Winter School, Würzburg
9-13 January 2012

Mathematics of Solid and Liquid Crystals

John Ball

Oxford Centre for Nonlinear PDE

Plan of course

Lectures 1-3

Mathematics of crystalline solids

Colloquium + lectures 4-5

Mathematics of liquid crystals

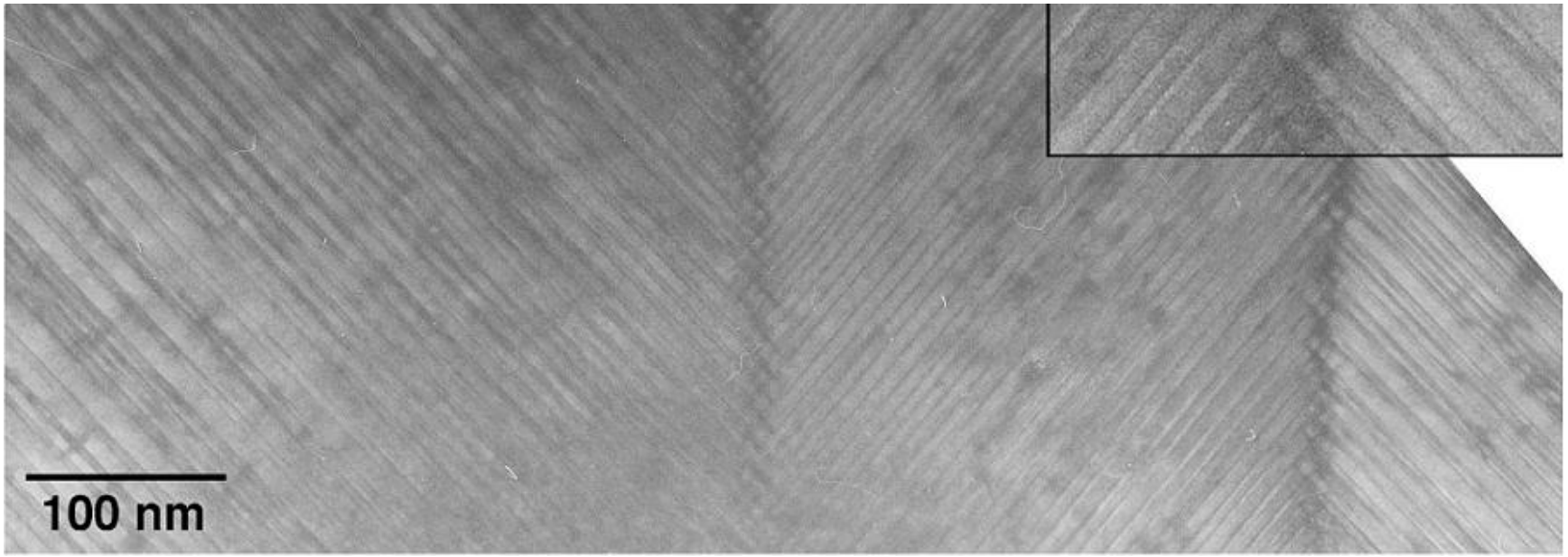
Plan for lectures 1-3

1. Modelling of solid phase transformations via nonlinear elasticity.
   Mathematical tools for describing microstructure.
   Classical austenite-martensite interfaces.

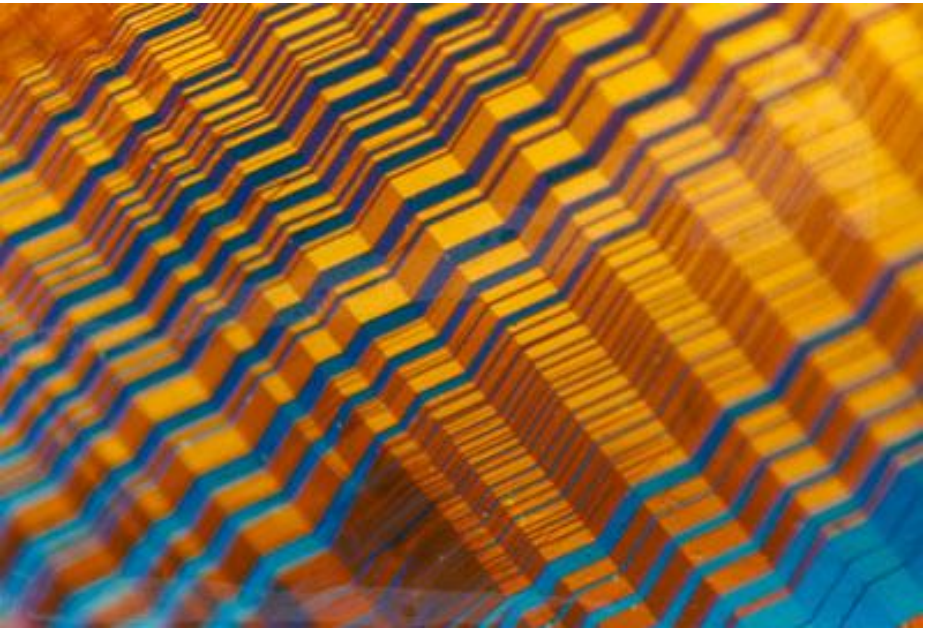
2. Macrotwins,
   Nonclassical austenite-martensite interfaces
   Nucleation of austenite in martensite

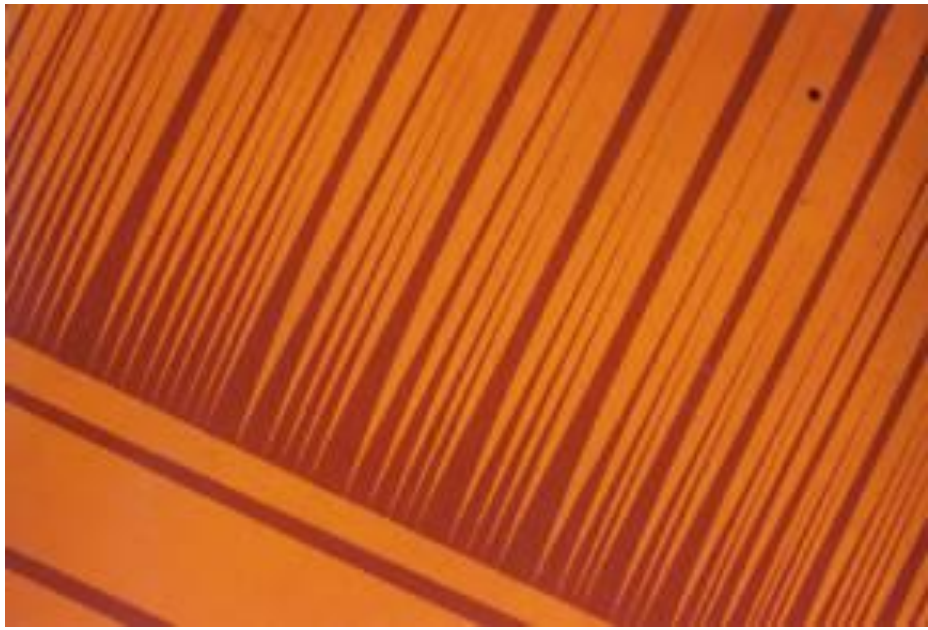
3. Incorporating interfacial energy.

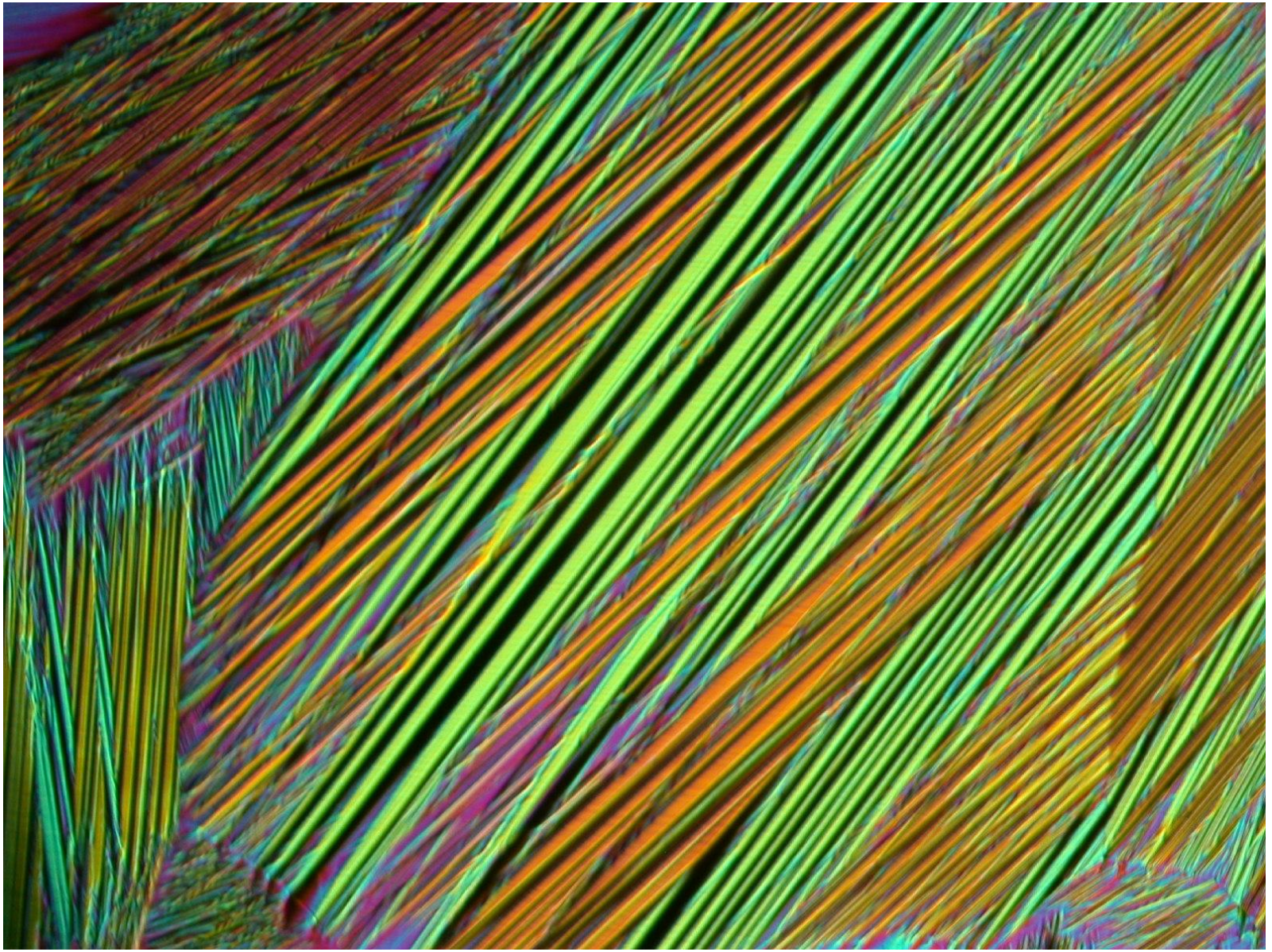
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



Martensitic microstructures in CuAlNi (Chu/James)







CuZnAl microstructure: Michel Morin (INSA de Lyon)

Themes of lectures

1. Role of compatibility of gradients in microstructure morphology.
2. Why do we see these particular microstructures rather than different ones?

Critique

We use a static theory, whereas this is clearly a pattern formation problem, which 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.

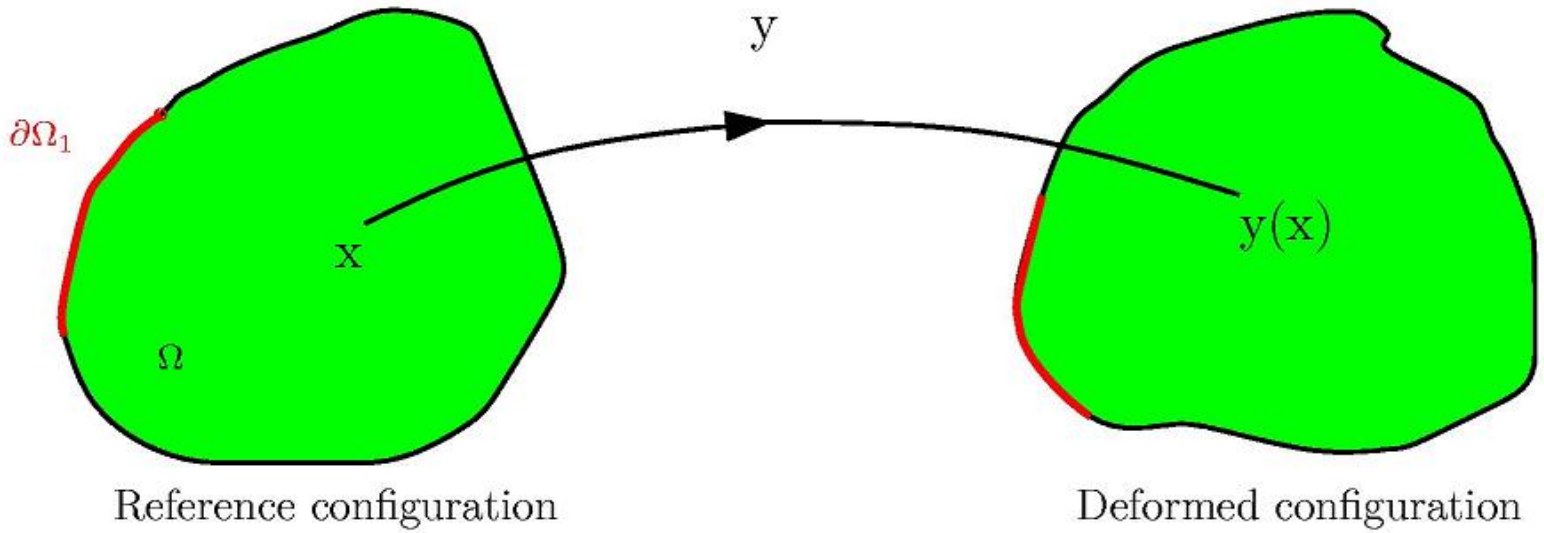
(a) what are appropriate dynamical equations?

(b) analysis currently intractable for any such model.

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).



$\Omega \subset \mathbf{R}^n$ bounded domain

Lipschitz boundary $\partial\Omega$

$$y : \Omega \to \mathbf{R}^m$$

Typically, $m = n = 2$ or 3.

$$Dy(x) = (\partial y_i / \partial x_j) \in M^{m \times n}$$

$$M^{m \times n} = \{\text{real } m \times n \text{ matrices}\}$$

Compatibility question

Given $F : \Omega \to M^{m \times n}$,

when is $F = Dy$ for some y?

A necessary condition that $F \in L^p(\Omega; M^{m\times n})$ satisfies $F = Dy$ for some $y \in W^{1,p}(\Omega; \mathbf{R}^m)$ is that

$$\frac{\partial F_{ij}}{\partial x_k} - \frac{\partial F_{ik}}{\partial x_j} = 0$$

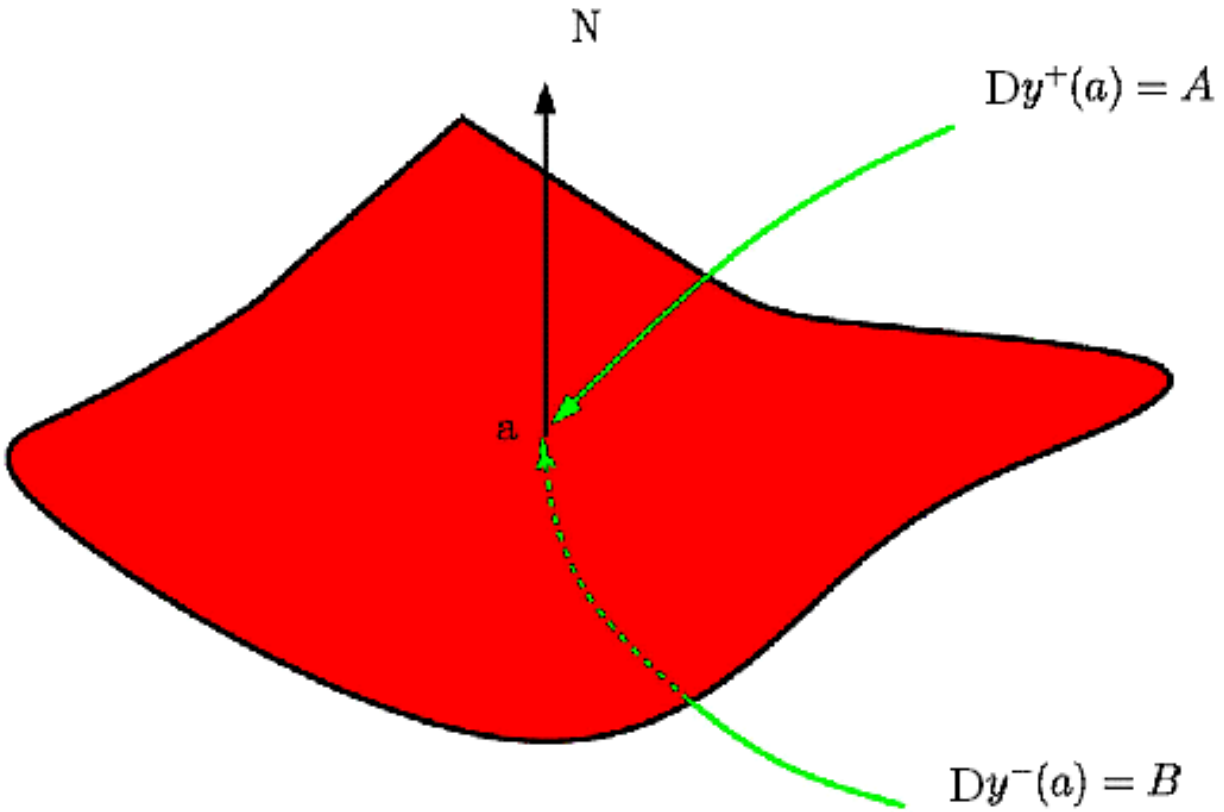
in the sense of distributions, i.e.

$$\int_\Omega \left(F_{ij} \frac{\partial \phi}{\partial x_k} - F_{ik} \frac{\partial \phi}{\partial x_j} \right) dx = 0$$

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

The condition is sufficient if Ω is simply connected.

Hadamard jump condition



y piecewise C^1

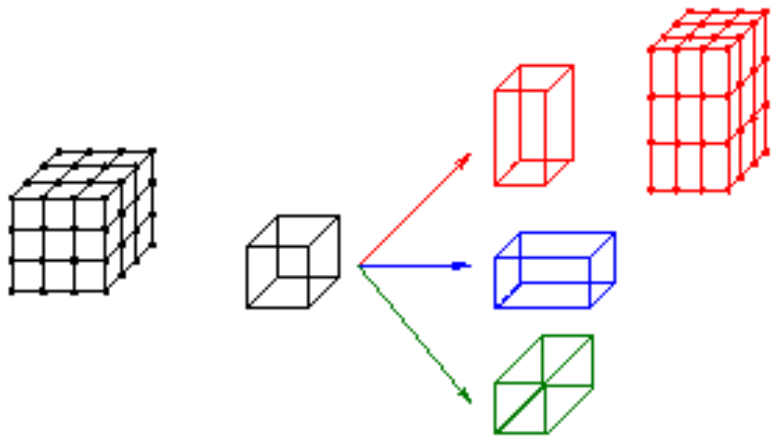
$$A - B = c \otimes N$$

Martensitic Transformations

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

e.g. cubic to tetragonal

$\theta > \theta_c$
cubic
austenite



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

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

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

Typically we assume that

$$\psi(A, \theta) \to \infty \text{ as } \det A \to 0+,$$

so that infinite energy is required to compress the body to zero volume.

