leq C_2 - \ln(\lambda_{\min}(Q) + \frac{1}{3})$$

for constants C_1, C_2.

The proof uses our initial construction of a function $\rho \in \mathcal{A}_Q$ to get the upper bound, and the dual variational principle to get the lower bound.

Other predictions

1. All stationary points uniaxial and phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

2. Minimizers ρ^* of $U(\rho) - \theta\eta(\rho)$ correspond to minimizers over Q of $\psi_B(Q, \theta)$. As already mentioned, these ρ^* were calculated and shown to be uniaxial by Fatkullin and Slastikov (2005), and by Liu, Zhang & Zhang (2005).

3. Existence when $L_4 \neq 0$ under suitable inequalities on the L_i, because $I_4 = Q_{lk}Q_{ij,l}Q_{ij,k} \geq -\frac{1}{3}|\nabla Q|^2$.

4. Near $Q = 0$ we have (see also Katriel *et al*) the expansion

$$\frac{1}{\theta k_B}\psi_B(Q,\theta) = \ln 4\pi + \left(\frac{15}{4} - \frac{\kappa}{2\theta k_B}\right)\mathrm{tr}\,Q^2 - \frac{225}{42}\mathrm{tr}\,Q^3 + \frac{225}{112}(\mathrm{tr}\,Q^2)^2 + \ldots$$

The ratio of the coefficients of the last two terms gives $\frac{b}{c} = 2$, while experimental values reported in the literature are for MBBA 1.19, and for 5CB 0.82.

Given appropriate boundary conditions, do minimizers of

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + \psi_E(Q,\nabla Q),\theta]\, dx$$

have eigenvalues which are *bounded away from* $-\frac{1}{3}$, i.e. for some $\varepsilon > 0$

$$-\frac{1}{3}+\varepsilon \leq \lambda_{\mathsf{min}}(Q(x)) \leq \lambda_{\mathsf{max}}(Q(x)) < \frac{2}{3}-\varepsilon \text{ for a.e. } x \in \Omega?$$

If not, this would mean that a minimizer of I would have an unbounded integrand. Surely this is inconsistent with being a minimizer ....

Similar nonlinear elasticity problem: Do minimizers for suitable boundary conditions of

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

with $W(A) \to \infty$ as $\det A \to 0+$ satisfy

$$\det Dy(x) \geq \varepsilon > 0 \text{ a.e. } x \in \Omega$$

for some $\varepsilon > 0$?

This seems to be very difficult.

One might think that for a minimizer to have the integrand infinite somewhere is some kind of contradiction, but in fact this is a common phenomenon in the calculus of variations, even in one dimension.

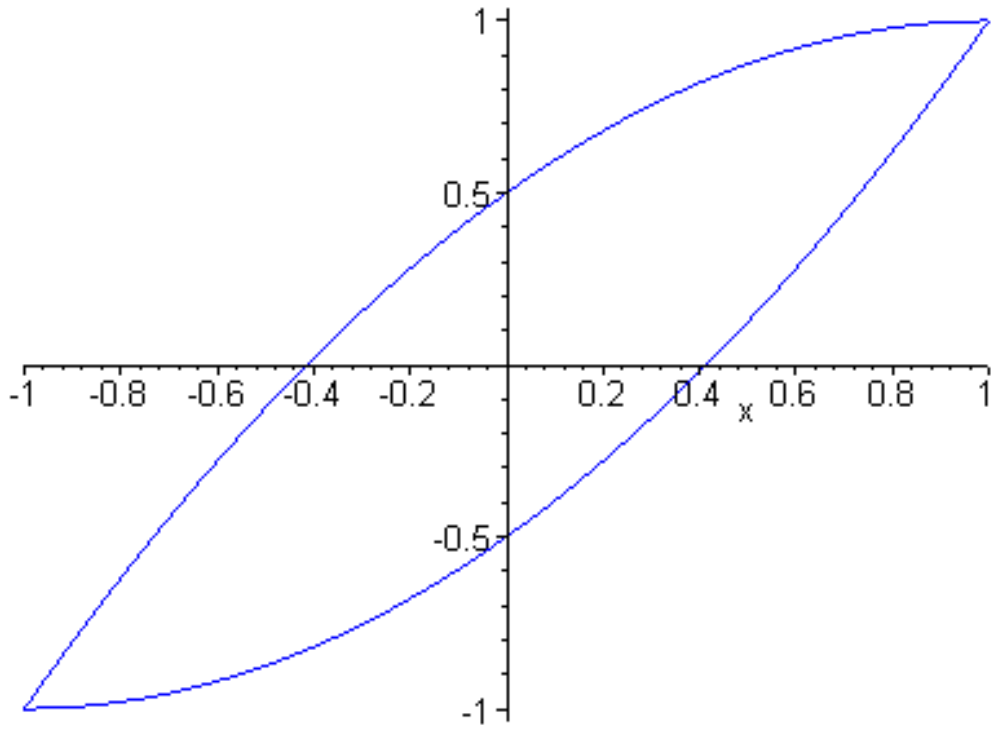
Example (B & Mizel)
Minimize

$$I(u) = \int_{-1}^{1} [(x^4 - u^6)^2 u_x^{28} + \epsilon u_x^2]\, dx$$

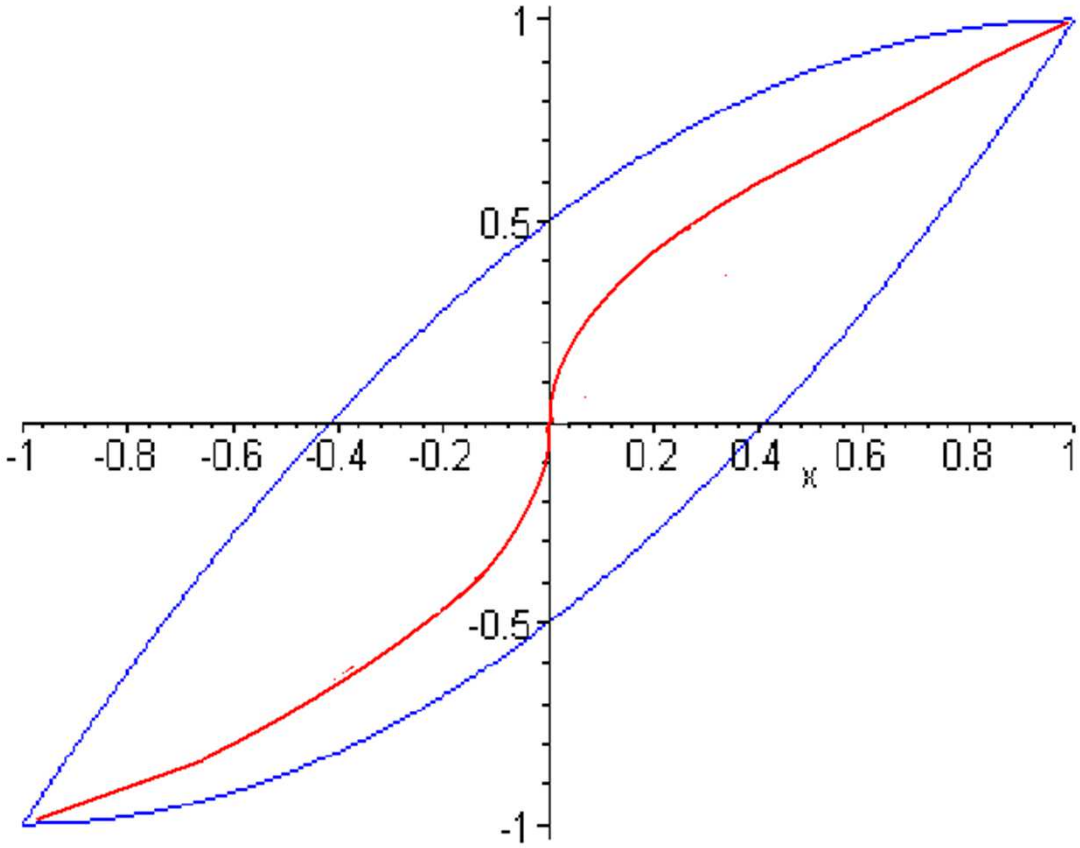
subject to

$$u(-1) = -1,\ u(1) = 1,$$

with $0 < \epsilon < \epsilon_0 \approx \cdot 001$.



Result of finite-element minimization, minimizing $I(u_h)$ for a piecewise affine approximation u_h to u on a mesh of size h, when h is very small. The method converges and produces two curves $u^{\pm}$.