We can then set $\psi(A, \theta) = \infty$ for $\det A \leq 0$, so that $\psi : M^{3\times 3} \times [\theta_1, \theta_2] \to [0, \infty]$ is continuous.

There is a substantial literature on the question of how this condition can be supplemented so that deformations with finite energy are invertible maps from - $\to \mathbf{R}^3$, so that interpenetration of matter does not occur.

Frame-indifference requires

$$\psi(RA, \theta) = \psi(A, \theta) \text{ for all } R \in SO(3).$$

If the material has cubic symmetry then also

$$\psi(AQ, \theta) = \psi(A, \theta) \text{ for all } Q \in P^{24},$$

where P^{24} is the group of rotations of a cube.

Energy-well structure

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

Assume

austenite

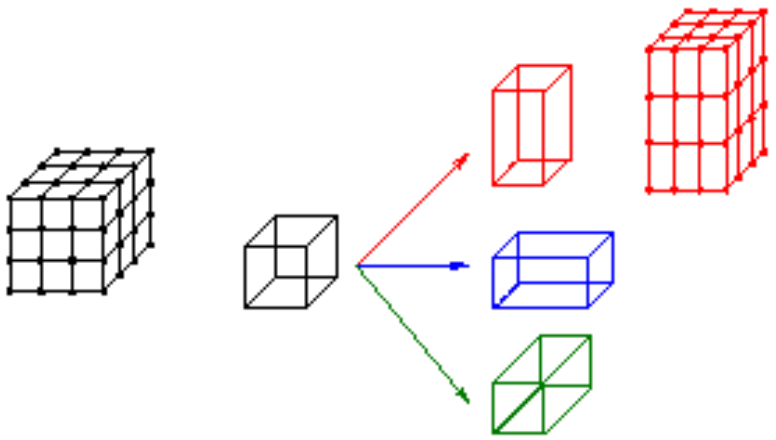
$$K(\theta) = \begin{cases} \alpha(\theta)\mathrm{SO}(3) & \theta > \theta_c \\ \mathrm{SO}(3) \cup \bigcup_{i=1}^{N} \mathrm{SO}(3)U_i(\theta_c) & \theta = \theta_c \\ \bigcup_{i=1}^{N} \mathrm{SO}(3)U_i(\theta) & \theta < \theta_c, \end{cases}$$

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

martensite

Assuming the austenite has cubic symmetry, and given the transformation strain U_1 say, the N variants U_i are the distinct matrices QU_1Q^T, where $Q \in P^{24}$.

Cubic to tetragonal (e.g. $Ni_{65}Al_{35}$)

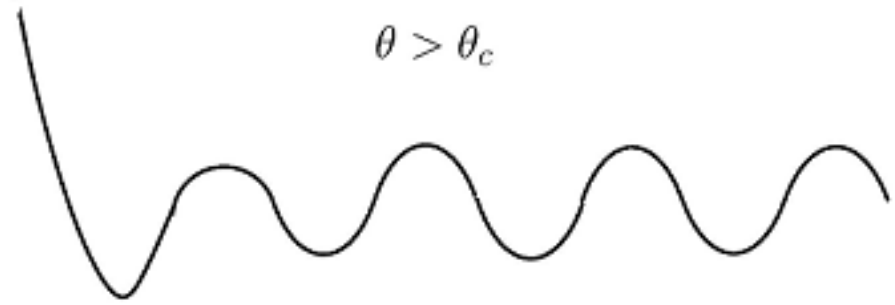


$N = 3$

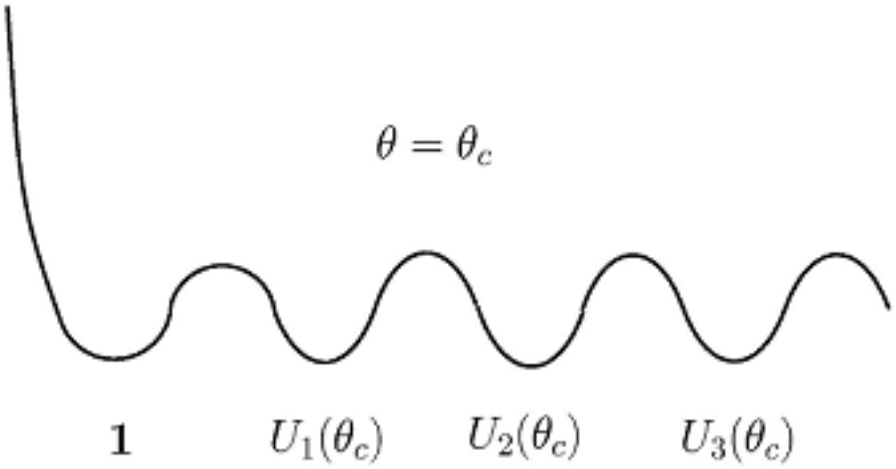
$$U_1 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_1)$$

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

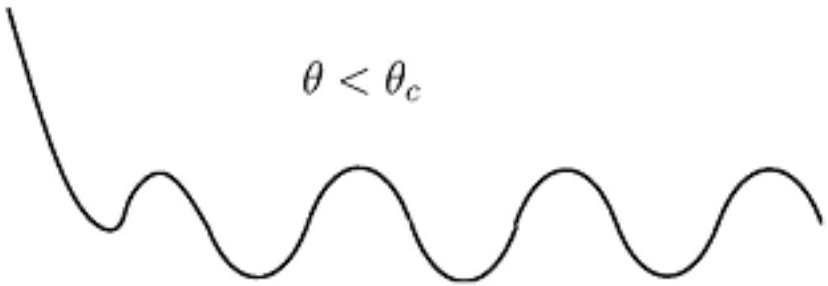
$$U_3 = \mathrm{diag}\,(\eta_1, \eta_1, \eta_2)$$



Exchange of stability



Can assume $\min_A \psi(A, \theta) = 0$ for all θ.



Why use nonlinear elasticity?

1. Conceptually simpler
2. Large rotations occur in martensitic transformations. If these are linearized then phantom stresses are predicted.

The use of nonlinear elasticity to describe martensitic transformations and their microstructure is due to B/James (1987), following work of many authors applying nonlinear elasticity to crystals, especially J.L. Ericksen. There is a 'linearized' version of the theory due to Khachaturyan and Roitburd.

Rank-one connections between energy-wells

Given $U = U^T > 0$ and $V = V^T > 0$, when is there a rank-one connection between $SO(3)U$ and $SO(3)V$?

That is , when are there rotations R_1, R_2 and vectors c, N such that

$$R_1 U = R_2 V + c \otimes N$$

Theorem. *Let $D = U^2 - V^2$ have eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$. Then $SO(3)U$ and $SO(3)V$ are rank-one connected if and only if $\lambda_2 = 0$. There are exactly two solutions provided $\lambda_1 < \lambda_2 = 0 < \lambda_3$, and the corresponding N's are orthogonal if and only if $\operatorname{tr} U^2 = \operatorname{tr} V^2$, i.e. $\lambda_1 = -\lambda_3$.*

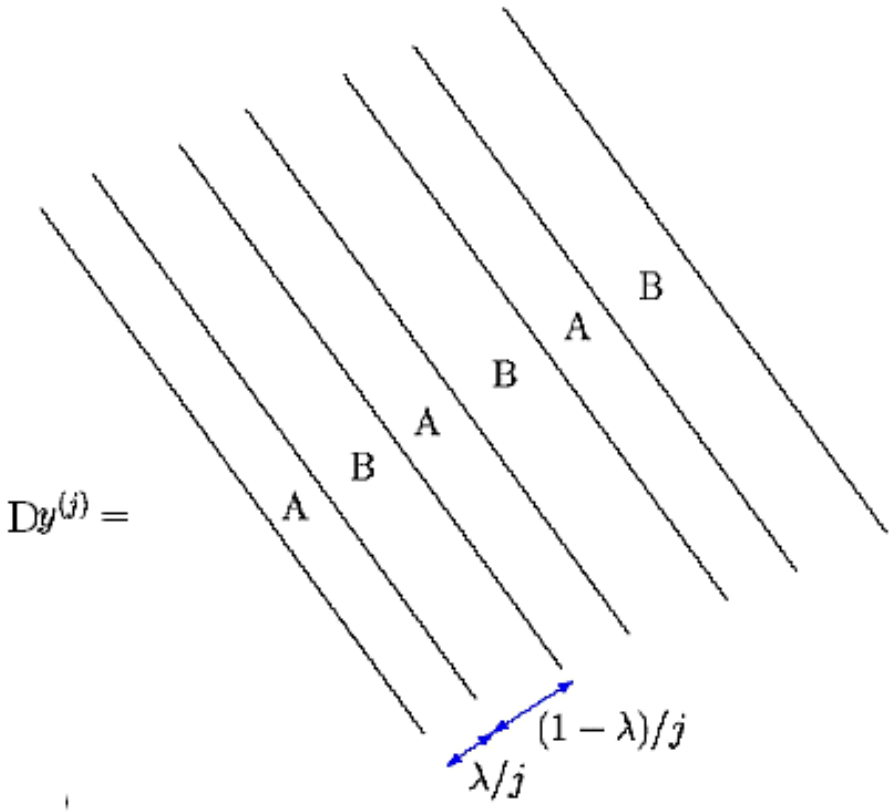
Twins

In the case of martensitic variants with $U = U_i, V = U_j$, $i \neq j$, we have $U = QVQ^T$ for some rotation Q and so the condition $\operatorname{tr} U^2 = \operatorname{tr} V^2$ is automatically satisfied. Rank-one connections correspond to twins and the corresponding twin normals are always orthogonal.

In this case there is a simpler criterion for the existence of rank-one connections due to Forclaz, namely that

$$\det(U - V) = 0$$

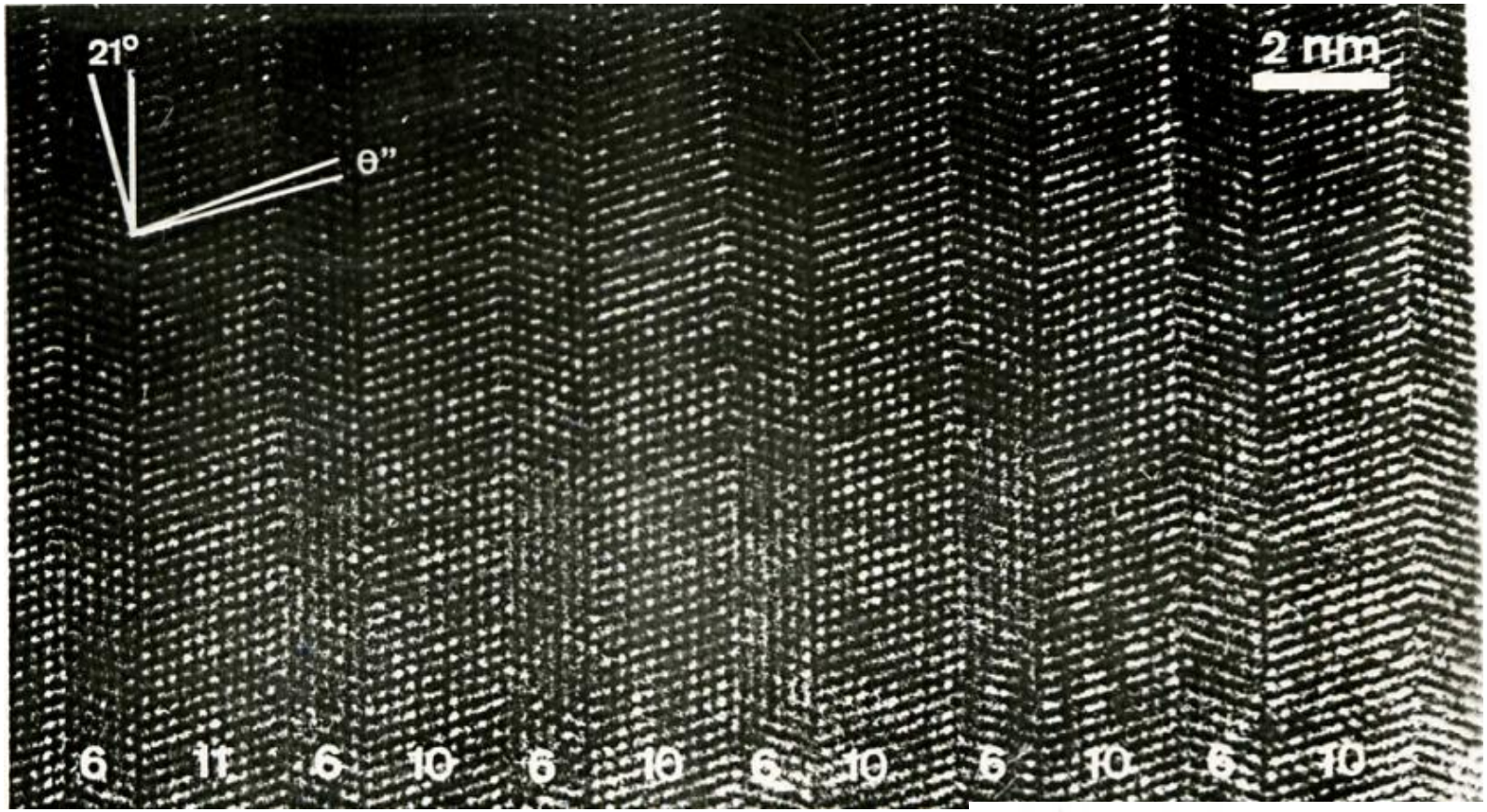
Weak convergence = convergence of averages



Simple laminate

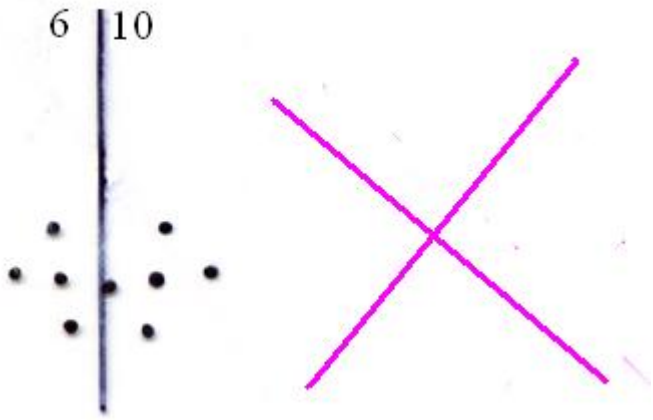
$$A - B = c \otimes N$$

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



Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

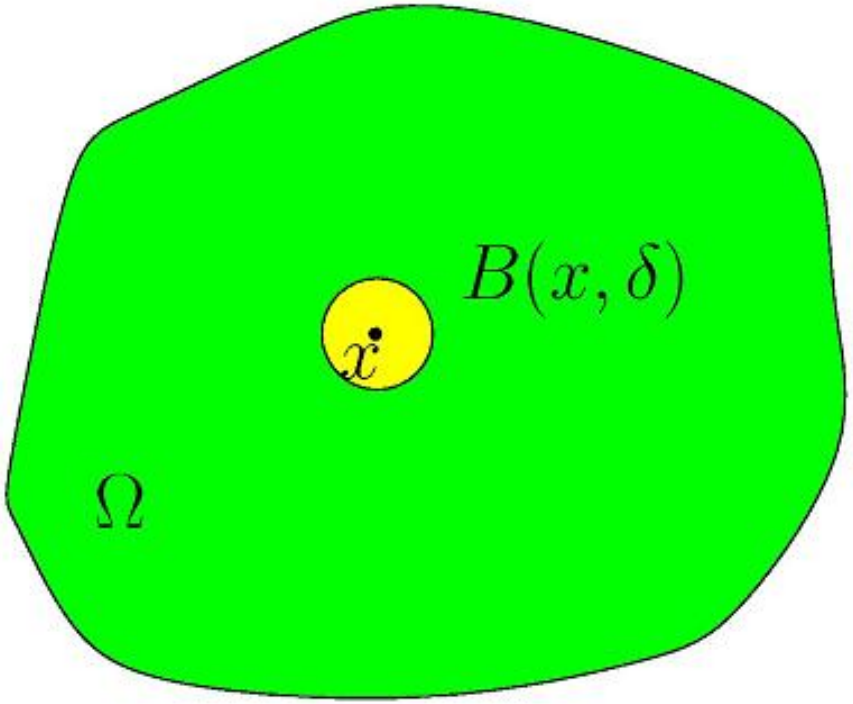
Baele, van Tenderloo, Amelinckx



Formulation of energy minimization problem in terms of Young measures

For ψ appropriate for martensite the minimum of $I_\theta(y) = \int_\Omega \psi(\nabla y(x), \theta)\, dx$ subject to suitable boundary conditions is not in general attained by ordinary deformations y, but rather by possibly infinitely fine microstructures generated by minimizing sequences $y^{(j)}$ of I_θ. These can be described by gradient Young measures.

Gradient Young measures



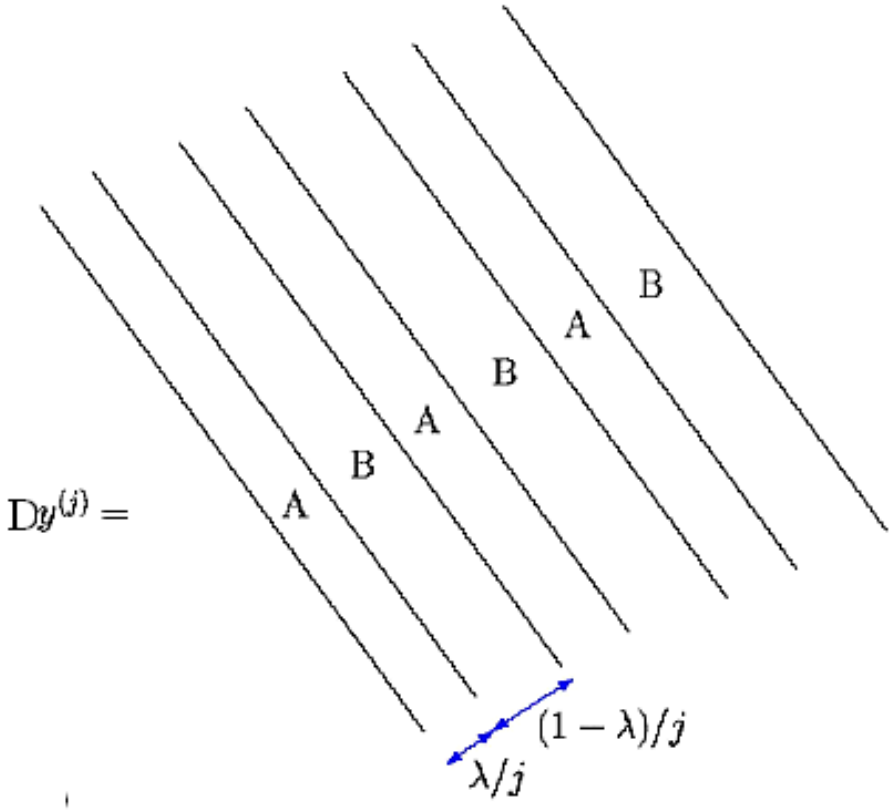
Fix x, j, δ.

$$E \subset M^{m\times n}$$

$$\nu_x^{j,\delta}(E) = \frac{\text{Volume}\{z \in B(x,\delta) \text{ with } Dy^{(j)}(z) \in E\}}{\text{Volume } B(x,\delta)}$$

$$\nu_x = \lim_{\delta\to 0}\lim_{k\to\infty} \nu_x^{j_k,\delta}$$ Young measure corresponding to $Dy^{(j_k)}$.

Gradient Young measure of simple laminate



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

Quasiconvexity

An integrand $f = f(A)$ is quasiconvex if

$$\int_\Omega f(Dz(x))\,dx \geq \int_\Omega f(A)\,dx = (\text{Volume } \Omega) f(A)$$

whenever $z : \Omega \to \mathbf{R}^m$ is smooth with $z(x) = Ax$ for all $x \in \partial\Omega$.

The condition does not depend on Ω.

Quasiconvexity is the central convexity condition of the calculus of variations

Roughly, quasiconvexity is necessary and sufficient for

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

to attain a minimum subject to given boundary conditions.

The existence of rank-one connections between martensitic energy-wells implies that $\psi(\cdot,\theta)$ is not rank-one convex, hence not quasiconvex. So we expect the minimum of I_θ not to be attained in general. The gradients $Dy^{(j)}$ of minimizing sequences for I_θ will not converge, but generate a microstructure (with a corresponding Young measure).

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

If $f : M^{m\times n} \to [0,\infty]$ then its quasiconvexification is defined to be the function

$$f^{\mathrm{qc}} = \sup\{g \le f : g \text{ finite and quasiconvex}\}$$

$E \subset M^{m\times n}$ is quasiconvex if there exists a quasiconvex $f : M^{m\times n} \to [0,\infty)$ with $f^{-1}(0) = E$.

If $K \subset M^{m\times n}$ is compact, its quasiconvexification is the set

$$K^{\mathrm{qc}} = \bigcap\{E \supset K : E \text{ quasiconvex}\}$$

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

There is no known characterization of quasiconvexity.

No local characterization (for example, inequalities on f and its derivatives at an arbitrary matrix A) exists (Kristensen).

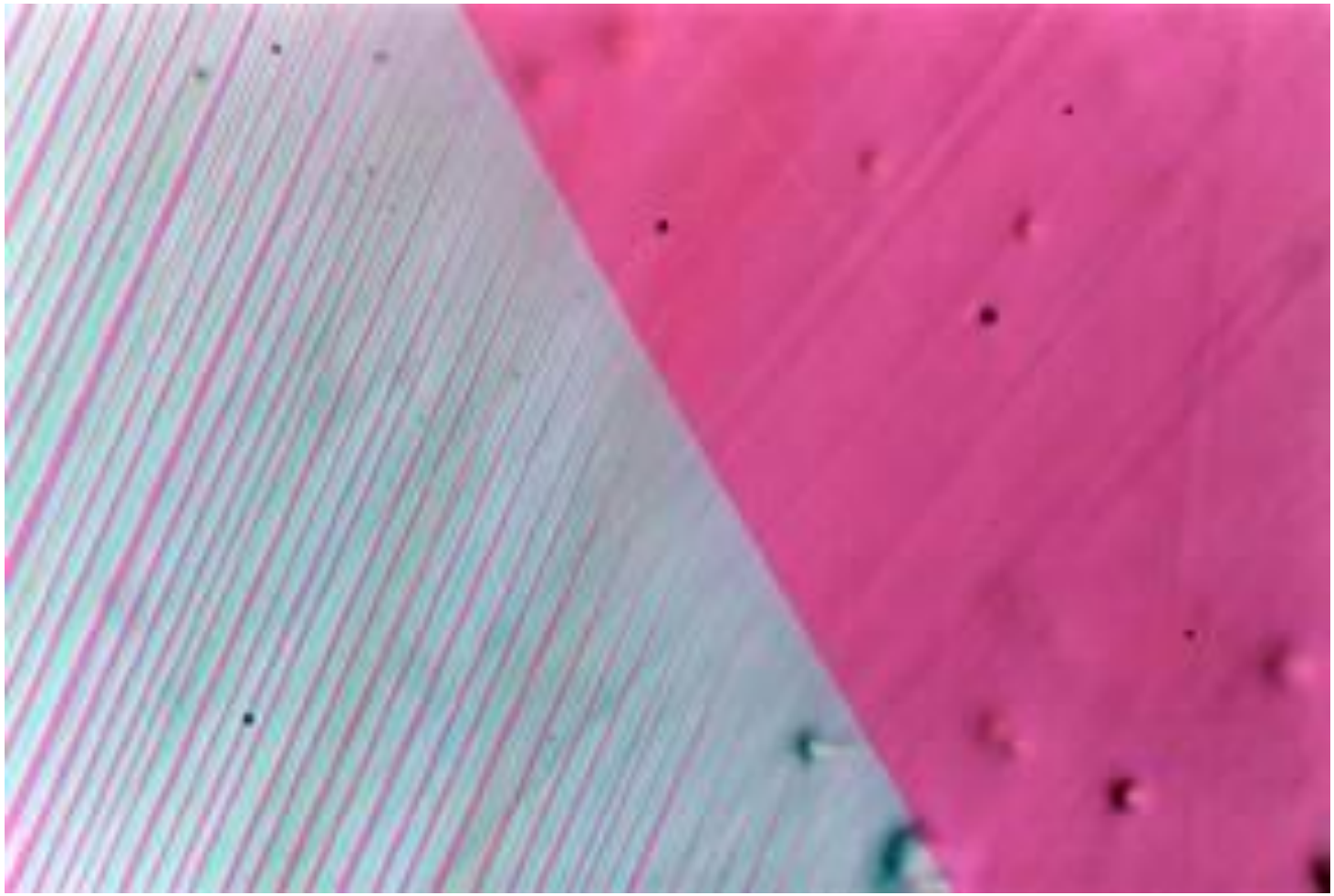
Classical austenite-martensite interfaces

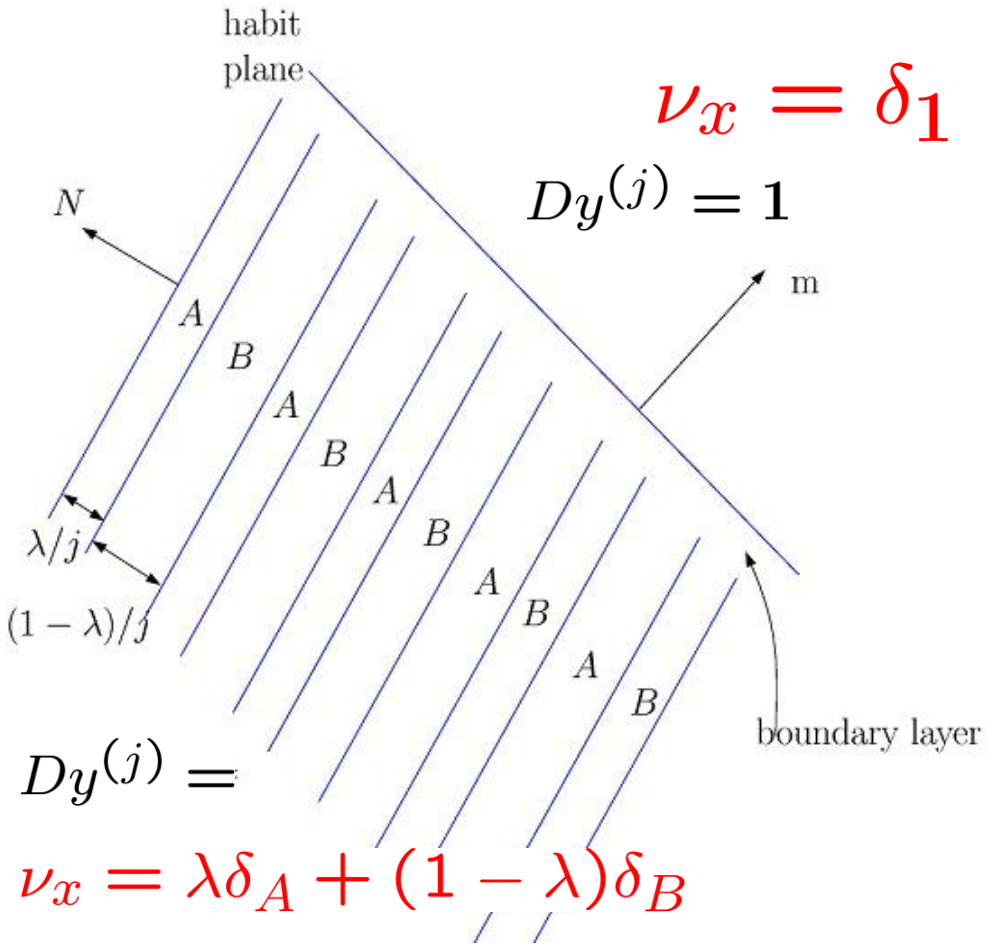
How does austenite transform to martensite as θ passes through θ_c?

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)

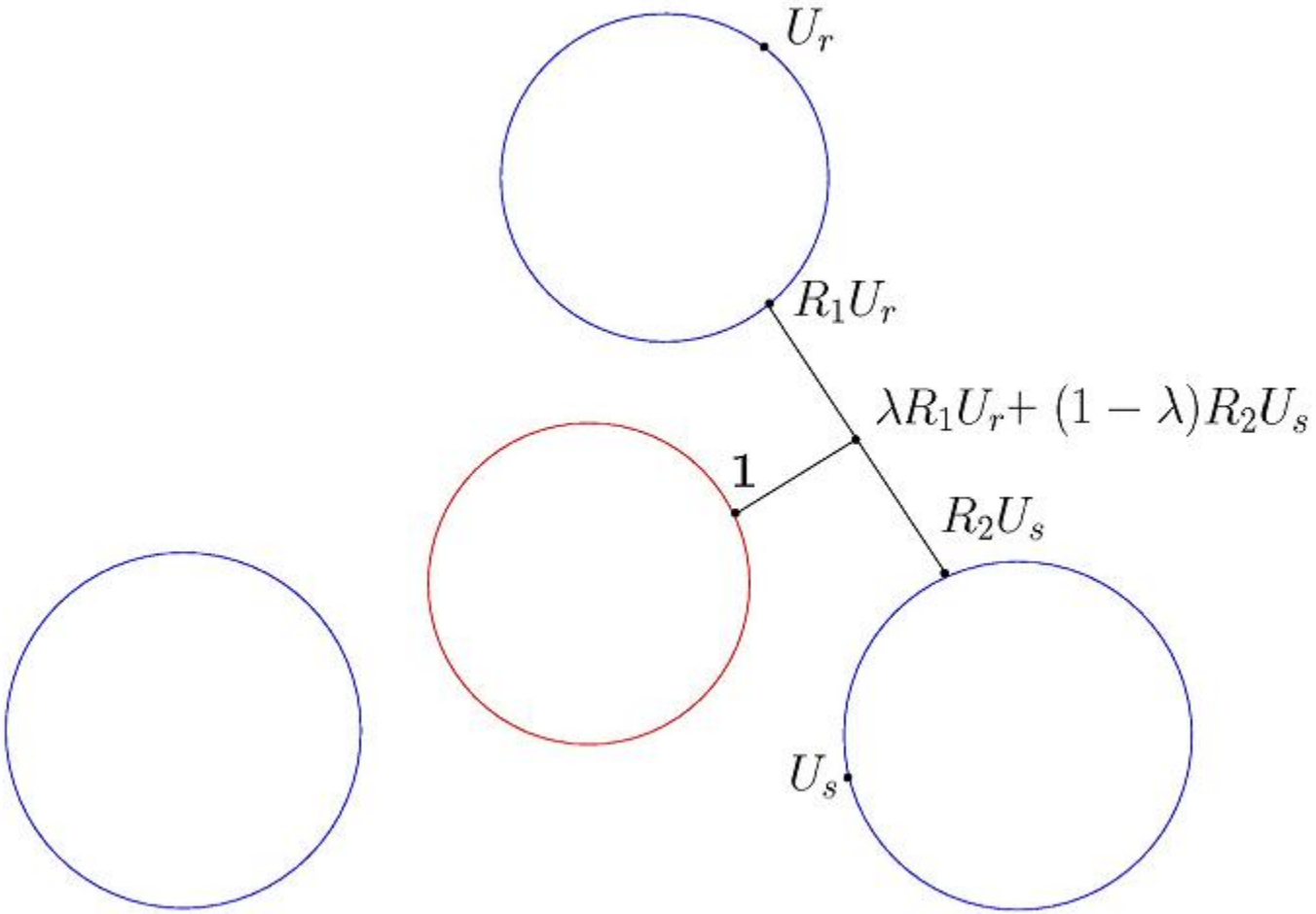


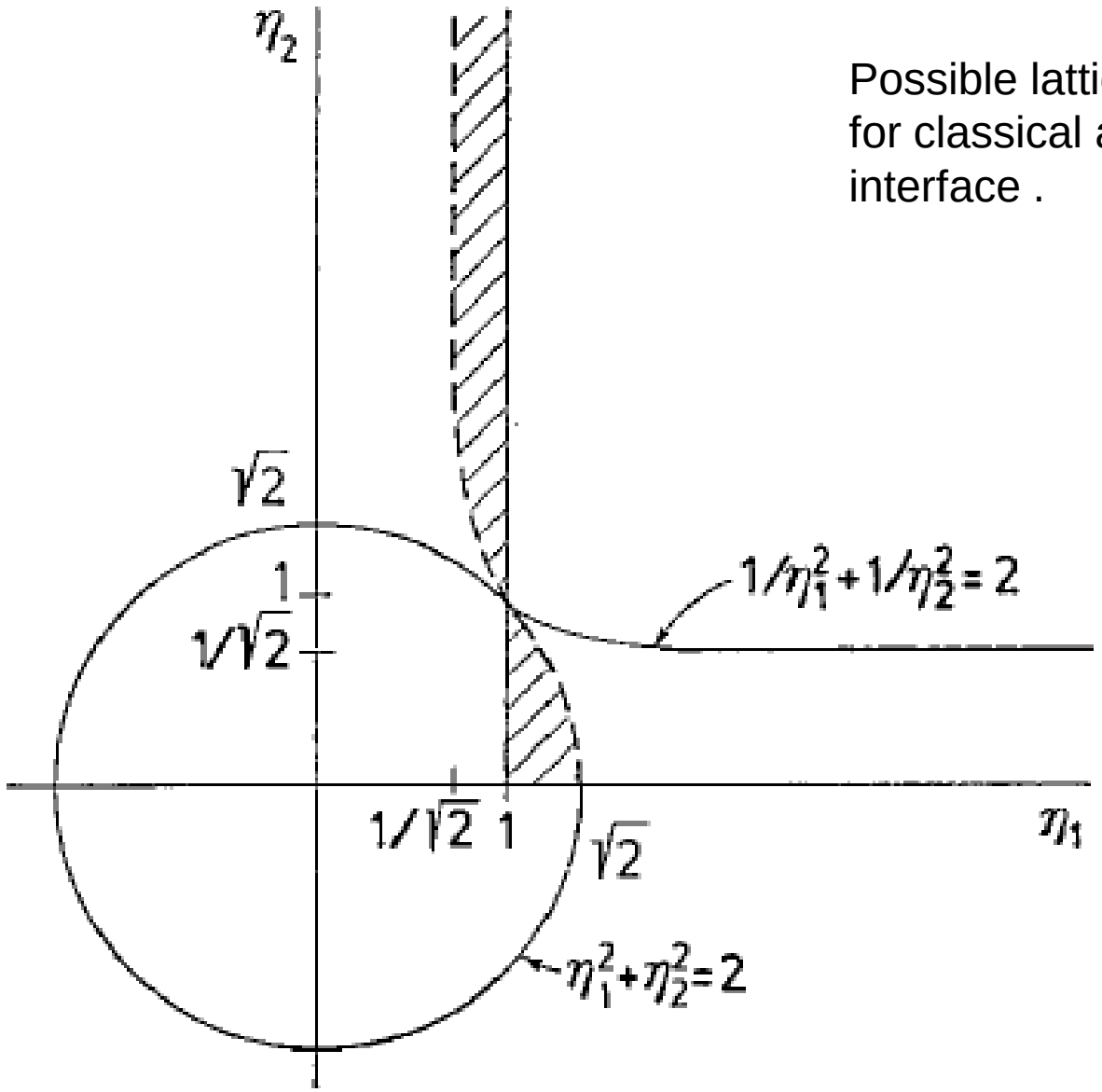


Gives formulae of the crystallographic theory of martensite (Wechsler, Lieberman, Read)

24 habit planes for cubic-to-tetragonal

Rank-one connections for A/M interface



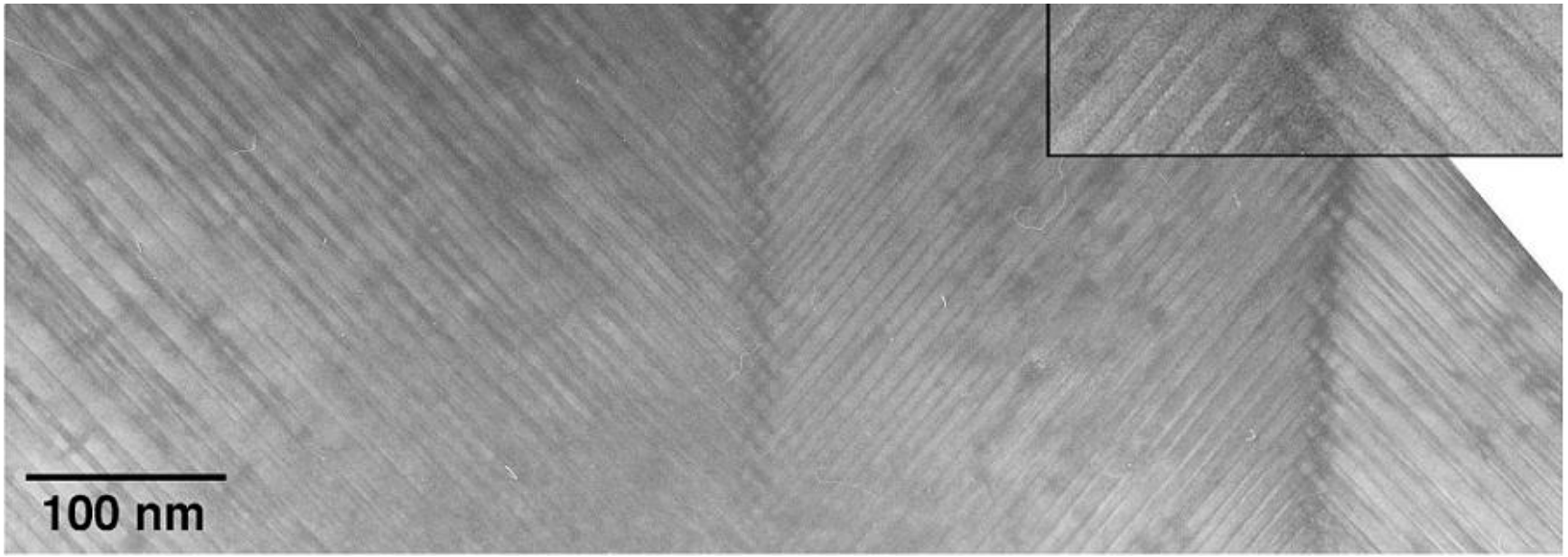


Possible lattice parameters
for classical austenite-martensite
interface .