However the real minimizer is u^*, which has a singularity

$$u^*(x) \sim |x|^{\frac{2}{3}} \text{sign}\, x \text{ as } x \sim 0.$$

Theorem (JB/Majumdar) *Let Q minimize*

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + K(\theta)|\nabla Q|^2]\, dx,$$

subject to $Q(x) = Q_0(x)$ for $x \in \partial\Omega$, where $K(\theta) > 0$ and $Q_0(\cdot)$ is sufficiently smooth with $\lambda_{\min}(Q_0(x)) > -\frac{1}{3}$. Then

$$\lambda_{\min}(Q(x)) > -\frac{1}{3} + \varepsilon,$$

for some $\varepsilon > 0$ and Q is a smooth solution of the corresponding Euler-Lagrange equation.

Proof: Project using the nearest point projection onto the convex set

$$K = \{Q : f(Q) \leq M\}$$

for large M. It can be shown that this reduces *both* terms in the integral.

Open problem. Prove this for the case of three or more elastic constants. The above method does not work. In the three elastic constant case Evans & Tran prove partial regularity, but not $\lambda_{\min}(Q(x)) > -\frac{1}{3} + \varepsilon$.

Developments.

1. Jamie Taylor (2015) has generalized the construction of the singular potential to a broad class of moment problems, with various applications.

2. For studies of dynamics using the singular potential see
E. Feireisl, E. Rocca, and G. Schimperna, Annali di Matematica Pura ed Applicata (2013)
M. Wilkinson, Arch. Rat. Mech. Anal. (2015)

4. The description of defects

Summary of LC models

For simplicity we drop the explicit dependence on the temperature θ.

Landau - de Gennes

$$I_{LdG}(Q) = \int_\Omega \left(\psi_B(Q) + \sum_{i=1}^{4 \text{ or } 5} L_i I_i \right) dx,$$

where $\psi_B(Q)$ has one of the forms discussed,

$$I_1 = Q_{ij,j}Q_{ik,k}, \quad I_2 = Q_{ik,j}Q_{ij,k},$$
$$I_3 = Q_{ij,k}Q_{ij,k}, \quad I_4 = Q_{lk}Q_{ij,l}Q_{ij,k},$$
$$I_5 = \varepsilon_{ijk}Q_{il}Q_{jl,k},$$

and the L_i are constants with $L_5 = 0$ for nematics.

Uniaxial ansatz $Q = s(n \otimes n - \frac{1}{3}1)$ for constant $s > 0$ leads to the

Oseen-Frank energy

$$I_{OF}(n) = \int_\Omega W(n, \nabla n)\, dx,$$

The work of Lamy (2014) shows/suggests that few equilibrium solutions of LdG are uniaxial (whereas most are nearly uniaxial).

where

$$W(n, \nabla n) = K_1(\operatorname{div} n)^2 + K_2(n \cdot \operatorname{curl} n + q_0)^2 + K_3|n \times \operatorname{curl} n|^2 + (K_2 + K_4)(\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2),$$

and the K_i and q_0 are constants with $q_0 = 0$ for nematics.

If $s = s(x)$ we get the Ericksen energy

$$I_E(s, n) = \int_\Omega W(s, \nabla s, n, \nabla n)\, dx.$$

Natural function spaces.

Landau - de Gennes: $Q \in W^{1,2}(\Omega, \mathcal{E})$, where $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$.

Oseen-Frank: $n \in W^{1,2}(\Omega, S^2)$. Indeed if $q_0 = 0$ then under the Ericksen inequalities

$$2K_1 > K_2 + K_4, \quad K_2 > |K_4|, \quad K_3 > 0$$

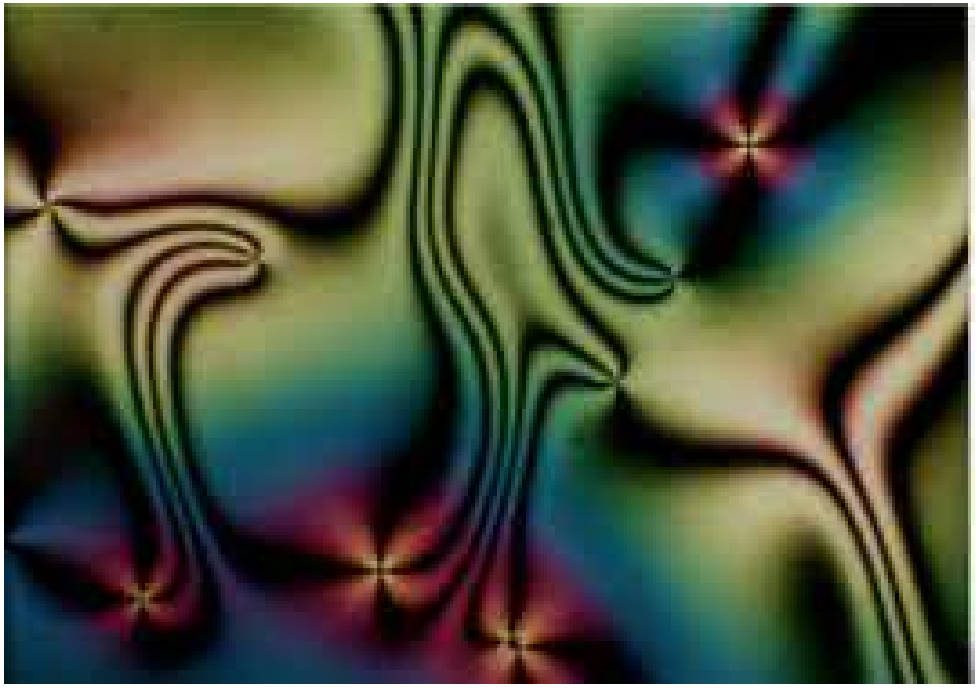
we have that

$$C'|\nabla n|^2 \leq W(n, \nabla n) \leq C|\nabla n|^2.$$

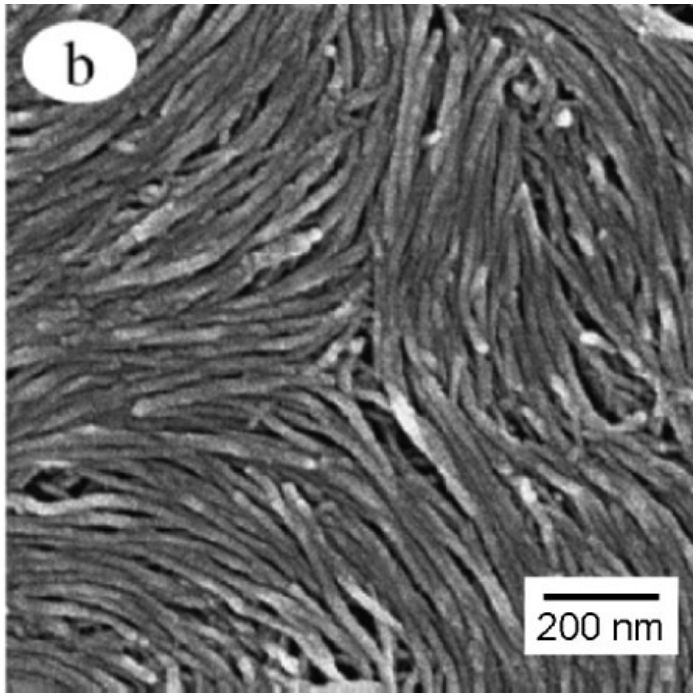
Ericksen: $(s, n) \in W^{1,2}(\Omega, \mathbb{R}) \times W^{1,2}(\Omega, S^2)$.

Defects

Roughly these can be thought of as regions of sharp change in the director or line field.

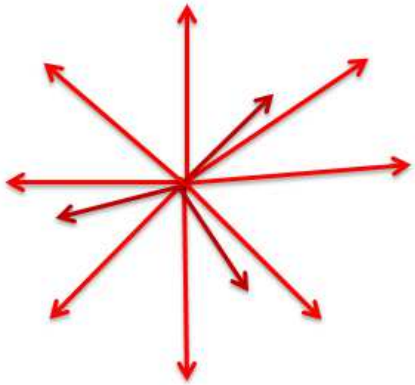


Schlieren texture of a nematic film
with surface point defects (boojums).
Oleg Lavrentovich (Kent State)



Zhang/Kumar 2007
Carbon nano-tubes as liquid crystals

Point defects



The Euler-Lagrange equation for

$$I_{OF} = \int_\Omega W(n, \nabla n)\, dx$$

has solutions representing point defects, e.g.

$$\tilde{n}(x) = \frac{x}{|x|} \quad \text{(radial hedgehog)}$$

$$\nabla \tilde{n}(x) = \frac{1}{|x|}(1 - n \otimes n)$$

$$|\nabla \tilde{n}(x)|^2 = \frac{2}{|x|^2}$$

$\int_0^1 r^{2-p} dr < \infty$ for $1 \leq p < 3$.