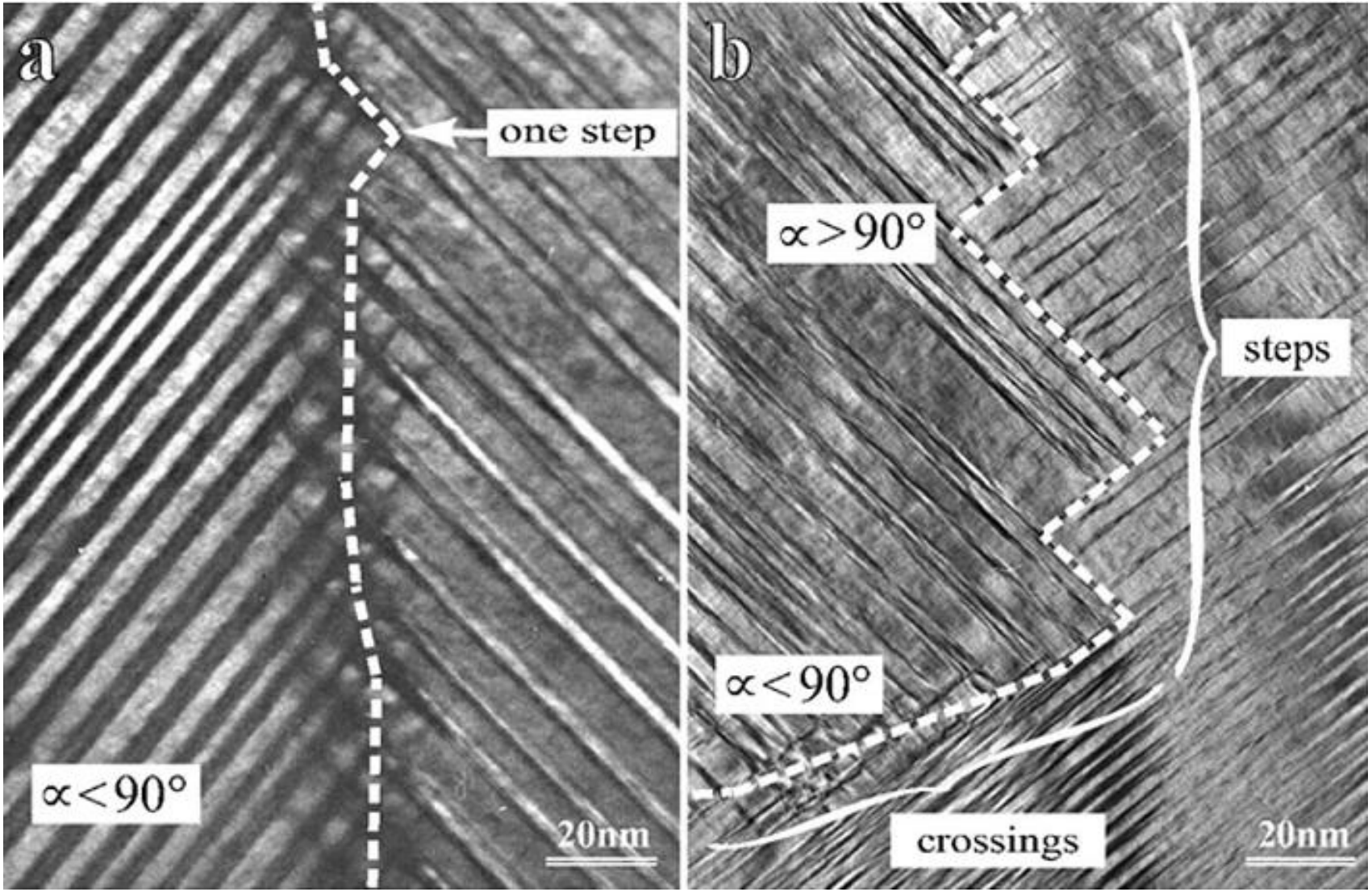
Macrotwins in $Ni_{65}Al_{35}$

JB, D. Schryvers, Ph. Boullay
(Antwerp)

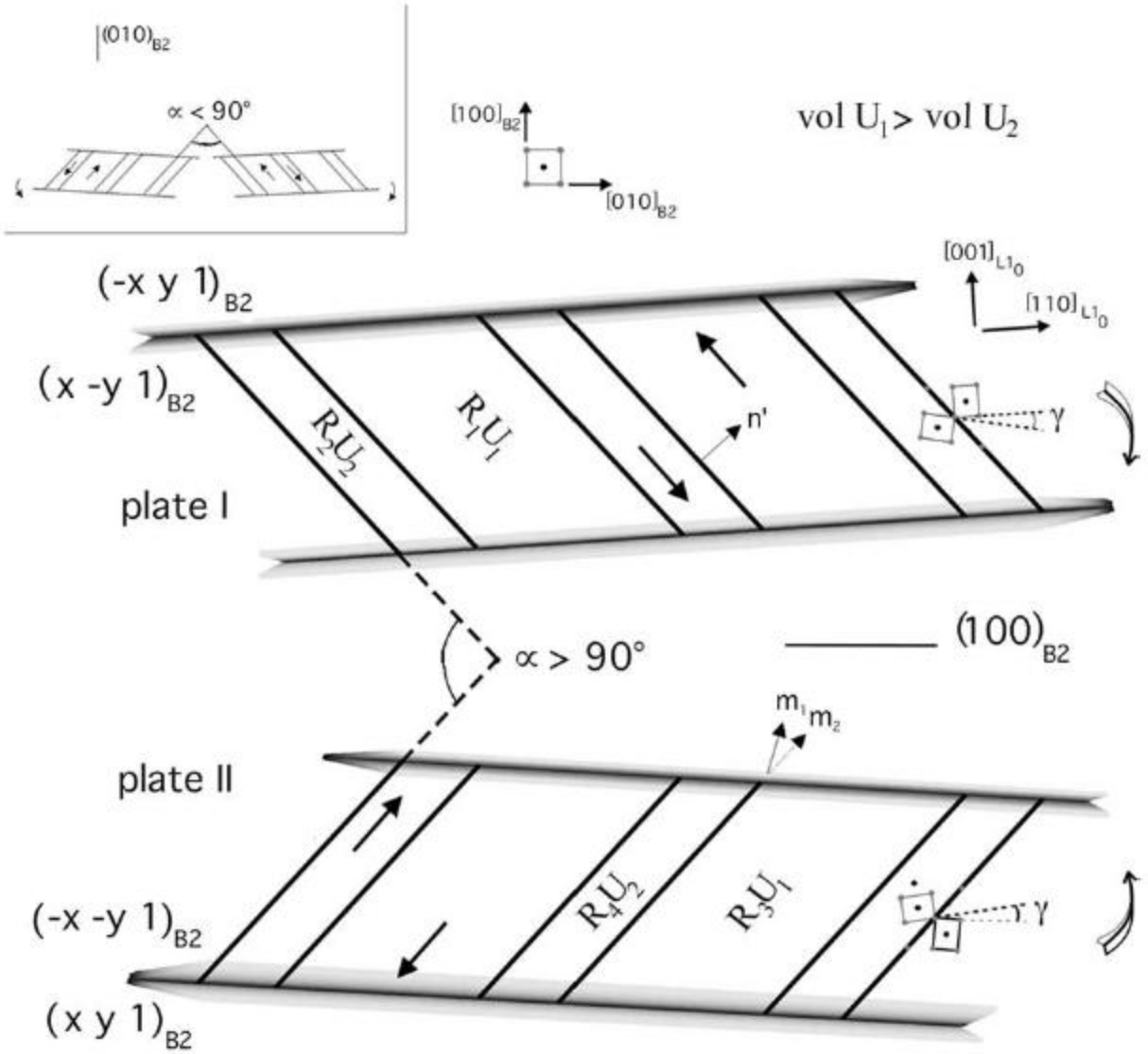
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



Crossings and steps



Macrotwin formation



Macroscopic deformation gradient in martensitic plate is

$$1 + b \otimes m$$

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

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

Different martensitic plates never compatible (Bhattacharya)

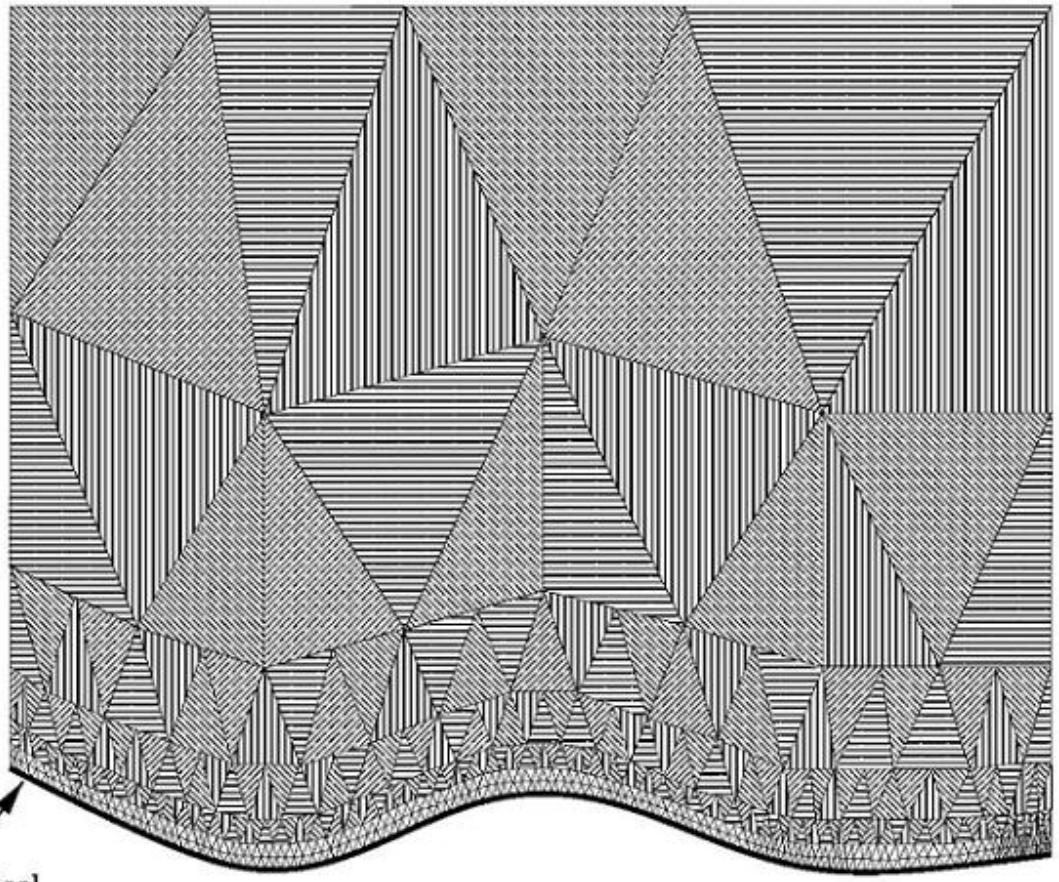
Table 1: Rotations Q_1 and Q_2 that bring Plate II into compatibility with Plate I ($\kappa_1 = \chi_1 = \nu_1 = 1$) and the corresponding macrotwin normals N_1 and N_2. The direction of rotation is that of a right-handed screw in the direction of the given axis. For the case $\kappa_2 = \nu_2 = 1, \chi_2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

JB/ Carsten Carstensen (Berlin),
Konstantinos Koumatos (Oxford),
Hanus Seiner (Prague).

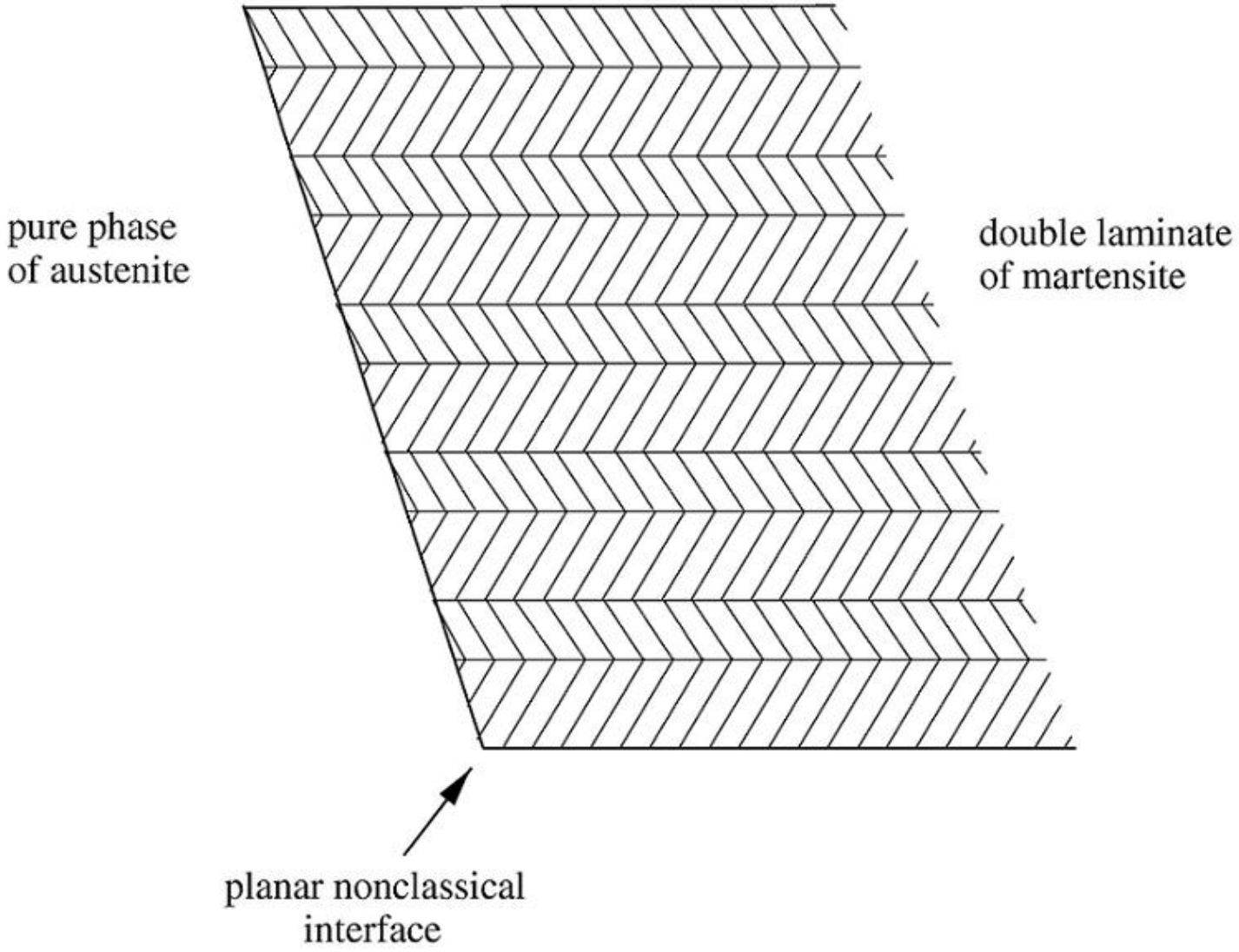
Nonclassical austenite-martensite interfaces (B/Carstensen 97)



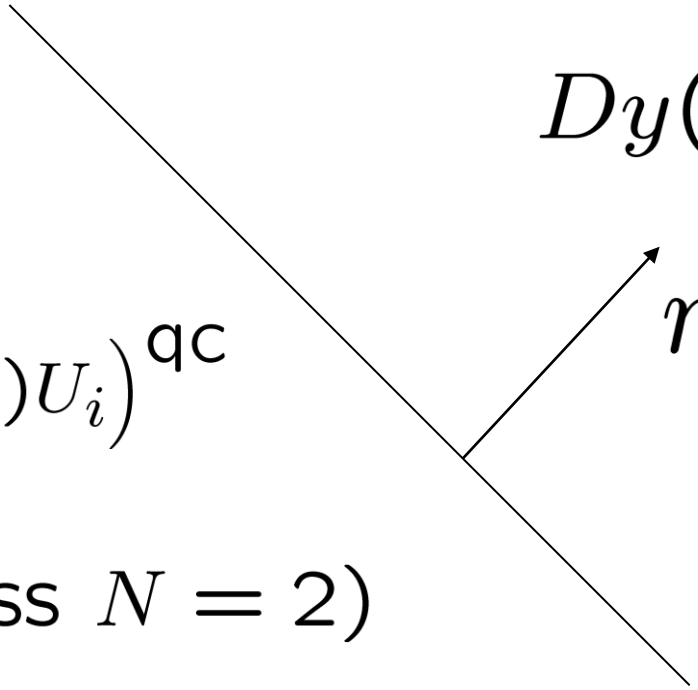
speculative nonhomogeneous martensitic microstructure with fractal refinement near interface

curved nonclassical interface

Nonclassical interface with double laminate



Nonclassical interface calculation



$Dy(x) = 1$

m

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

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

$\nu_x = \delta_1$

(unknown unless $N = 2$)

$\nu_x = \nu$

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

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

More on quasiconvexifications

Let $K \subset M^{m\times n}$ be compact. Then

$$\begin{aligned} K^{qc} &= \{F \in M^{m\times n} : F = \bar{\nu}, \nu \text{ a homogeneous} \\ &\qquad \text{gradient Young measure with } \operatorname{supp}\nu \subset K\} \\ &= \{F \in M^{m\times n} : \varphi(F) \le \max_{G\in K} \varphi(G) \text{ for all quasiconvex } \varphi\} \end{aligned}$$

φ is *polyconvex* if $\varphi(F) = g(\mathbf{J}(F))$ for some convex function g of the list $\mathbf{J}(F)$ of all minors of F. Thus if $m = n = 3$, φ is polyconvex if

$$\varphi(F) = g(F, \operatorname{cof} F, \det F)$$

for some convex g.

φ polyconvex $\Rightarrow$ φ quasiconvex.

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

$$K^{qc} \subset K^{pc}$$

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

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

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 $\varphi(G) = \sigma_{\mathsf{max}}(\mathrm{cof}\, G)$, which is a convex function
of $\mathrm{cof}\,(G)$ 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

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

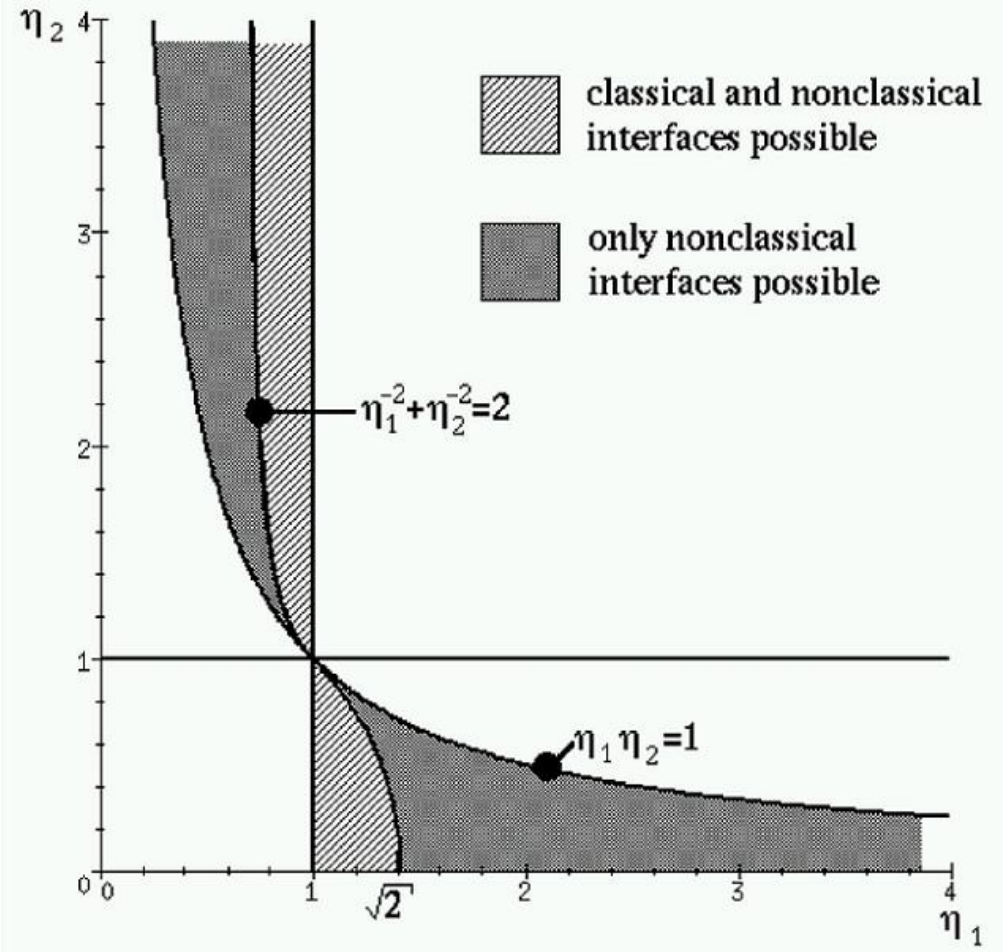
and the necessary conditions become

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

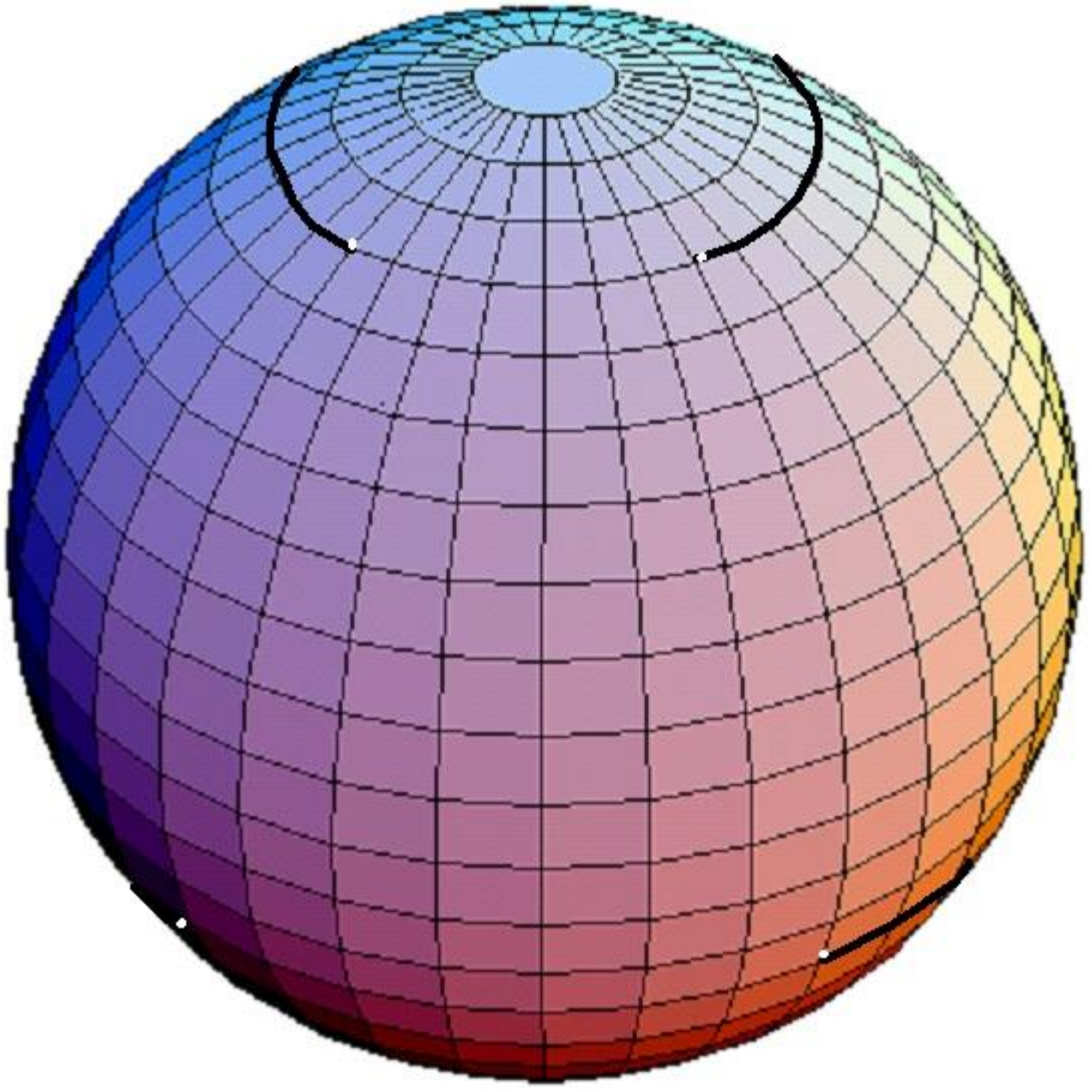
$$\eta_2 \leq \eta_1^{-1} \leq \eta_1 \text{ if } \eta_1 \geq \eta_2.$$

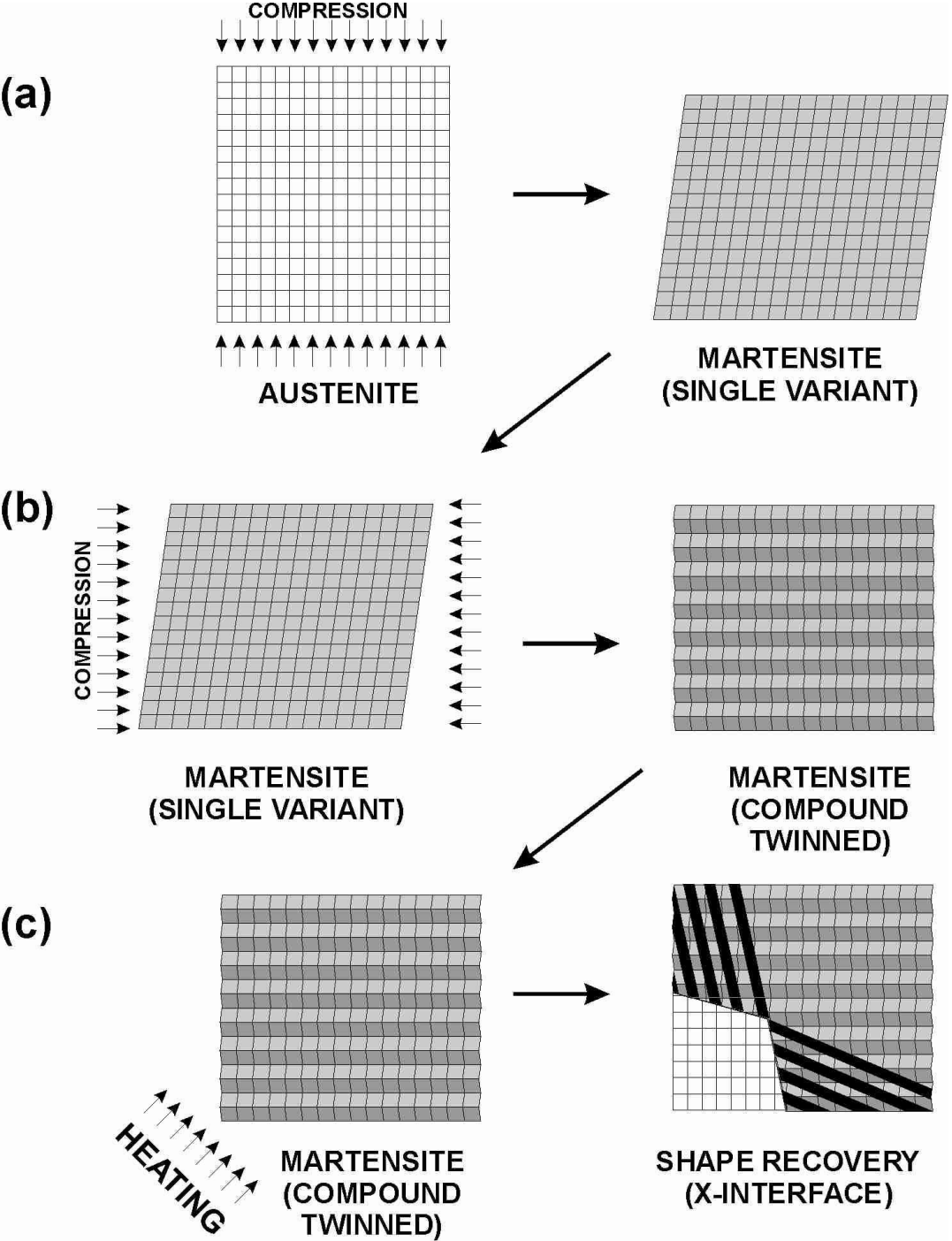
But these turn out to be exactly the conditions given by the two-well theorem to construct a rank-one connection from $(SO(3)U_1 \cup SO(3)U_2)^{qc}$ to the identity!
Hence the conditions are sufficient also.

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



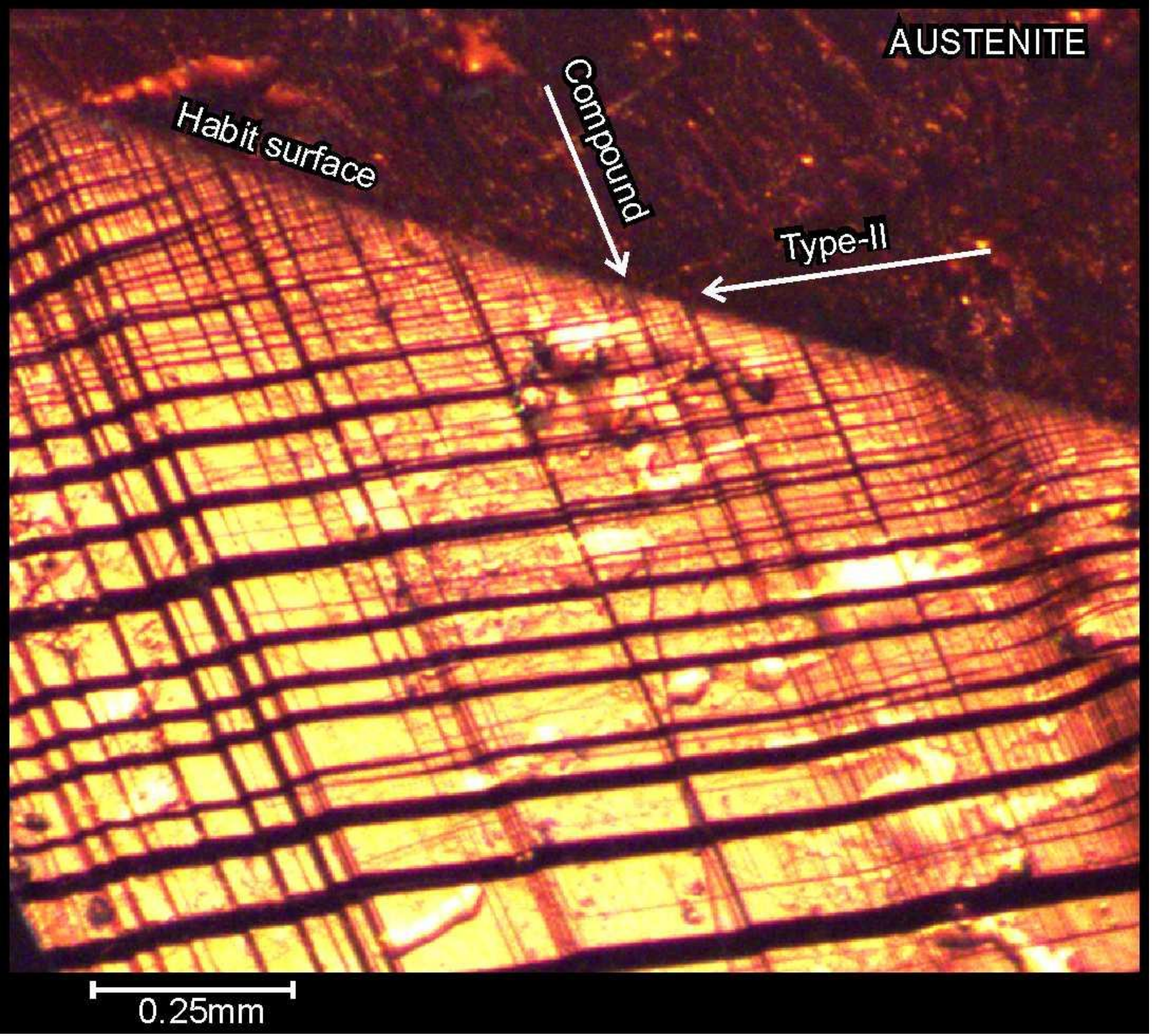
Interface normals





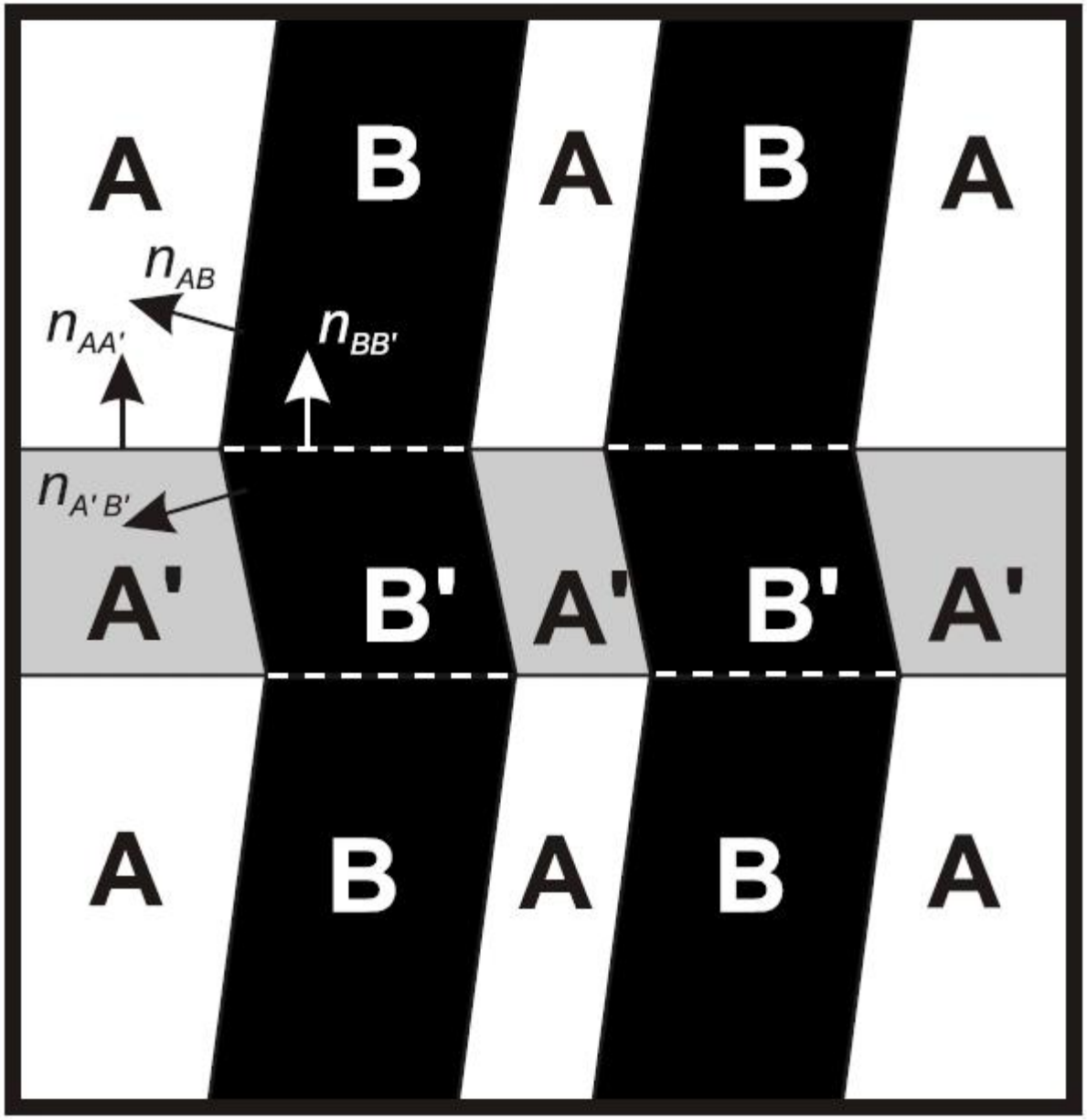
Experimental procedure (H. Seiner)

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

Cubic-to-orthorhombic energy wells

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

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

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

$$\alpha = 1.06372, \ \beta = 0.91542, \ \gamma = 1.02368$$

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

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

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

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

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

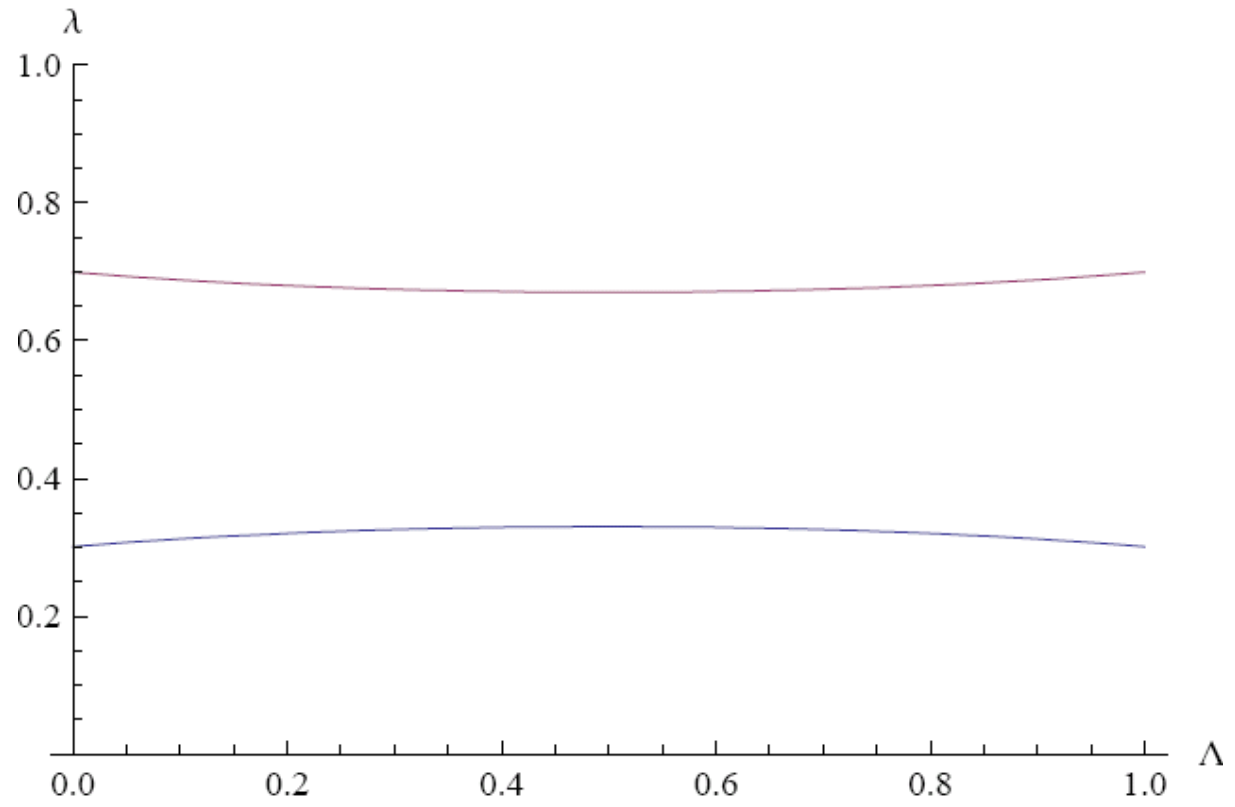
$$M = (1-\Lambda)M_{AB} + \Lambda R_{AA'} M_{A'B'}.$$