$\tilde{n} \in W^{1,p}$ for $1 \leq p < 3$ finite energy for quadratic models

If $q_0 = 0, K_1 = K_2 = K_3 = K,\ K_4 = 0$ (the *one constant approximation*) then $\tilde{\mathbf{n}}$ is the unique minimizer of $I_{OF} = K \int_\Omega |\nabla n|^2 d\mathbf{x}$ subject to its own boundary conditions (Brezis, Coron, Lieb 1986). In this case any minimizer is smooth except for a finite number of point defects (Schoen & Uhlenbeck 1982) at points $x(i)$ such that

$$n(x) \sim \pm R(i) \frac{x - x(i)}{|x - x(i)|} \text{ as } x \to x(i),$$

for some $R(i) \in SO(3)$.

Much less is known about point defects in the Oseen-Frank theory for the general case of unequal elastic constants. For example it is not known if a minimizer can have infinitely many point defects.

Helein (1987) proved that $\tilde{n}$ is not a minimizer if $8(K_1 - K_2) > K_3$, this condition being sharp (Cohen & Taylor (1990)).

Why is one-constant approximation easier?

Remark: for Oseen-Frank the Euler-Lagrange equation is

$$\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial n_{i,j}}\right) - \frac{\partial W}{\partial n_i} = \lambda(x) n_i,$$

where the Lagrange multiplier $\lambda(x)$ is given by

$$\lambda(x) = \left(\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial n_{k,j}}\right) - \frac{\partial W}{\partial n_k}\right) n_k.$$

$= 2K|\nabla n|^2$
for the one-constant approximation, but in general depends on second derivatives of n.

$\Delta n \cdot n = -|\nabla n|^2$
for $n \in S^2$

Description of defects in the Landau – de Gennes theory

Since weak solutions in Landau - de Gennes are smooth, modulo difficulties with the eigenvalue constraints, defects are not represented by singularities in Q. Rather they can be seen as singularities in the eigenvectors of Q, which can occur when eigenvalues coincide. (cf de Gennes, Biscari ...)

The situation might be different for free-energy densities $\psi(Q, \nabla Q)$ which are convex but not quadratic in ∇Q. For such integrands there is a counterexample of Šverák & Yan which has a singular minimizer of the form

$$Q(x) = |x| \left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} 1 \right).$$

Point defects in the Ericksen and Landau - de Gennes theories

Since weak solutions in Landau - de Gennes are smooth, point defects are not represented by point singularities in Q. In both the Landau - de Gennes and Ericksen theories there are solutions to the Euler-Lagrange equations representing *melting hedgehogs*, of the form

$$Q(x) = s(|x|)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathbf{1}\right),$$

where $s(0) = 0$.

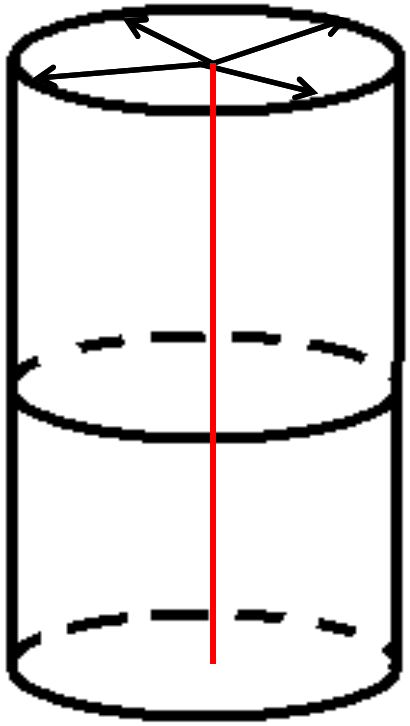
For the quartic bulk energy ψ_B and the one constant elastic energy such a solution is shown by Ignat, Nguyen, Slastikov & Zarnescu (2014) to be a local minimizer for $\Omega = \mathbb{R}^3$ subject to the condition at infinity

$$Q(x) \to s_{\text{min}} \left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathbf{1} \right) \text{ as } |x| \to \infty,$$

where $s_{\text{min}} = \frac{b+\sqrt{b^2-12ac}}{2c} > 0$, for temperatures close to the nematic initiation temperature.

However for lower temperatures the melting hedgehog is not a minimizer (Gartland & Mkaddem (1999)) and numerical evidence suggests a biaxial torus structure for the defect without melting.

Line defects

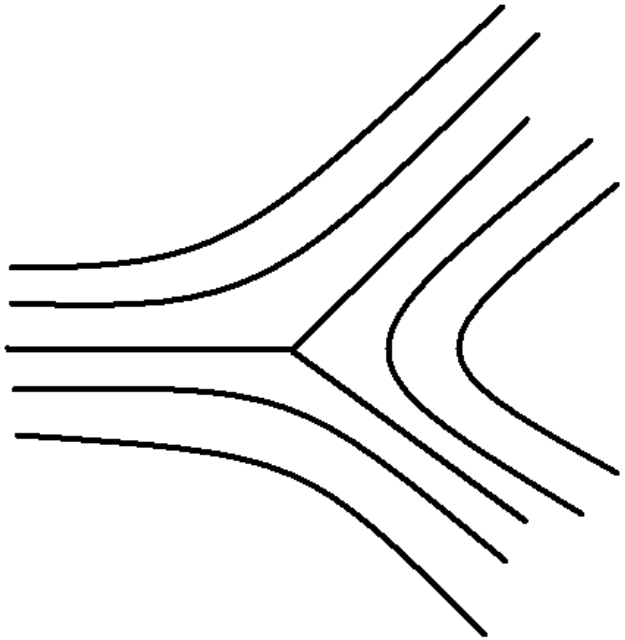


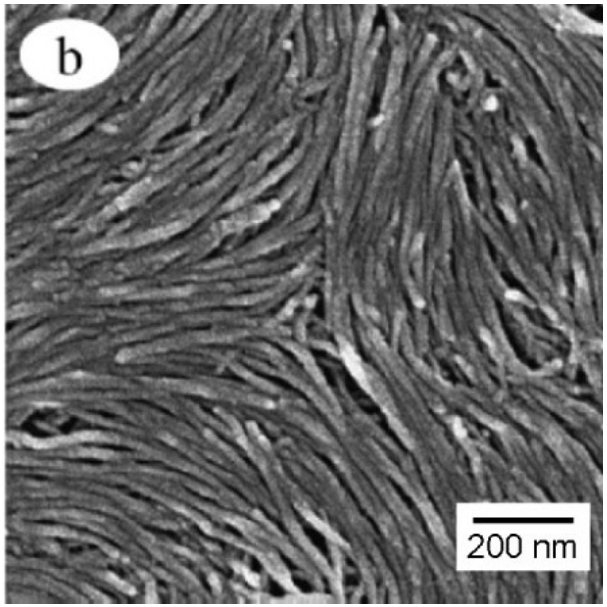
$$\hat{n}(x) = (\frac{x_1}{r}, \frac{x_2}{r}, 0) \quad r = \sqrt{x_1^2 + x_2^2}$$
$$|\nabla \hat{n}(x)|^2 = \frac{1}{r^2}$$

$$\hat{n}, \hat{Q} = s\left(\hat{n} \otimes \hat{n} - \frac{1}{3}\mathbf{1}\right) \in W^{1,p} \Leftrightarrow 1 \leq p < 2$$

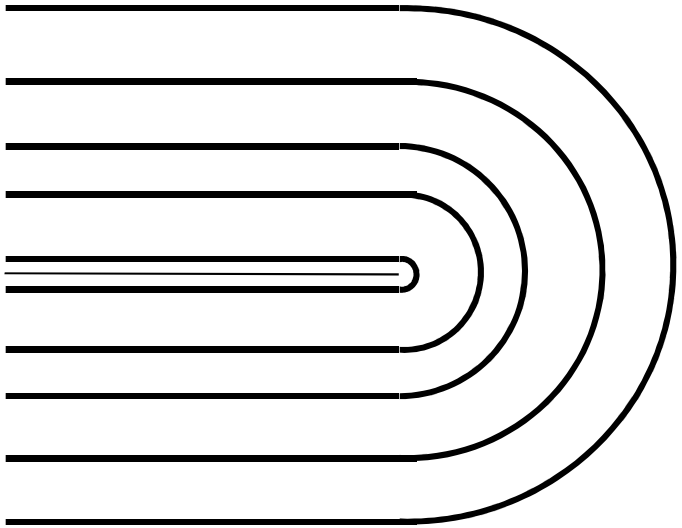
infinite energy for Oseen-Frank and constrained Landau-de Gennes quadratic models