For compatibility with the austenite we need

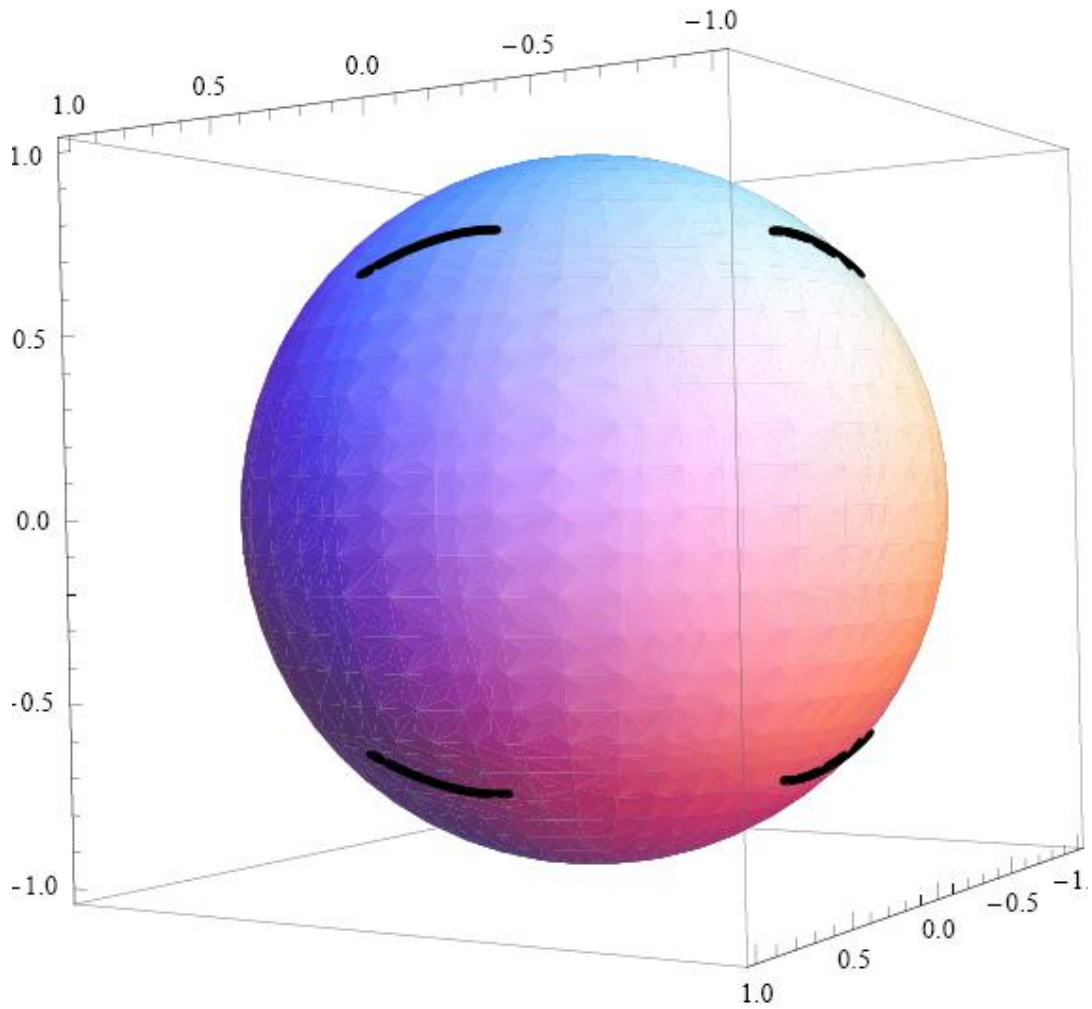
$$\lambda_{\text{mid}}(M^T M) = 1$$

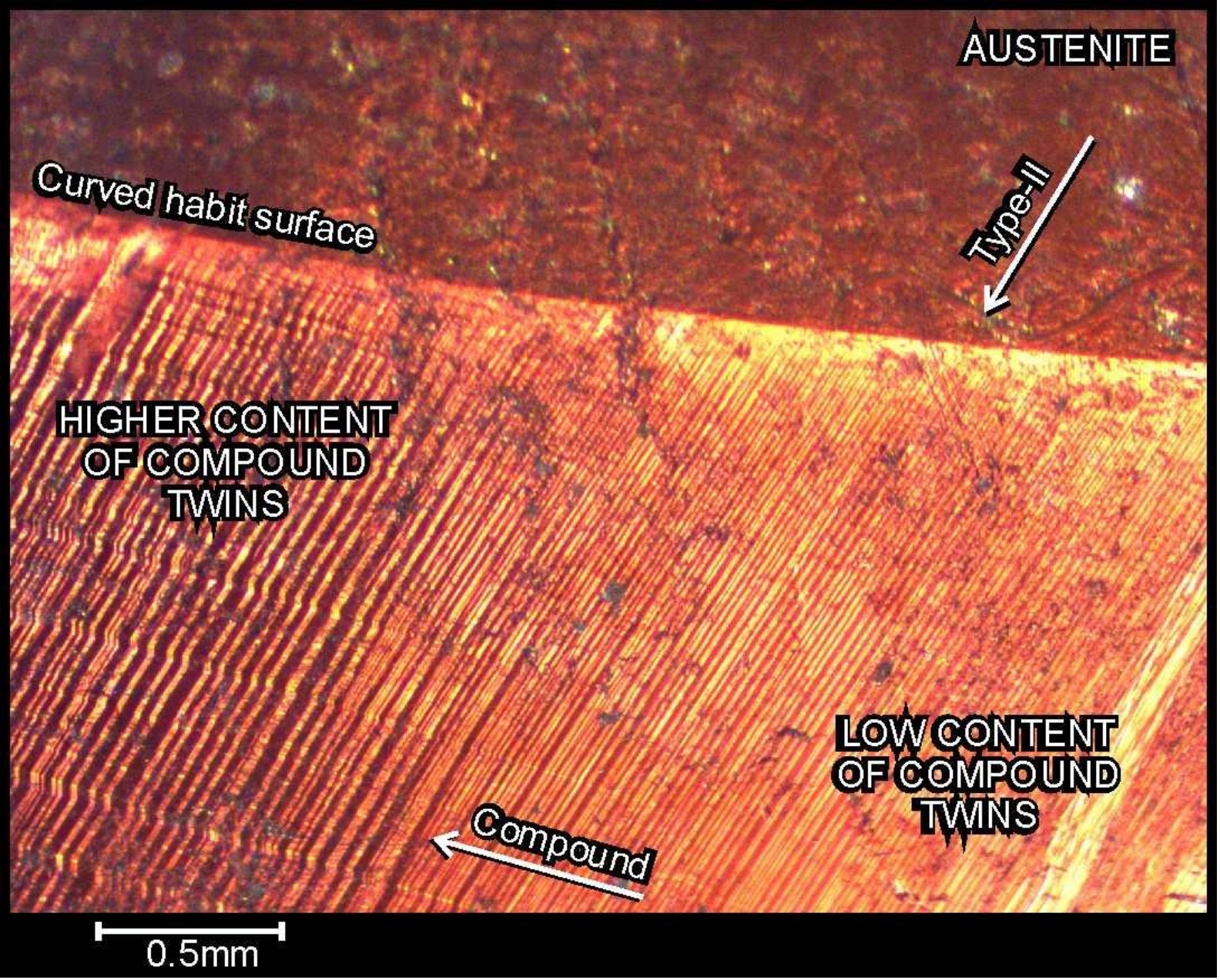
Possible volume fractions

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



Possible nonclassical interface normals





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

Construction of curved interface

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

Nucleation of austenite in mechanically stabilized martensite by localized heating

JB, Konstantinos Koumatos

Hanus Seiner

Mechanically stabilized martensite

The shape-recovery process in shape-memory alloys (SMAs) concerns the thermally driven transition from the low temperature phase (martensite) into the high-temperature phase (austenite). For many SMAs, the critical temperature for initiation of the shape-recovery process depends strongly on the microstructure of the martensite.

In particular, if the martensite is mechanically treated so that it is more difficult for it to make a compatible interface with the austenite, the critical temperature is shifted significantly upwards. This effect is called *the mechanical stabilization of martensite* and occurs for both single crystals and polycrystalline SMAs.

It is natural to seek an explanation for this effect in terms of local minimizers y of

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

Experimental observations

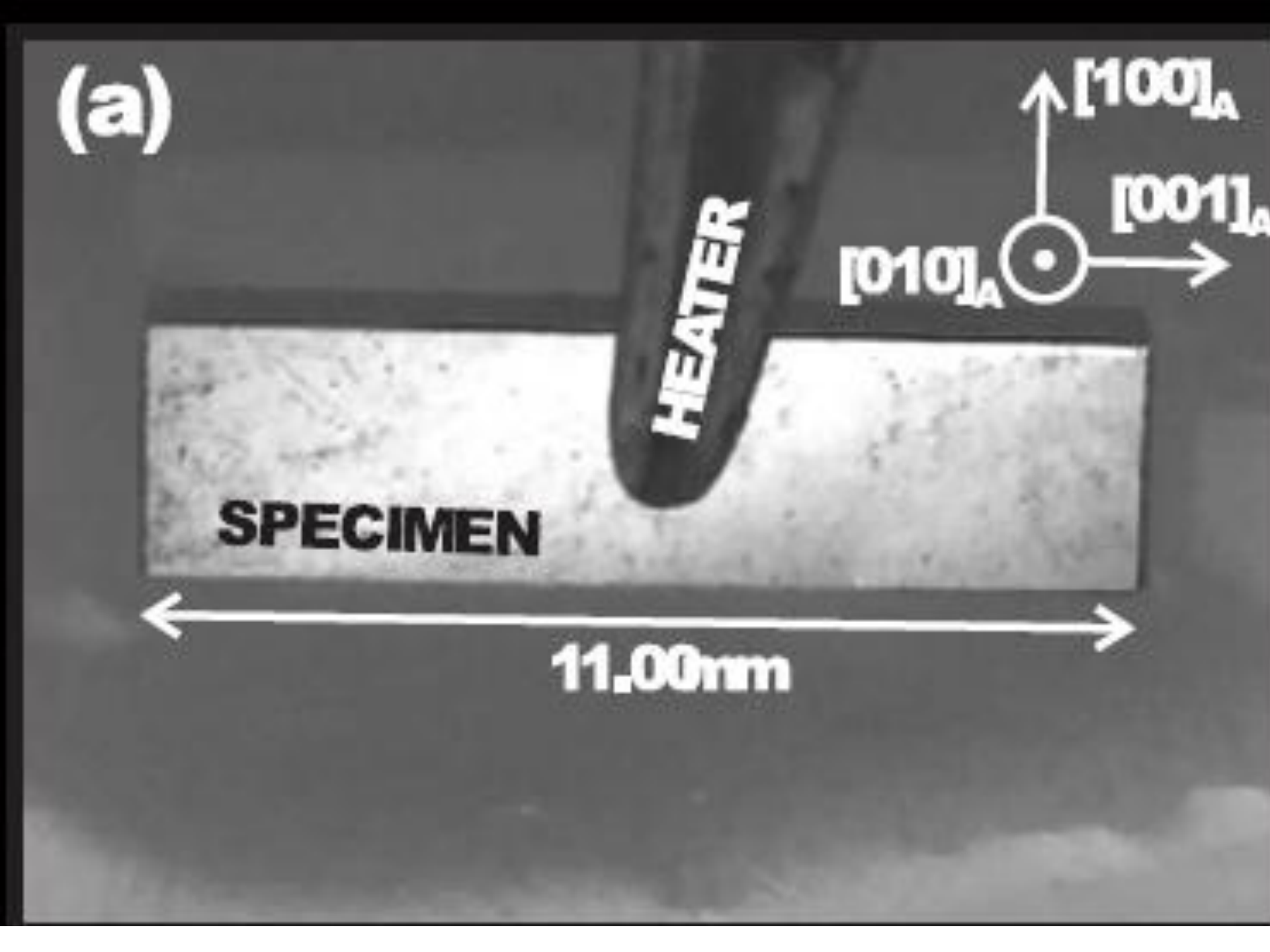
Specimen: single crystal of CuAlNi prepared by the Bridgeman method in the form of a prismatic bar of dimensions $12 \times 3 \times 3 mm^3$ in the austenite with edges approximately along the principal cubic directions.

By unidirectional compression along its longest edge, the specimen was transformed into a single variant of mechanically stabilized 2H martensite. Due to the mechanical stabilization effect the reverse transition did not occur during unloading.

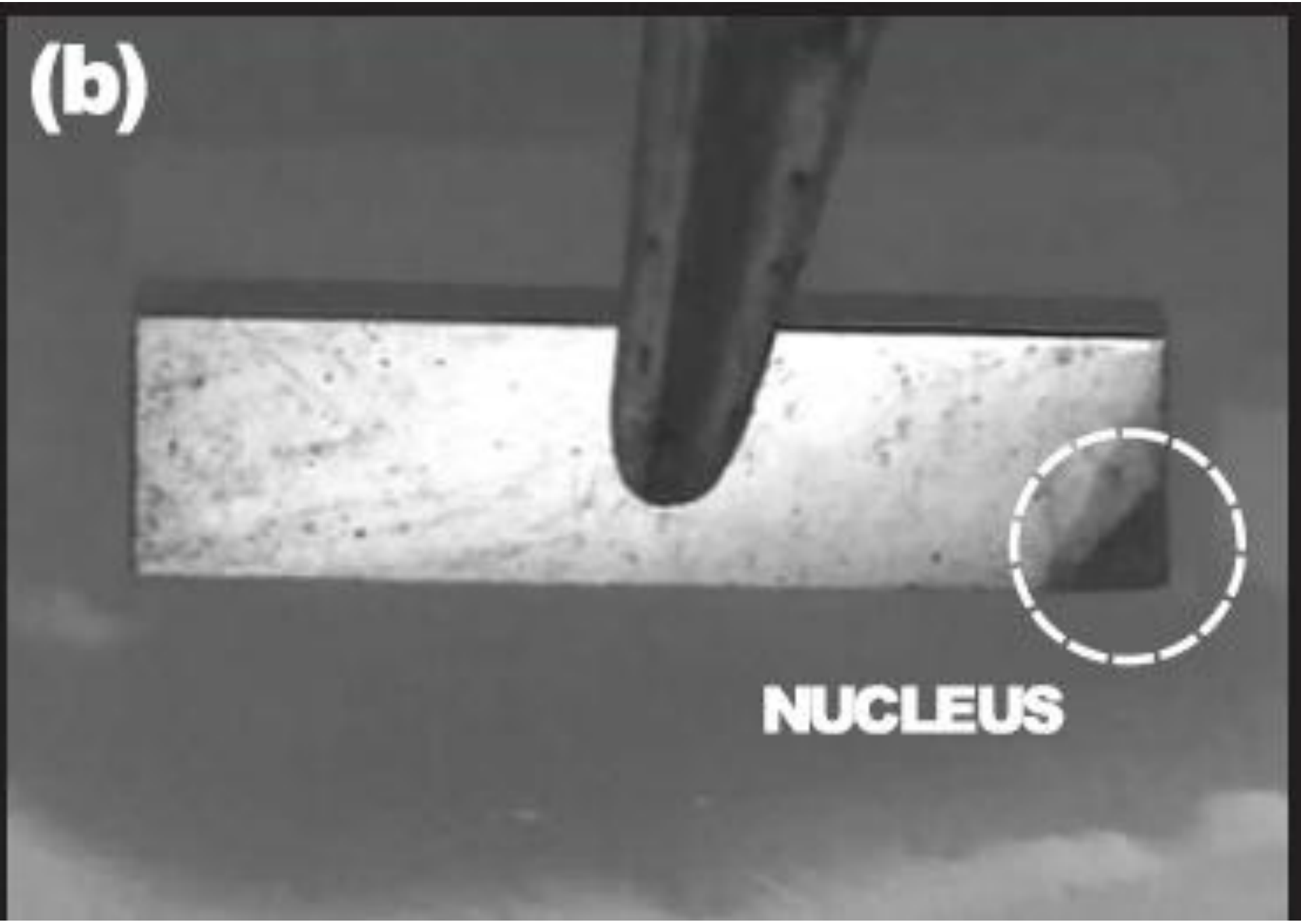
The martensite-to-austenite transition temperatures determined by DSC were $A_S = -6°C$ and $A_F = 22°C$. The critical temperature T_C for the transition from the stabilized martensite induced by homogeneous heating for this specimen was $\sim$60°C. This was estimated from optical observations of the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

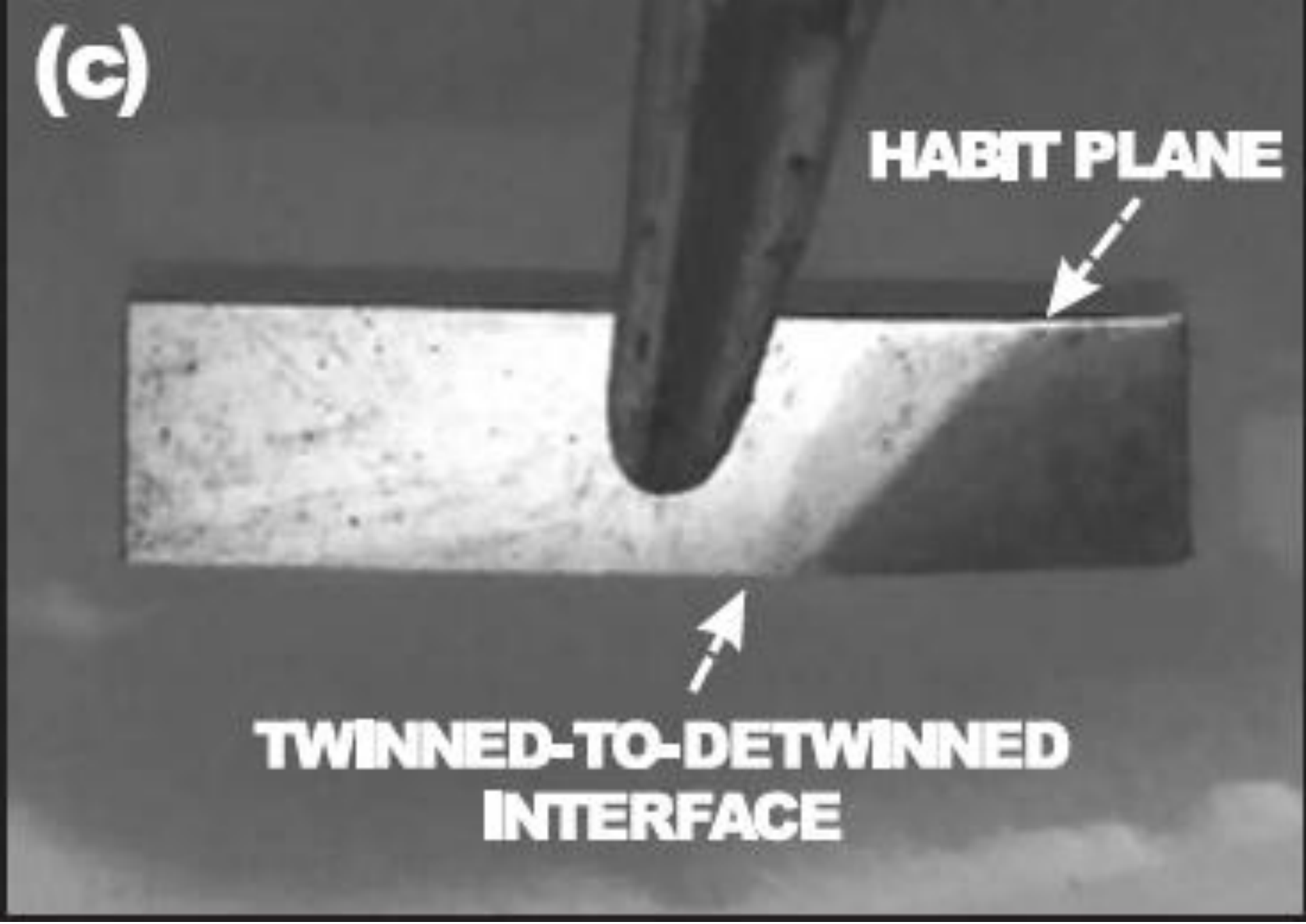
Localized heating experiment

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


(a)
[100]A
[001]A
[010]A
HEATER
SPECIMEN
11.00mm

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 $> T_C$).


(b)
NUCLEUS


(c)
HABIT PLANE
TWINNED-TO-DETWINNED
INTERFACE

In terms of Young measures the total free energy takes the form

$$I_\theta(\nu) = \int_\Omega \int_{M^{3\times 3}} \psi(A,\theta)\, d\nu_x(A)\, dx$$

We fix θ to be the temperature of the probe. Then it is reasonable to assume that $\min_A \psi(A,\theta) = -\delta < 0$ and that

$$\psi(A,\theta) = \begin{cases} -\delta & \text{if } A \in SO(3) \qquad\qquad \text{(austenite)}, \\ 0 & \text{if } A \in \bigcup_{i=1}^{6} SO(3)U_i \quad \text{(martensite)}. \end{cases}$$

Here the U_i are the six orthorhombic variants given by

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

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

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 (cf Ball & Marsden 1981) 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.

Then $I = I_\theta$ becomes

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

where

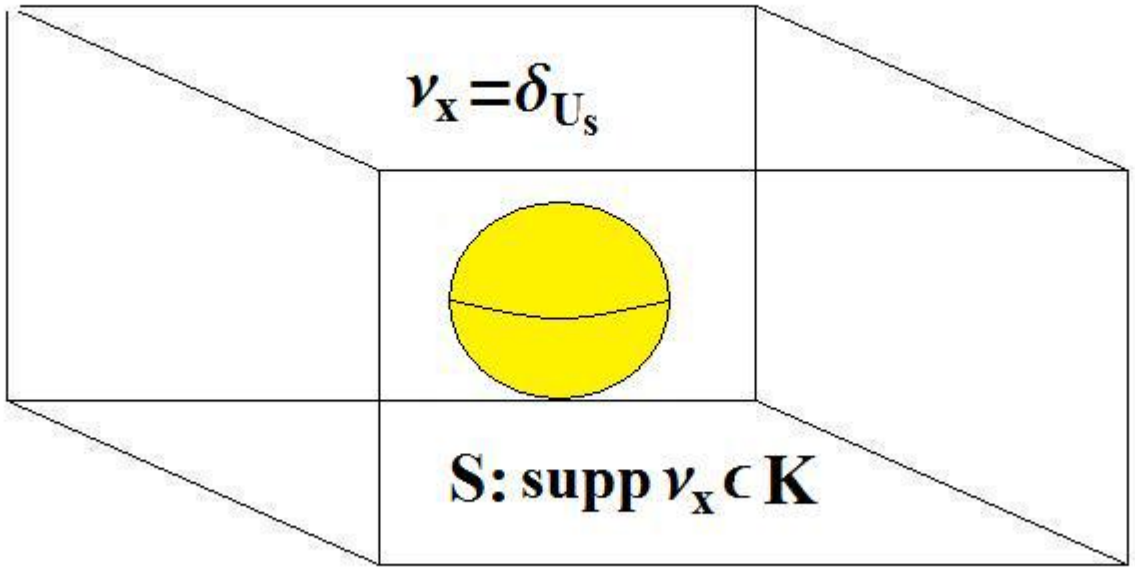
$$W(A) = \begin{cases} -\delta & A \in SO(3) \\ 0 & A \in \bigcup_{i=1}^{6} SO(3)U_i \\ +\infty & \text{otherwise} \end{cases},$$

and $\delta > 0$.

So $W(A) < \infty$ on

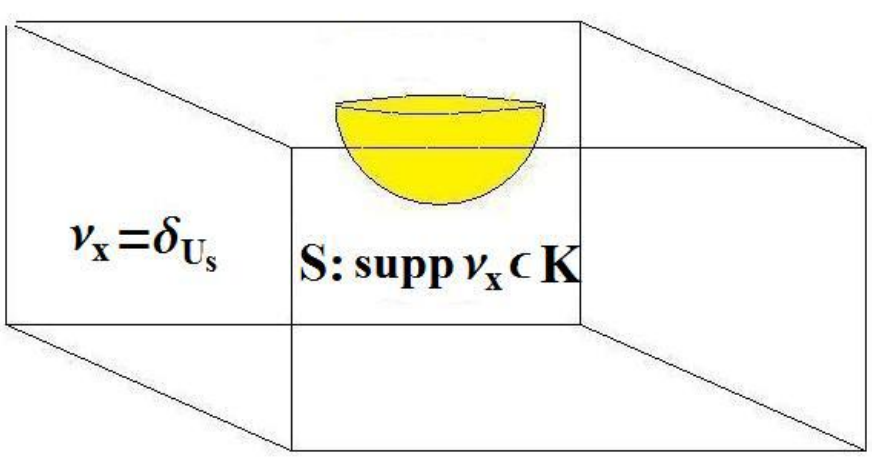
$$K = SO(3) \cup \bigcup_{i=1}^{6} SO(3)U_i$$

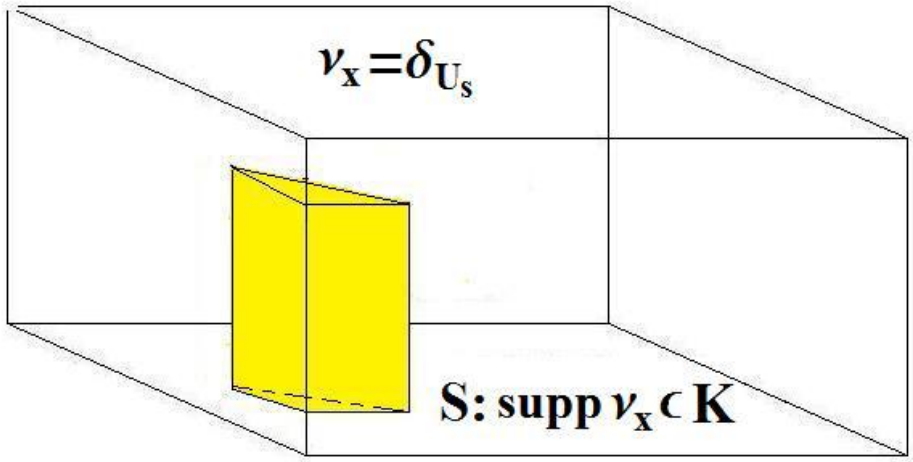
Nucleation impossible in the interior



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

Nucleation impossible at faces or edges

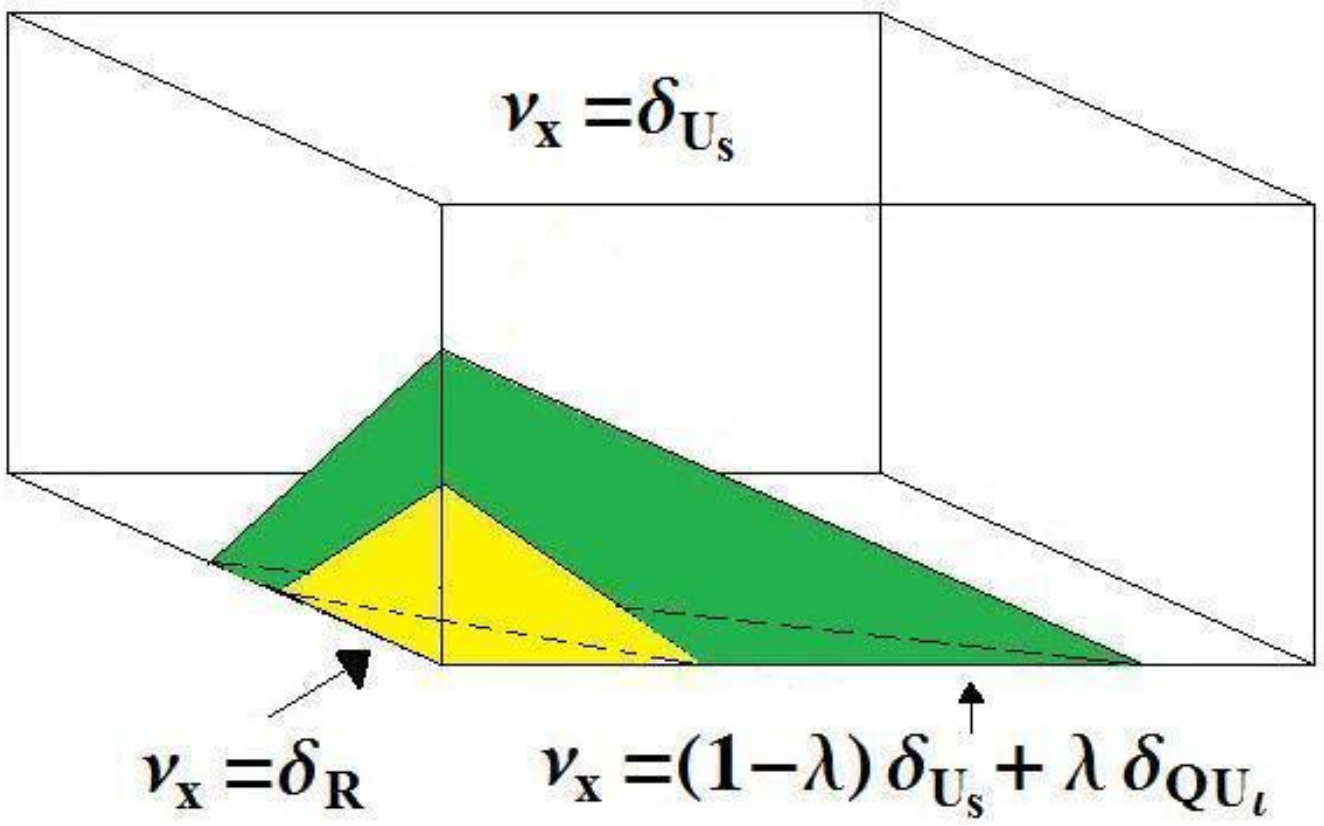




Similarly in these cases we have

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

Nucleation possible at a corner

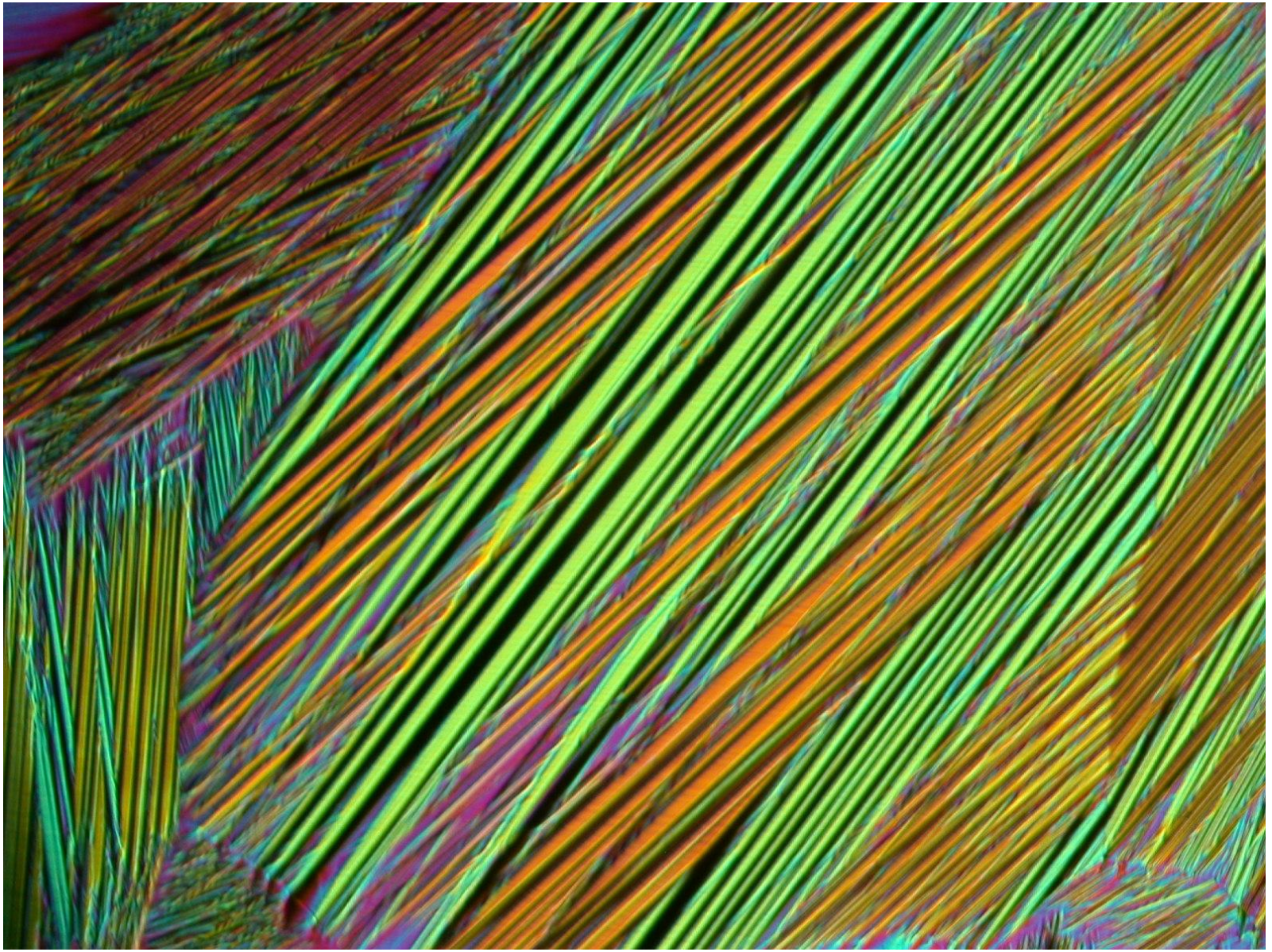


$I(\nu) < I(\delta_{U_s})$

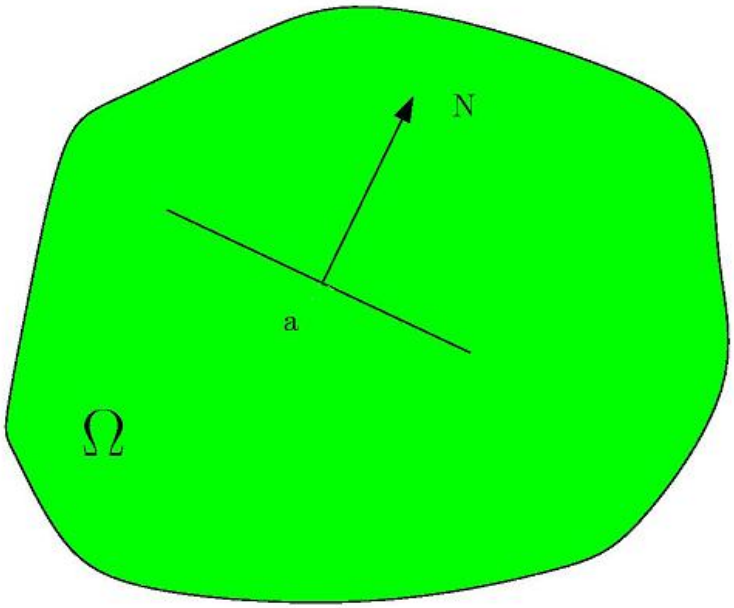
I *not* quasiconvex at a corner.

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?
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.

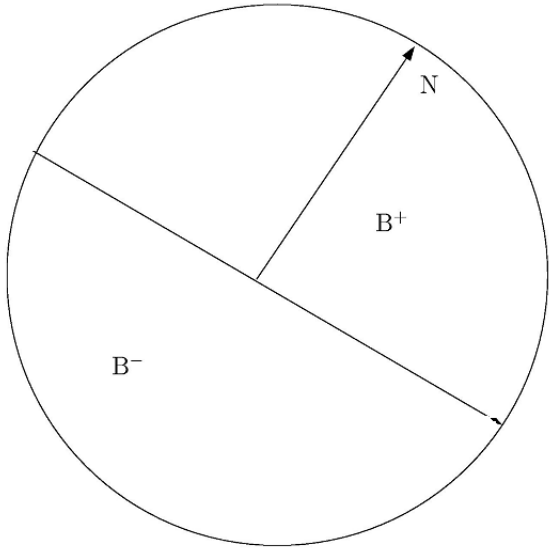


CuZnAl microstructure: Michel Morin (INSA de Lyon)



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

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



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

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

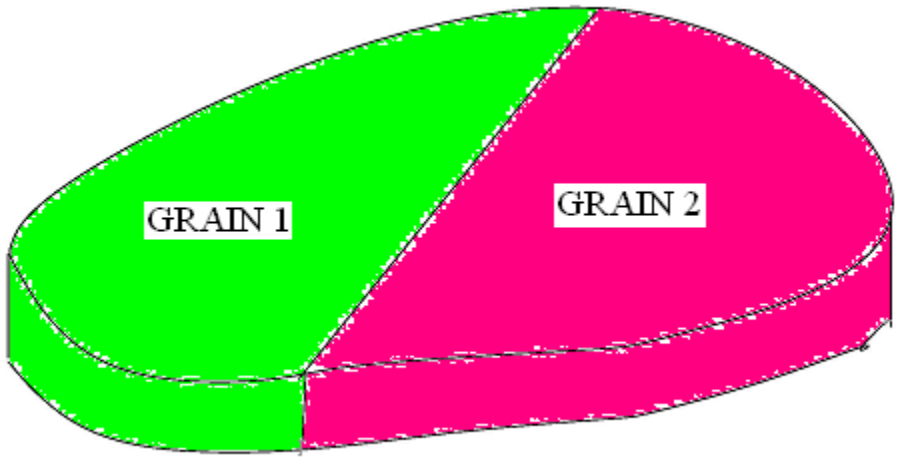
Theorem 1 (B/Carstensen). *There exists* $b \in \mathbf{R}^n$ *with* $b \otimes N \in Dy^+(a)^c - Dy^-(a)^c$.

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

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

Application to bicrystal microstructure

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



Grain 1

$\operatorname{supp} \nu_x \subset K(\theta)$

Grain 2

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

$$R_\alpha e_3 = e_3$$

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

In general one cannot have a pure variant of martensite in both grains, and if the interface between grains is suitably curved have a pure variant in either grain. This is some kind of justification as to why we typically see microstructure in grains.

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

Adding interfacial energy to the nonlinear elasticity model

The nonlinear elasticity model for martensitic transformations is based on a total free-energy functional

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

In general the minimum of I_θ is not attained, and minimizing sequences $y^{(j)}$ generate an infinitely fine microstructure, some of whose features can be described by a gradient Young measure $(\nu_x)_{x\in\Omega}$.