Index one half defects

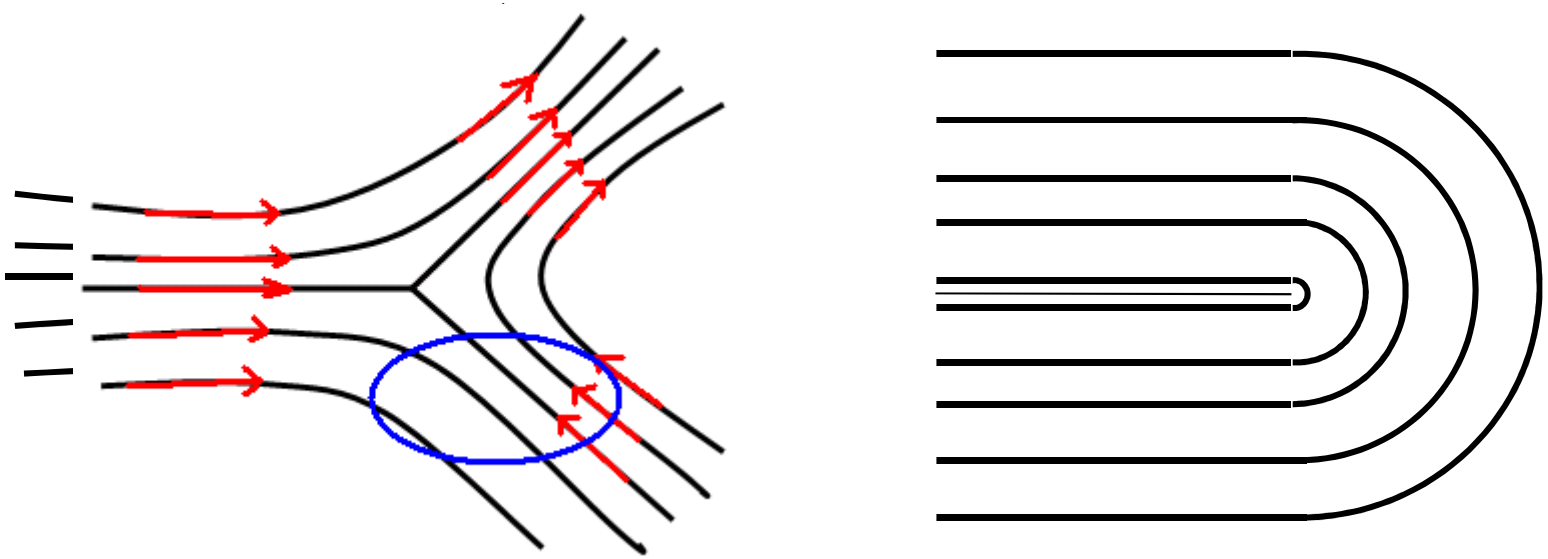




Zhang/Kumar 2007
Carbon nano-tubes
as liquid crystals



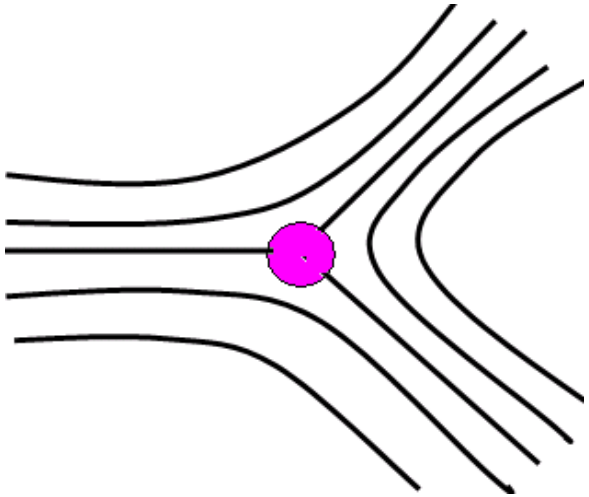
The index one half singularities are non-orientable



$Q \notin W^{1,2}$ since otherwise orientable

Can one change Q (while remaining uniaxial) in a core around the defect in such a way that the energy becomes finite?

Yes for the cylindrical hedgehog by 'escape into the third dimension'.



No for the index $\frac{1}{2}$ defects because then Q would be nonorientable and in $W^{1,2}$, contradicting the orientability result for simply-connected domains.

Lessons from solid mechanics

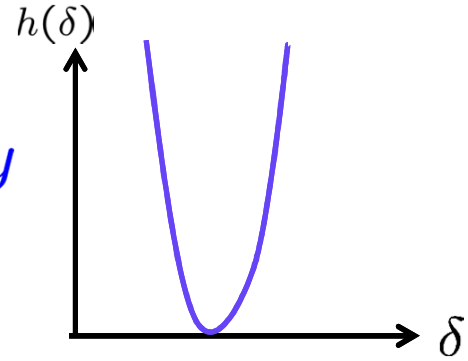
For nonlinear elasticity, with free-energy functional

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

minimizers can have singularities, and the predictions of the model depend on the function space.

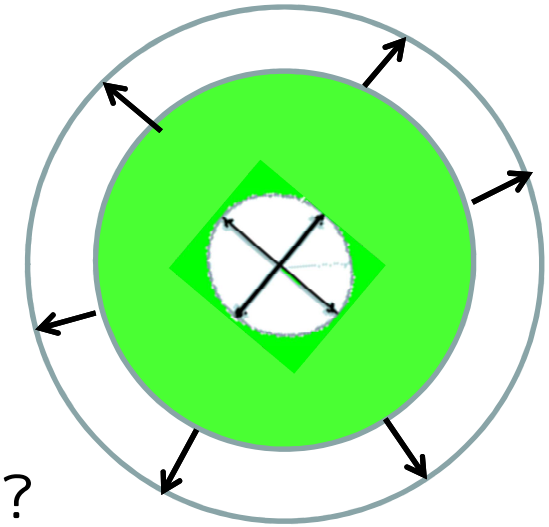
e.g. cavitation: given $\lambda > 0$ the minimizer of

$$I(y) = \int_{B(0,1)} [|Dy|^2 + h(\det Dy)]\, dx \quad + \kappa \text{ area } S_y$$

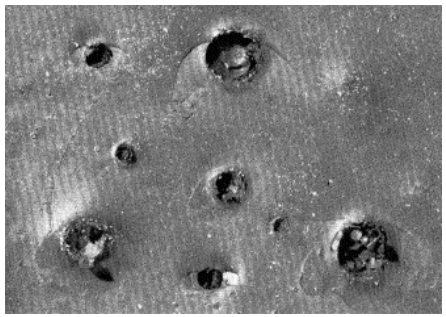


among smooth y subject to $y(x) = \lambda x$ for $|x| = 1$ is $y^*(x) = \lambda x$.

But among radial deformations $y(x) = \frac{r(|x|)}{|x|}x$ in $W^{1,2}$ the minimizer for large enough λ satisfies $r(0) > 0$.



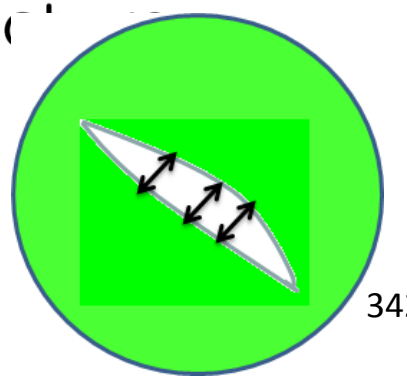
(Lavrentiev phenomenon)



But is $W^{1,2}$ the largest such function space?

No, because the body could develop fra[illegible]

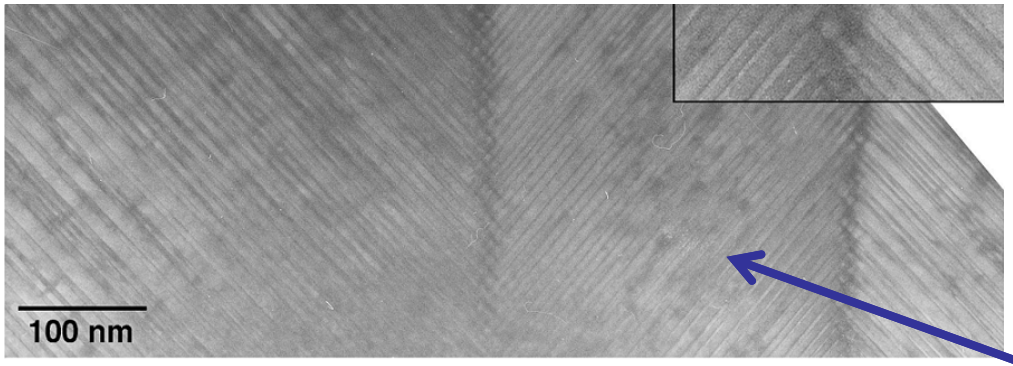
surfaces across which y is discontinuous.



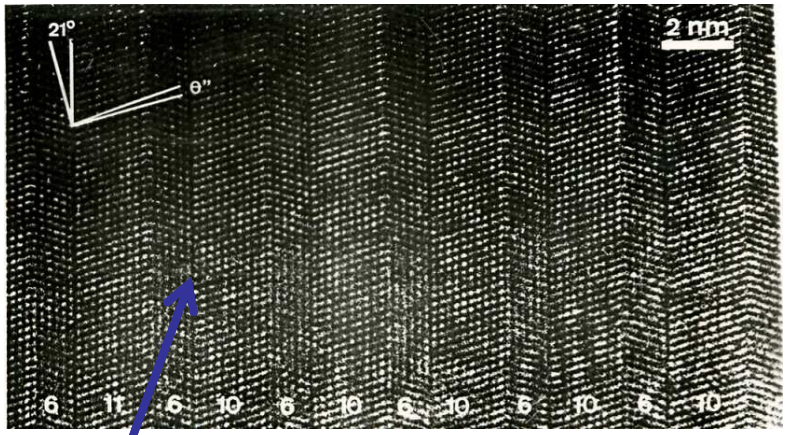
Francfort-Marigo theory of fracture.

$y \in SBV$ (special functions of bounded variation), jump set S_y

As we have seen, there can also be planar discontinuities in Dy representing phase boundaries.

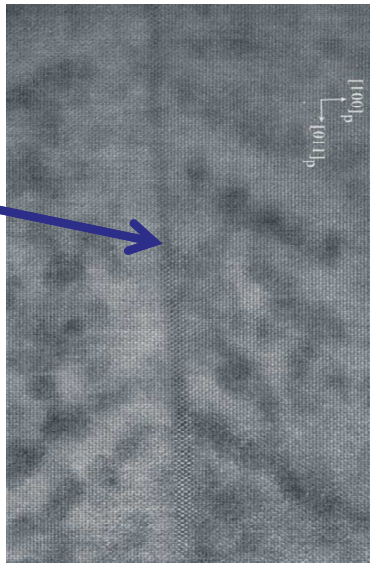


Macrotwins in $Ni_{65}Al_{35}$
single crystal (D. Schryvers)



NiMn, Baele, van Tenderloo, Amelinckx

Sharp, and diffuse interfaces



Perovskite. Salje.

And there are models similar to Landau - de Gennes allowing both sharp and diffuse interfaces, e.g.

$$I(y) = \int_\Omega [\psi(Dy) + \varepsilon |D^2 y|^2]\, dx + \kappa \,\text{area}\, S_{Dy}.$$

(Ball & Mora-Corral 2009)

The important conclusion to draw for liquid crystals is that the function space is part of the model. (Proof. Change the function space and the predictions change.)

Indeed the Lavrentiev phenomenon (the infimum of the total free energy is different in different function spaces is different) occurs in the Oseen-Frank theory. In fact we have that for the unit ball B

$$\inf_{n\in X,\, n|_{\partial B}=x} \int_B K|\nabla n|^2\,dx \begin{cases} = \infty & \text{if } X = C^1 \\ < \infty & \text{if } X = W^{1,2} \end{cases}$$

(Hardt & Lin 1986 give an example with smooth degree zero boundary data for which both infima are finite but that in $W^{1,2}$ is lower.)

Director modeling of line defects with finite energy

That these defects have infinite energy arises from the quadratic growth in ∇n of $W(n, \nabla n)$.

But there is no reason to suppose that $W(n, \nabla n)$ is quadratic for large $|\nabla n|$ (such as near defects).

So a possible remedy would be to assume that $W(n, \nabla n)$ has *subquadratic* growth, i.e.

$$W(n, \nabla n) \leq C(|\nabla n|^p + 1),$$

where $1 \leq p < 2$, which would make line defects have finite energy.

For example, we can let

$$W_\alpha(n, \nabla n) = \frac{2}{p\alpha}\left((1 + \alpha W(n, \nabla n))^{\frac{p}{2}} - 1\right),$$

where $\alpha > 0$ is small. Then $W_\alpha(n, \nabla n) \to W(n, \nabla n)$ as $\alpha \to 0$. Also, assuming the Ericksen inequalities, W_α satisfies the growth conditions

$$C'_\alpha(|\nabla n|^p - 1) \leq W_\alpha(n, \nabla n) \leq C_\alpha |\nabla n|^p,$$

for positive constants C_α, C'_α. Setting

$$I_\alpha(n) = \int_\Omega W_\alpha(n, \nabla n)\, dx,$$

we obtain that $I_\alpha(\widehat{n}) < \infty$ as desired. Also $W_\alpha(n, \cdot)$ is convex.

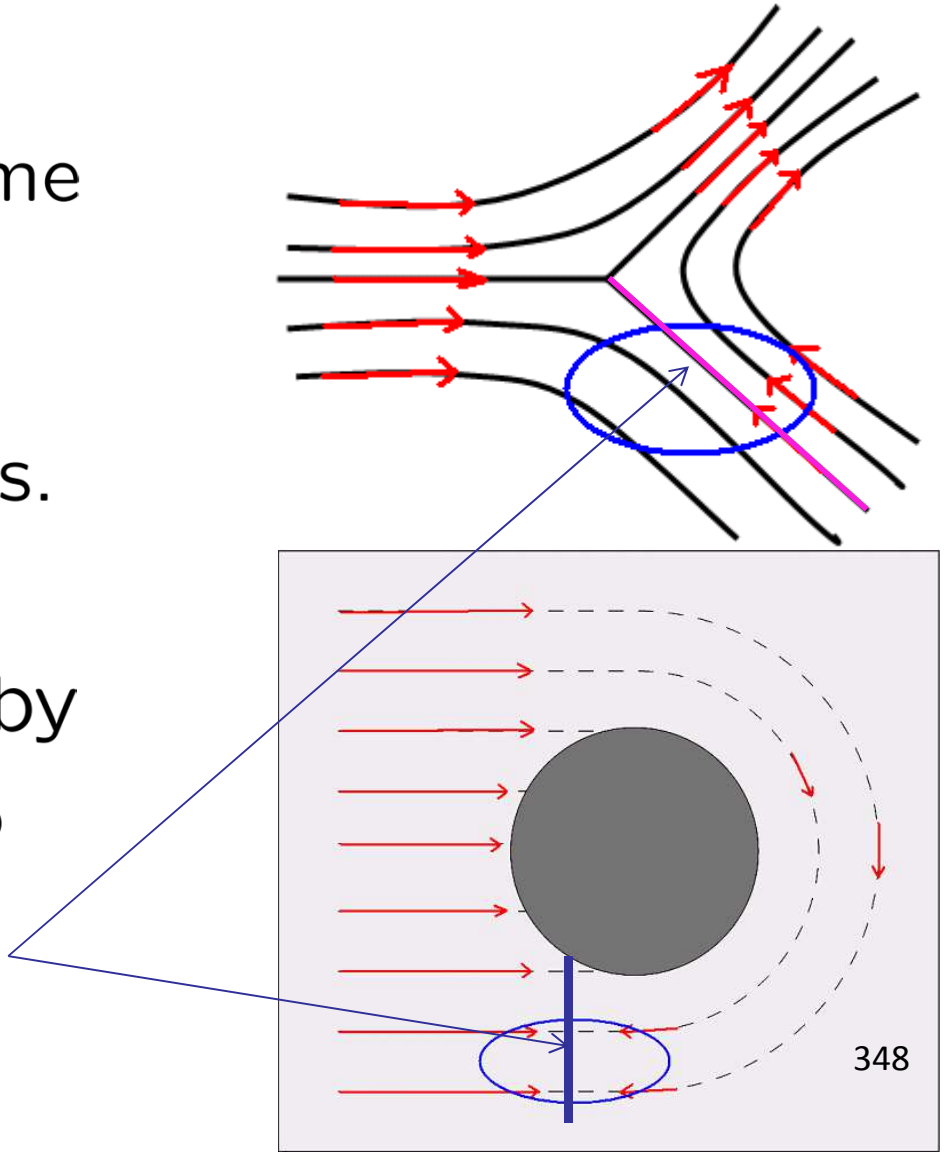
Boundary conditions:
If $\Omega \subset \mathbb{R}^3$ has smooth boundary and a sufficiently smooth unit vector field N is given on the boundary $\partial\Omega$, then it is known (Hardt & Lin 1987) that there is a unit vector field $n \in W^{1,2}(\Omega; S^2)$ with $n = N$ on $\partial\Omega$.

However, if, for example, $\Omega = (0,1)^3$ is a cube and N is the inward normal to the boundary, then (Bedford) there is no such n. Thus the Oseen-Frank theory does not apply to homeotropic boundary conditions on a cube, although a theory with subquadratic growth would be OK.

But the index $\frac{1}{2}$ singularities cannot be modelled this way because they are not *orientable*.

As we have seen the same issue arises for smooth line fields in non simply-connected regions.

This can be handled by allowing n to jump to $-n$ across suitable surfaces.



Theorem (Bedford). *Let* $\mathbf{Q} = s\left(n \otimes n - \frac{1}{3}\mathbf{1}\right) \in W^{1,2}(\Omega; M^{3\times 3})$, *where* $s \neq 0$ *is constant. Then there exists a unit vector field* $m \in SBV$ *such that* $m \otimes m = n \otimes n$, *and* $m_+ = -m_-$ *across any jump.*

This applies to the second situation above but not to index $\frac{1}{2}$ defects, for which an extension to $W^{1,p}$, $1 < p < 2$, would be required.

Ericksen theory. Here we can model point and line defects by finite energy configurations in which n is discontinuous and $s = 0$ at the defect (melting core). In this case there is no need to change the growth rate at infinity.

For example, if we consider the special case when

$$I_{LdG}(Q) = \int_\Omega [K|\nabla Q|^2 + \psi_B(Q)]\, dx,$$

then the uniaxial ansatz

$$Q(x) = s(x)\left(n(x) \otimes n(x) - \frac{1}{3}\mathbf{1}\right)$$

gives the functional

$$I_E(s,n) = \int_\Omega [K(|\nabla s|^2 + 2s^2|\nabla n|^2) + \psi_B(s)]\, dx,$$

where $\psi_b(s) = \widehat{\psi}(\frac{2s^2}{3}, \frac{2s^3}{27})$.

Then n can have a singularity at a point or curve which has finite energy because s can tend to zero sufficiently fast as the point or curve is approached to make $I_E(s, n)$ finite. However for non simply-connected domains or index $\frac{1}{2}$ defects there is the same orientability problem as in the Oseen-Frank theory, which can be 'cured' by allowing jumps from n to $-n$ across surfaces.

Theorem [Bedford] *Let* $Q \in W^{1,2}(\Omega; M^{3\times 3})$ *be uniaxial with* $s \in C(\Omega)$. *Then* $s \in W^{1,2}(\Omega)$ *and there exists a vector field*

$$m \in SBV_{\text{loc}}(\Omega \setminus \{s = 0\}; S^2)$$

such that $m \otimes m = n \otimes n$.

There is also the possibility of 'genuine' planar defects in this theory (see later).

Planar defects (JB/Bedford)

Let's explore whether it might be reasonable to consider a free-energy functional for nematic and cholesteric liquid crystals of free-discontinuity type

$$I(n) = \int_\Omega W(n, \nabla n)\, dx + \int_{S_n} f(n_+, n_-, \nu)\, d\mathcal{H}^2,$$

for $n \in SBV(\Omega, S^2)$, where ν is the normal to the jump set S_n. Here $W(n, \nabla n)$ is assumed to have the Oseen-Frank form or be modified so as to have subquadratic growth as suggested previously.

Admissible interfacial energies

Suppose that $f : S^2 \times S^2 \times S^2 \to [0, \infty)$ is continuous and frame-indifferent, i.e.

$$f(Rn_+, Rn_-, R\nu) = f(n_+, n_-, \nu) \qquad (1)$$

for all $R \in SO(3), n_+, n_-, \nu \in S^2$, and that f is invariant to reversing the signs of n_+, n_-, reflecting the statistical head-to-tail symmetry of nematic and cholesteric molecules, so that

$$f(-n_+, n_-, \nu) = f(n_+, -n_-, \nu) = f(n_+, n_-, \nu). \qquad (2)$$

Theorem. *A necessary and sufficient condition that a continuous* $f : S^2 \times S^2 \times S^2 \to [0, \infty)$ *satisfies* (1) *and* (2) *is that*

$$f(n_+, n_-, \nu) = \\ g((n_+ \cdot n_-)^2, (n_+ \cdot \nu)^2, (n_- \cdot \nu)^2, (n_+ \cdot n_-)(n_+ \cdot \nu)(n_- \cdot \nu))$$

for a continuous function $g : D \to [0, \infty)$, *where*

$$D = \{(\alpha, \beta, \gamma, \delta) : \alpha, \beta, \gamma \in [0, 1], \delta^2 = \alpha\beta\gamma, \alpha+\beta+\gamma-2\delta \leq 1\}.$$

An equivalent representation is in terms of the matrices $M_+ = n_+ \otimes n_+, M_- = n_- \otimes n_-,\ N = \nu \otimes \nu$, namely

$$f(n_+, n_-, \nu) = g(M_+ \cdot M_-, M_+ \cdot N, M_- \cdot N, \mathrm{tr}\,(M_+ M_- N)).$$

In fact the theorem, though without the characterization of the domain of g, follows from a representation theorem (Smith 1971) for isotropic functions of symmetric matrices.

Possible candidates for planar defects.

1. Nematic elastomers

The energy functional for nematic elastomers proposed by Bladon, Terentjev, Warner (1993) is given by

$$I(y,n) = \int_\Omega \frac{\mu}{2}\left(Dy(Dy)^T \cdot L_{a,n}^{-1} - 3\right)\, dx,$$

where

$$L_{a,n} = a^{\frac{2}{3}} n \otimes n + a^{-\frac{1}{6}}(\mathbf{1} - n \otimes n)$$

and $\mu > 0, a > 0$ are material parameters.

The material is assumed incompressible, so that $\mathbf{y}$ is subjected to the constraint $\det Dy = 1$.

Stripe domains in nematic elastomer
Kundler & Finkelmann
Mathematical theory due to De Simone & Dolzmann

By minimizing the integrand over $n \in S^2$ we obtain the purely elastic energy

$$I(y) = \int_\Omega W(Dy)\, dx, \qquad (1)$$

where

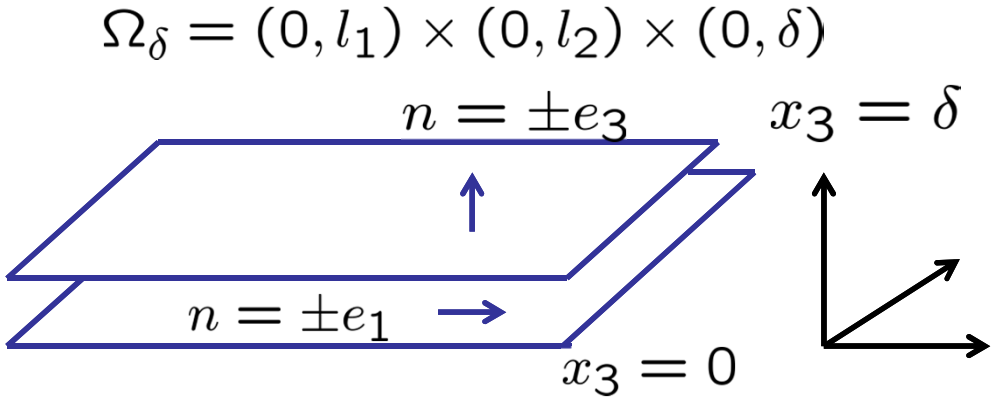
$$W(A) = \frac{\mu}{2}\left(a^{-\frac{2}{3}} v_1^2(A) + a^{\frac{1}{3}}(v_2^2(A) + v_3^2(A))\right),$$

and $v_1(A) \geq v_2(A) \geq v_3(A) > 0$ denote the singular values of A, that is the eigenvalues of $\sqrt{A^T A}$.

As discussed by De Simone & Dolzmann (2002) the free-energy function (1) is not quasiconvex, and admits minimizers in which ∇y jumps across planar interfaces, so that the minimizing n of the integrand also jumps. Of course the functional ignores Frank elasticity, i.e. terms in ∇n, but the experimental observations might suggest that even with such terms allowing jumps in n may be a useful approximation.

Order reconstruction

Barbero & Barberi (1983)
Palffy-Muhoray, Gartland
& Kelly (1994)



(a) Analysis using Landau - de Gennes

Boundary conditions:
$Q(x_1, x_2, 0) = Q^{(0)}, \;\; Q(x_1, x_2, \delta) = Q^{(1)},$
for a.e. $(x_1, x_2) \in (0, l_1) \times (0, l_2)$, where
$Q^{(0)} = s_1 \left(e_1 \otimes e_1 - \frac{1}{3}\mathbf{1} \right), \;\; Q^{(1)} := s_2 \left(e_3 \otimes e_3 - \frac{1}{3}\mathbf{1} \right),$
and Q periodic in x_1, x_2.

Assume that $L_4 = 0$ with the Longa inequalities

$$L_3 > 0, \;\; -L_3 < L_2 < 2L_3, \;\; -\frac{3}{5}L_3 - \frac{1}{10}L_2 < L_1,$$

which imply that

$$\psi_E(\nabla Q) \geq \alpha |\nabla Q|^2$$

for some $\alpha > 0$.

Rescale, defining

$$P(x_1, x_2, x_3) = Q(x_1, x_2, \delta x_3),$$

so that $I_{LdG}(Q) = \delta^{-1} E^{\delta}(P)$, where

$$E^{\delta}(P) = \int_D [\delta^2 \psi_B(P) + \psi_E(\delta P_{,1}, \delta P_{,2}, P_{,3})] \, dx$$

and $D = (0, l_1) \times (0, l_2) \times (0, 1)$.

Theorem. *Let P^δ be a minimizer of E^δ. Then as $\delta \to 0$*

$$P^\delta \to \bar{P},\ P^\delta_{,3} \to \bar{P}_{,3},\ \delta P^\delta_{,1} \to 0,\ \delta P^\delta_{,2} \to 0 \ \ \textit{in}\ L^2(D;S),$$

where

$$\bar{P}(x) = (1 - x_3)Q^{(0)} + x_3 Q^{(1)},$$

and $S = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$.

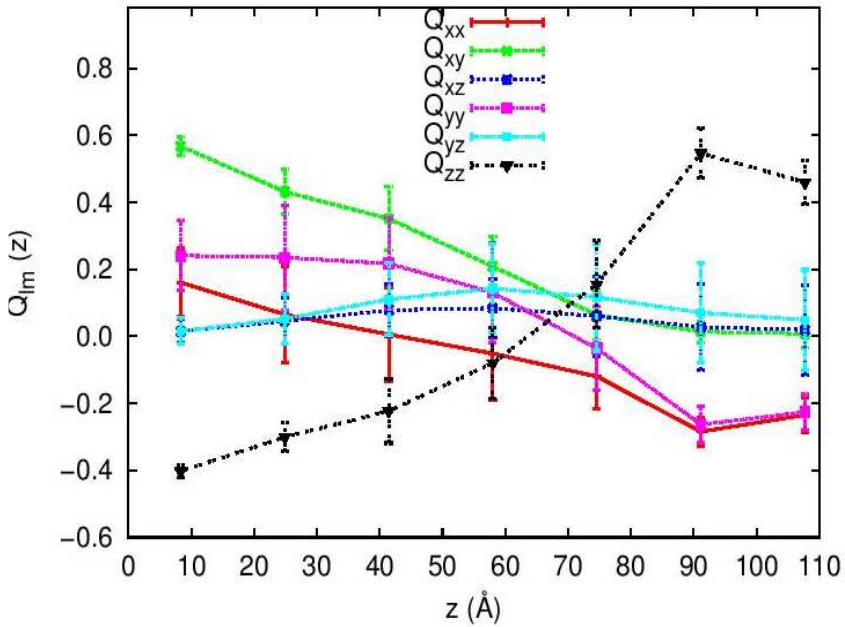
So for sufficiently small δ, Q is given approximately by

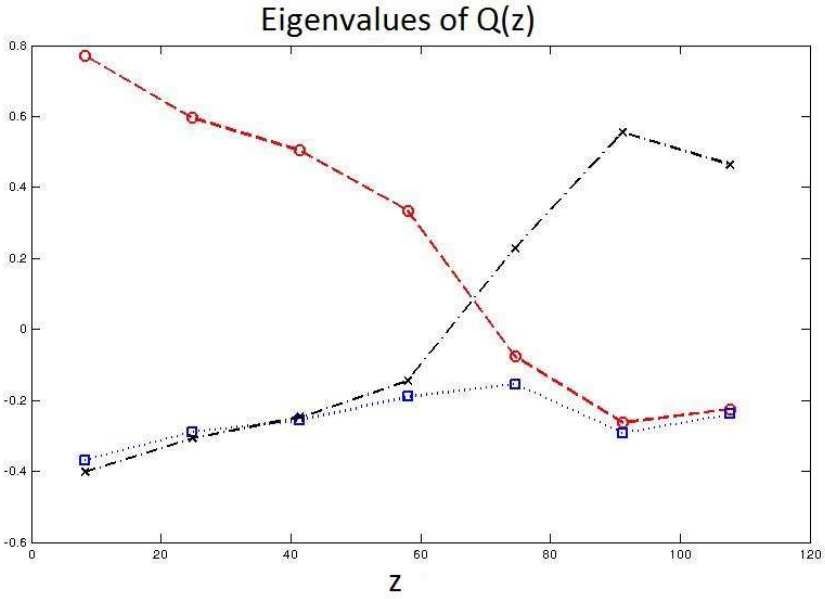
$$Q(x) = (1 - \delta^{-1}x_3)Q^{(0)} + \delta^{-1}x_3 Q^{(1)},$$

for which the director (the eigenvector of Q corresponding to the largest eigenvalue)

$$n(x) = \begin{cases} e_1 & \text{if } 0 \le x_3 \le \frac{s_1}{s_1+s_2}\delta \\ e_3 & \text{if } \frac{s_1}{s_1+s_2}\delta \le x_3 \le 1. \end{cases}$$

has a discontinuity on the plane $x_3 = \frac{s_1}{s_1+s_2}\delta$.





A. Pizzirusso, R. Berardi, L. Muccioli, M. Riccia, and C. Zannoni. Predicting surface anchoring: molecular organization across a thin film of 5CB liquid crystal on silicon. Chem. Sci., 3:573–579, 2012.

(b) Analysis using director model

Consider for simplicity the functional

$$I(n) = \int_{\Omega_\delta} K'|\nabla n|^2\,dx + k' \int_{S_n} (1-(n_+\cdot n_-)^2)^{\frac{r}{2}})\,d\mathcal{H}^2,$$

where $k' > 0$ and $0 < r < 1$, with boundary conditions $n(x_1, x_2, 0) = \pm e_1$, $n(x_1, x_2, \delta) = \pm e_3$ and $l_1 = l_2 = 1$.

Formally this can be obtained from the Landau - de Gennes functional

$$I(Q) = \int_{\Omega_\delta} K|\nabla Q|^2\,dx + k \int_{S_Q} |Q_+ - Q_-|^r\,d\mathcal{H}^2,$$

by making the uniaxial ansatz

$$Q(x) = s\left(n(x) \otimes n(x) - \frac{1}{3}\mathbf{1}\right),$$

where $|n(x)| = 1$ and $s \in (0,1)$ is constant, with $K' = 2Ks^2$, $k' = 2^{\frac{r}{2}} s^r k$.

Some care is needed when interpreting the boundary conditions and periodicity, since it is possible that Q might jump at the boundary $\partial\Omega_\delta$ of Ω_δ. This is handled by minimizing $I(Q)$ among $Q \in SBV_{\text{loc}}(\mathbb{R}^2 \times (-1, \delta+1); M^{3\times 3})$ satisfying

$$Q(x_1, x_2, x_3) = s\left(e_1 \otimes e_1 - \frac{1}{3}\mathbf{1}\right) \text{ for } -1 < x_3 < 0,$$

$$Q(x_1, x_2, x_3) = s\left(e_3 \otimes e_3 - \frac{1}{3}\mathbf{1}\right) \text{ for } \delta < x_3 < \delta+1,$$

and $Q(x_1 + l_1, x_2, x_3) = Q(x_1, x_2 + l_2, x_3) = Q(x_1, x_2, x_3)$ for all $(x_1, x_2, x_3) \in \mathbb{R}^2 \times (-1, \delta + 1)$. With this interpretation S_Q can be partly on $\partial\Omega_\delta$.

Candidates for minimizers of I are the two smooth Q given by

$$Q^{\pm}(x) = \frac{s}{2}\begin{pmatrix} \frac{1}{3} + \cos\frac{\pi x_3}{\delta} & 0 & \pm\sin\frac{\pi x_3}{\delta} \\ 0 & -\frac{2}{3} & 0 \\ \pm\sin\frac{\pi x_3}{\delta} & 0 & \frac{1}{3} - \cos\frac{\pi x_3}{\delta} \end{pmatrix},$$

which are the minimizers of $\int_{\Omega_\delta} |\nabla Q|^2 dx$ among uniaxial $Q \in W^{1,2}(\Omega_\delta; M^{3\times 3})$ satisfying the boundary conditions, and which correspond to the two Oseen-Frank solutions in which the line field rotates anticlockwise (resp. clockwise) in the (x_1, x_3) plane from horizontal to vertical.

Theorem. *For any $\delta > 0$ there exists at least one minimizer $Q \in SBV(\Omega_\delta : M^{3\times 3})$ of I subject to the boundary conditions.*

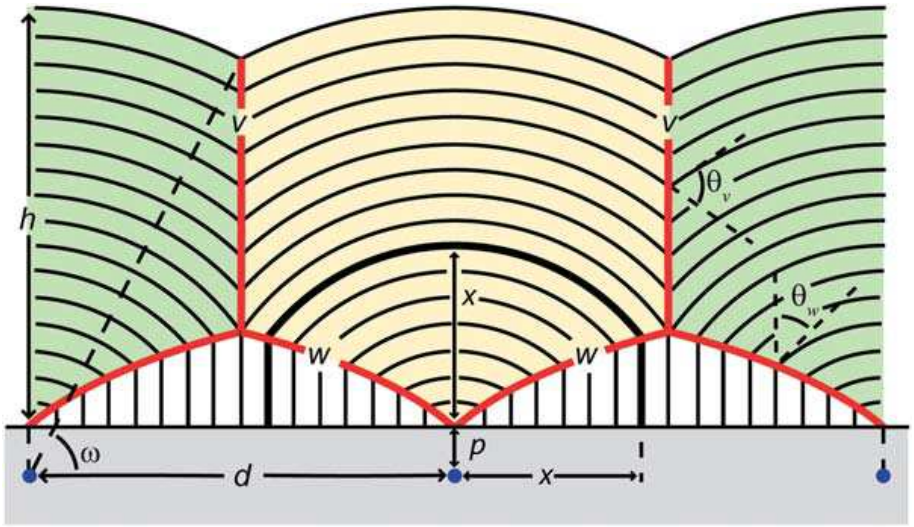
Conjecture. *There is a small $\delta_0 > 0$ such that if $\delta > \delta_0$ then $Q^{\pm}$ are the only minimizers, while if $0 < \delta < \delta_0$ then any minimizer Q has a single jump with jump set $S_Q = \{x : x_3 = \gamma(\delta)\}$, where $0 < \gamma(\delta) < \delta$.*

That $Q^{\pm}$ are not minimisers for δ sufficiently small is easily seen. In fact, $|\nabla Q^{\pm}| = \frac{C}{\delta}$ for some $C > 0$, so that $I(Q^{\pm}) = Ks^2\frac{C^2}{\delta}$. But if

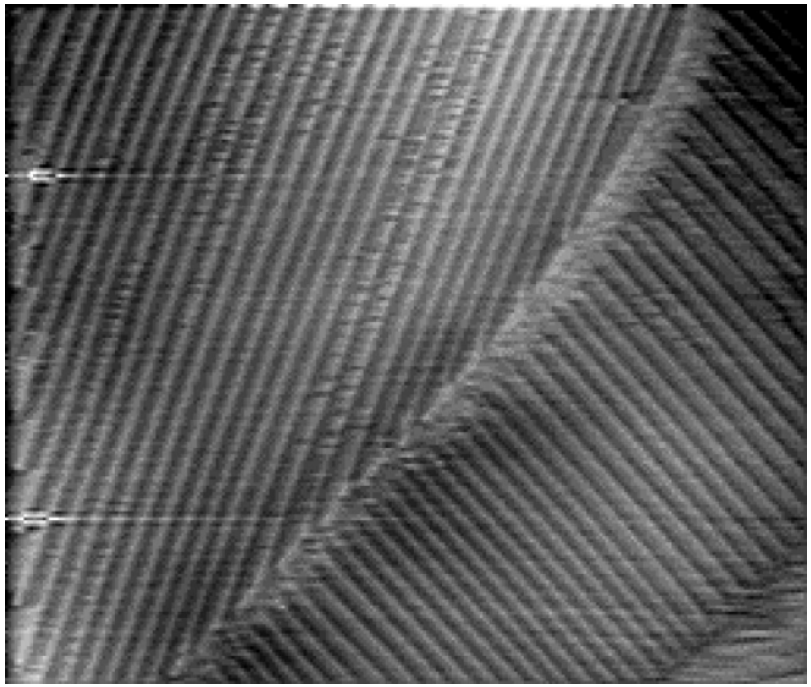
$$\hat{Q}(x) = \begin{cases} s\left(e_1 \otimes e_1 - \frac{1}{3}\mathbf{1}\right) & \text{if } 0 < x_3 < \frac{\delta}{2} \\ s\left(e_3 \otimes e_3 - \frac{1}{3}\mathbf{1}\right) & \text{if } \frac{\delta}{2} < x_3 < \delta \end{cases}$$

then $I(\hat{Q}) = ks^r 2^{\frac{r}{2}}$, so that $I(\hat{Q}) < I(Q^{\pm})$ if $s^{r-2}\frac{\delta k}{K} < 2^{-\frac{r}{2}}C^2$.

3. Smectic thin films



8CB smectic thin films
Zappone, Lacaze et al, 2010



AFM image
Michel, Lacaze
et al, 2004

Models of smectics

de Gennes approach: model using a complex order parameter $\Psi(x) = r(x)e^{i\phi(x)}$, in terms of which the molecular density is given by

$$\rho_0 + \rho(x) = \rho_0 + \mathrm{Re}\Psi(x) = \rho_0 + r(x)\cos\phi(x),$$

where $\rho_0 > 0$ is a constant average density. Thus $\rho(x)$ describes the fluctuations in the density due to the smectic layers, and $\nabla\phi$ gives the normals to the layers.

Various free-energy densities for smectics have been proposed (Chen & Lubensky, Kleman & Parodi, Leslie, Stewart & Nakagawa, Mcmillan, Zhang ...). We will restrict attention to smectic A liquid crystals, for which it is often assumed that $r(x)$ is constant, with the free-energy density being expressed in terms of n and ϕ. For example, the free-energy functional proposed by Kleman & Parodi is given by

$$I(n,\phi) = \int_\Omega \left(W(n, \nabla n) + \frac{1}{2}\mathbf{B}(n - \nabla\phi) \cdot (n - \nabla\phi) \right) dx,$$

where $\mathbf{B} = B_\perp \mathbf{1} + (B_\parallel - B_\perp) n \otimes n$ and $B_\perp, B_\parallel$ are positive material constants.

E (1994) argued that a good approximation is given by

$$\int_\Omega (K_1(\operatorname{div} n)^2 + B_{\|}(|\nabla\phi| - 1)^2)\, dx,$$

together with the constraint

$$n = \frac{\nabla\phi}{|\nabla\phi|}$$

that rigidly enforces that the director points parallel to the normal.

Existence of a minimizer for the Kleman & Parodi model is easy, but for the reduced one unclear.

Modified Pevnyi, Selinger & Sluckin model (2014)

$$I(Q,\rho)=\int_\Omega\left(\psi_E(Q,\nabla Q)+B\left|D^2\rho+\frac{q^2}{3s}\left(3Q+s\mathbf{1}\right)\rho\right|^2+f(\rho)\right)\,d\mathbf{x}$$

$$+k\int_{S_Q}\left|Q_+-Q_-\right|^r\,d\mathcal{H}^2$$

$$Q(x)=s\left(n(x)\otimes n(x)-\tfrac{1}{3}\mathbf{1}\right)$$

Then under suitable hypotheses on ψ_E and f one can prove the existence of a minimizing pair Q,ρ in

$$\mathcal{A}:=\left\{Q\in SBV\left(\Omega,\mathbb{R}^{3\times3}\right),\rho\in W^{2,2}\left(\Omega,\mathbb{R}\right):\right.$$

$$\left.Q=s\left(n\otimes n-\frac{1}{3}\mathbf{1}\right),\ |n|=1,\ Q|_{\partial\Omega}=\overline{Q}\right\}$$