This is good because it provides an explanation of why very fine microstructures are observed, but bad

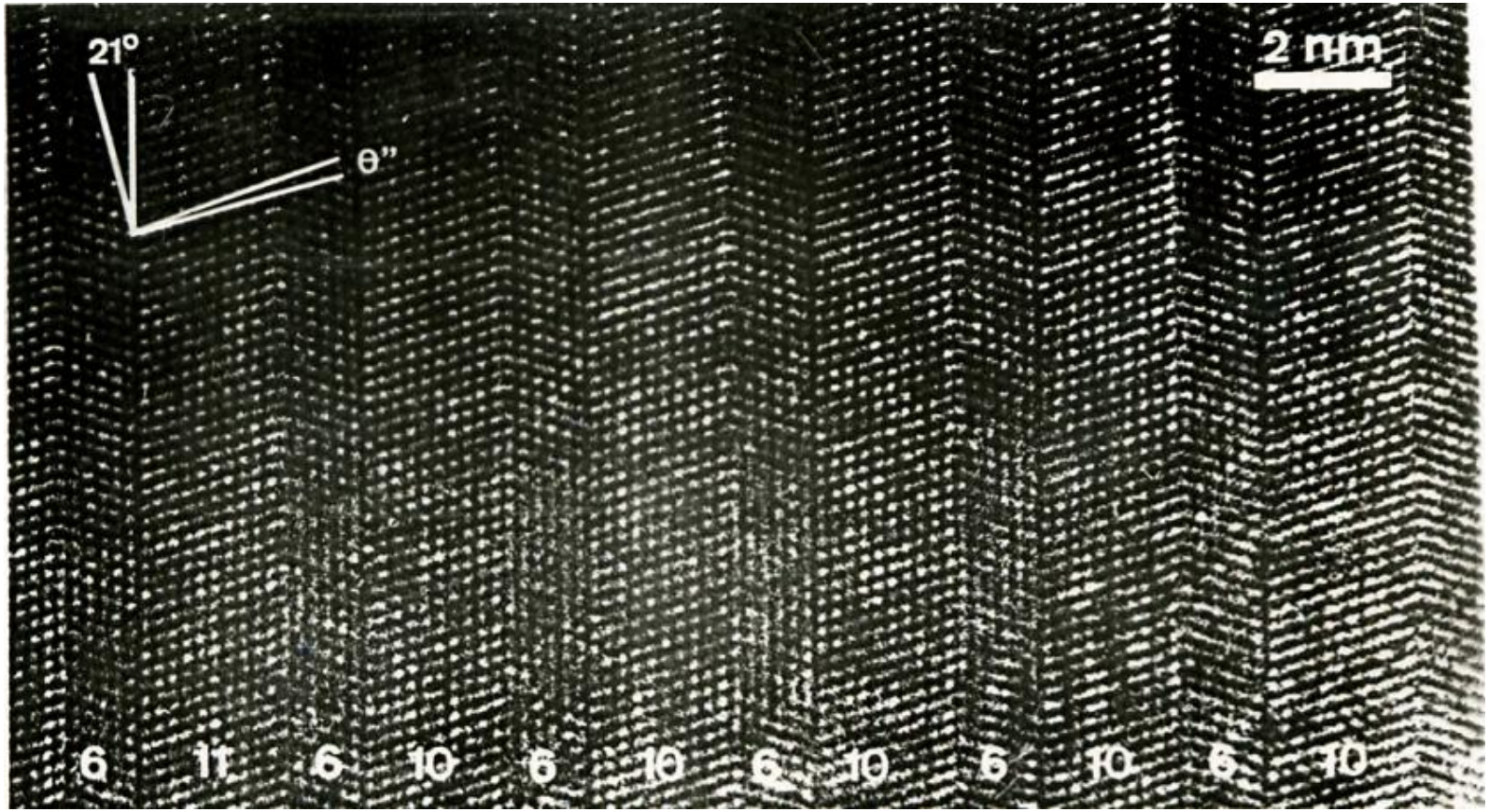
(a) because real microstructures are not infinitely fine, and have characteristic length-scales,

(b) because the minimum is not attained.

These issues can be addressed by adding to the free-energy functional a term representing interfacial energy, resulting from the different atomic environment at twin boundaries and/or lattice curvature.

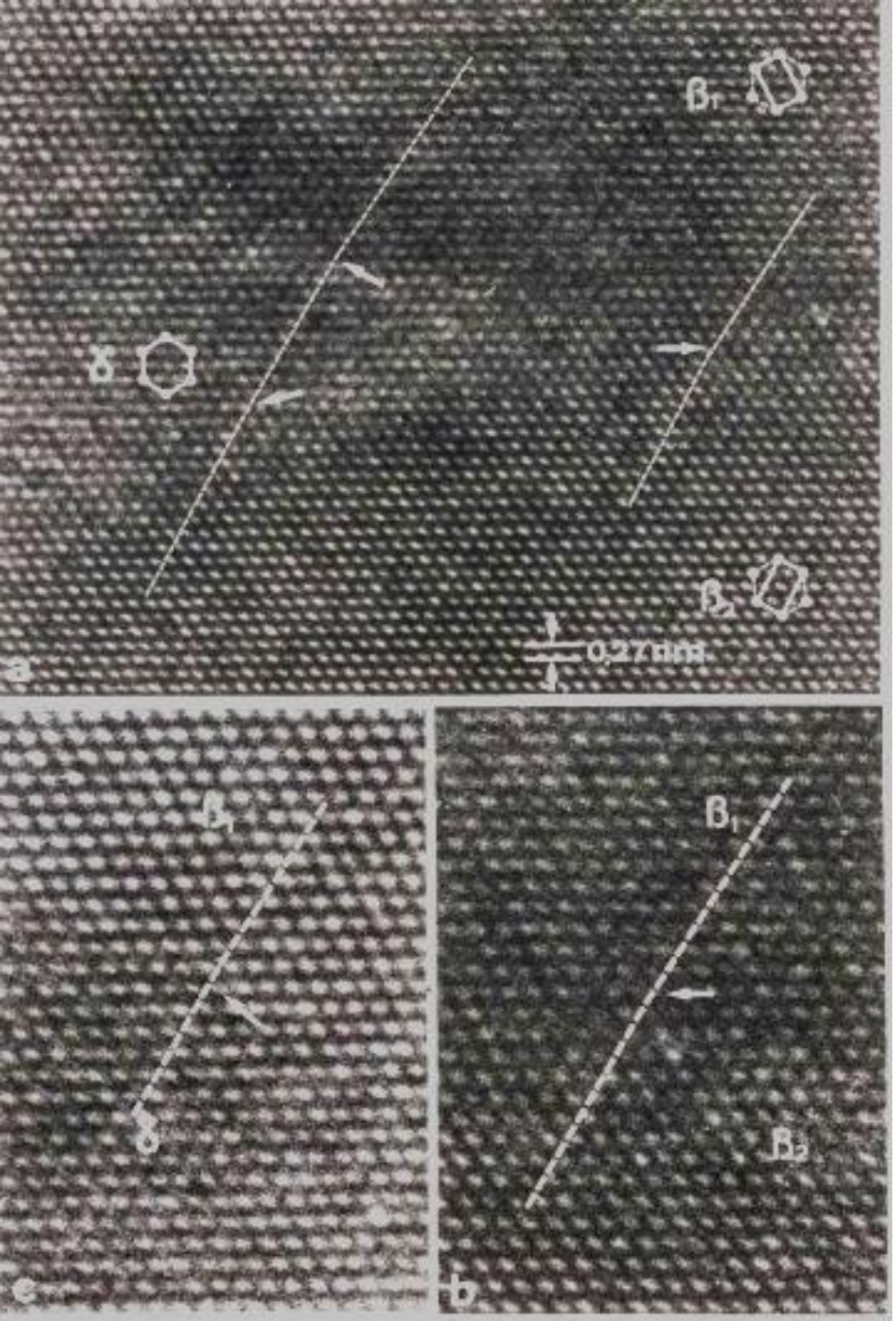
The natural way to try to understand what form the interfacial energy should take is via passage from an atomistic to a continuum model, but there is some confusion as to how this should be done.

Some interfaces are atomistically sharp



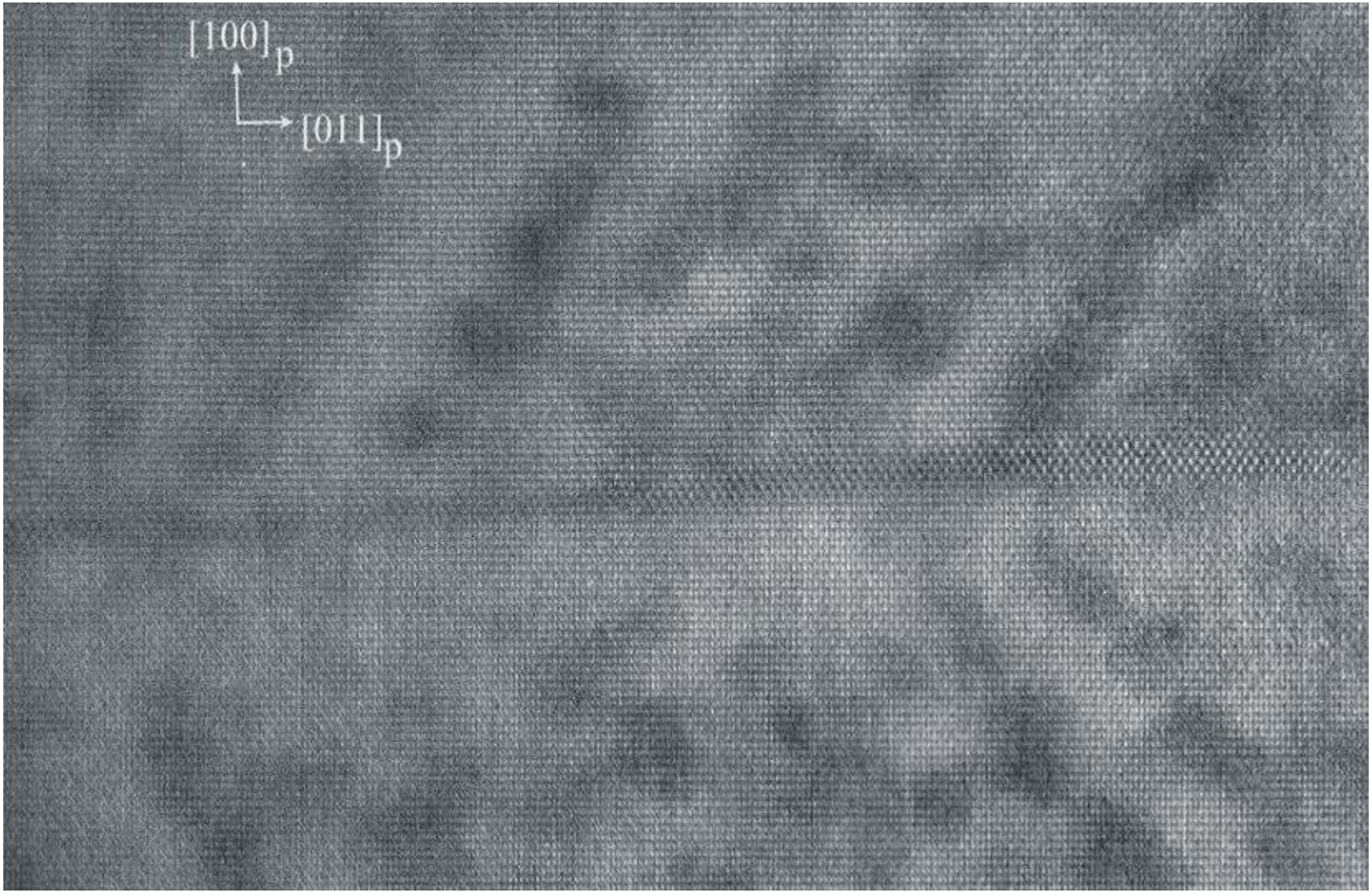
NiMn Baele, van Tenderloo, Amelinckx

while others are diffuse …



Diffuse (smooth) interfaces in $Pb_3V_2O_8$

Manolikas, van Tendeloo, Amelinckx

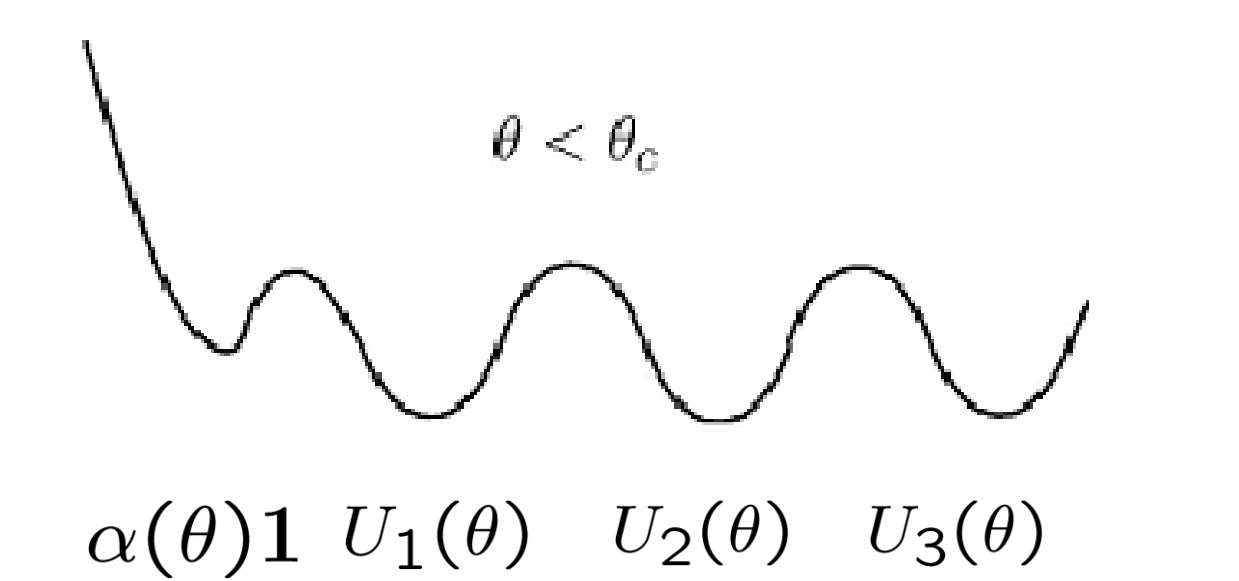


Diffuse interface in perovskite (courtesy Ekhard Salje)

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 $\alpha = \alpha(\theta)$.

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.

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

More precisely,

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

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

Remark.

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

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

by Friesecke, James, Müller Rigidity Theorem

Idea of proof

Reduce to problem of local minimizers for

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

studied by Taheri (2002), using

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

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

Smoothing of twin boundaries

Seek solution to equilibrium equations for

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

such that

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

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

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

Lemma

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

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

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

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

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

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

In particular

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

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 $\longrightarrow$ tetragonal or orthorhombic (under a nondegeneracy assumption) we have

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

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

Remarks

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

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

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

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

Sharp interface models

A natural idea is to minimize an energy such as

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

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

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

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

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

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

in the set

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

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

GSBV

The space $GSBV$ was introduced by Ambrosio & de Giorgi. BV is the space of maps y of bounded variation i.e. whose distributional derivative Dy is a bounded measure. The space SBV consists of those $y \in BV$ such that the measure Dy has no Cantor part. $GSBV$ consists of those y such that for every $\varphi \in C^1(\mathbf{R}^3)$ with $\nabla\varphi$ of compact support, $\varphi(y) \in SBV$.

More generally we can suppose the energy is given by

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

One-dimensional case

Minimize

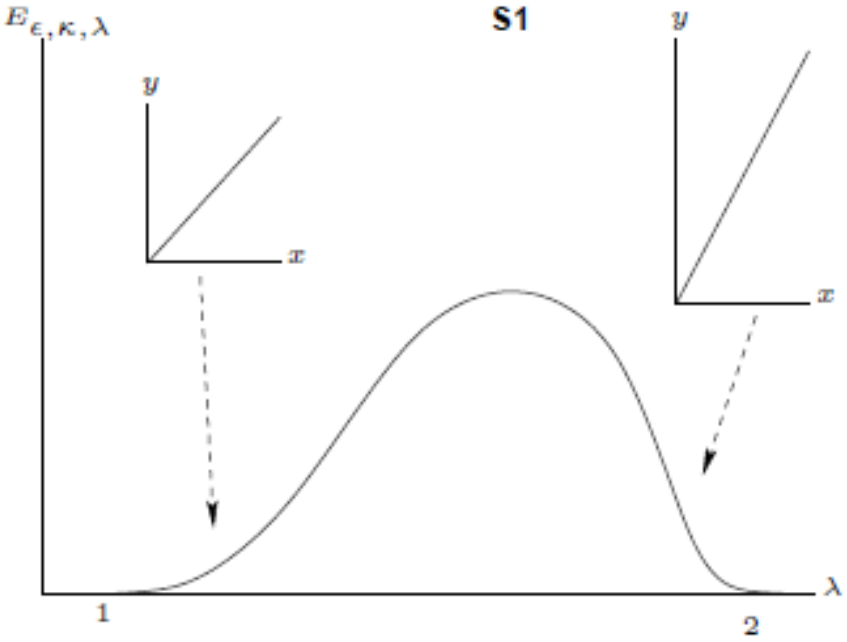
$$I_{\varepsilon,\kappa}(y) = \int_0^1 (W(y') + \varepsilon^2 |\nabla^2 y|^2)\, dx + \kappa \mathcal{H}^0(S_{y'})$$

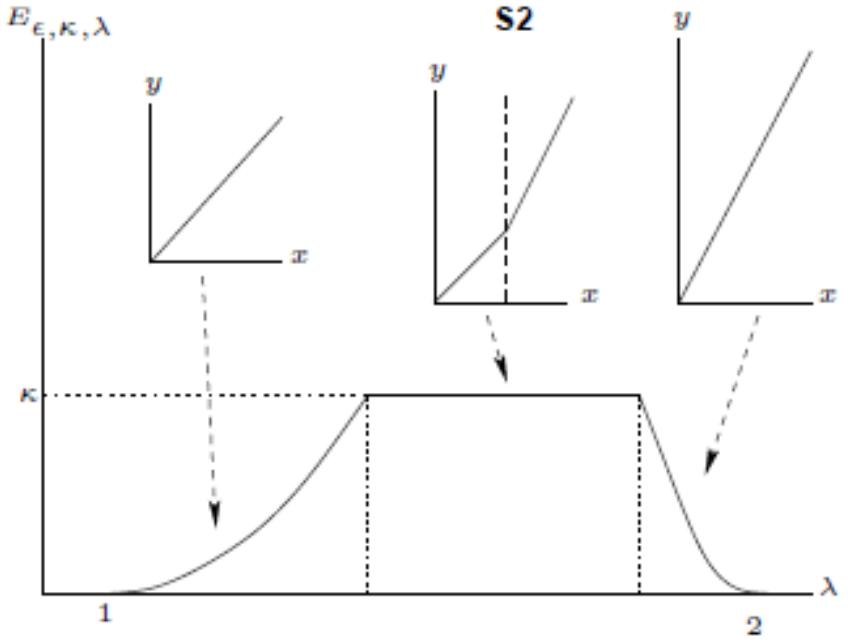
in

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

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

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


$E_{\epsilon,\kappa,\lambda}$
S1
y
x
y
x
λ
1
2


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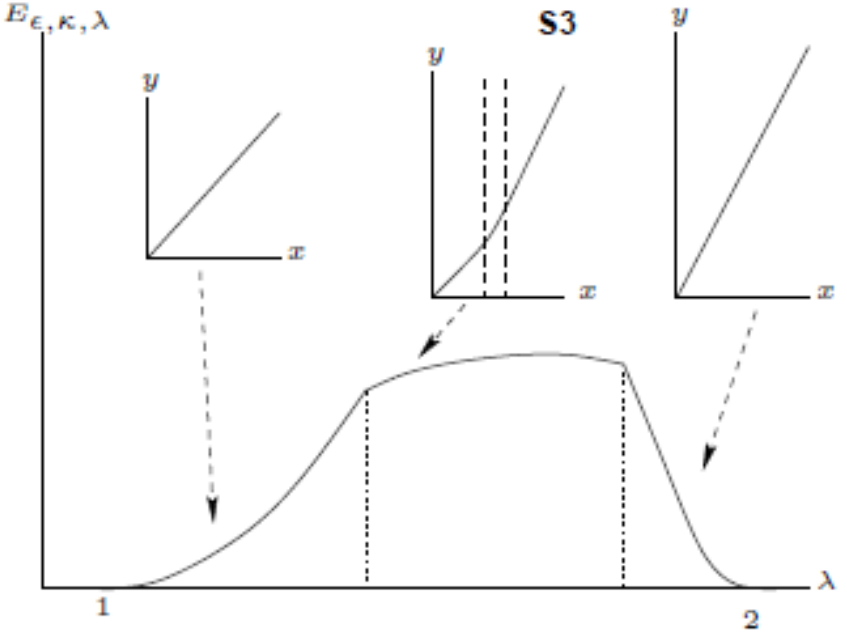
κ
λ
1
2


$E_{\epsilon,\kappa,\lambda}$
S3
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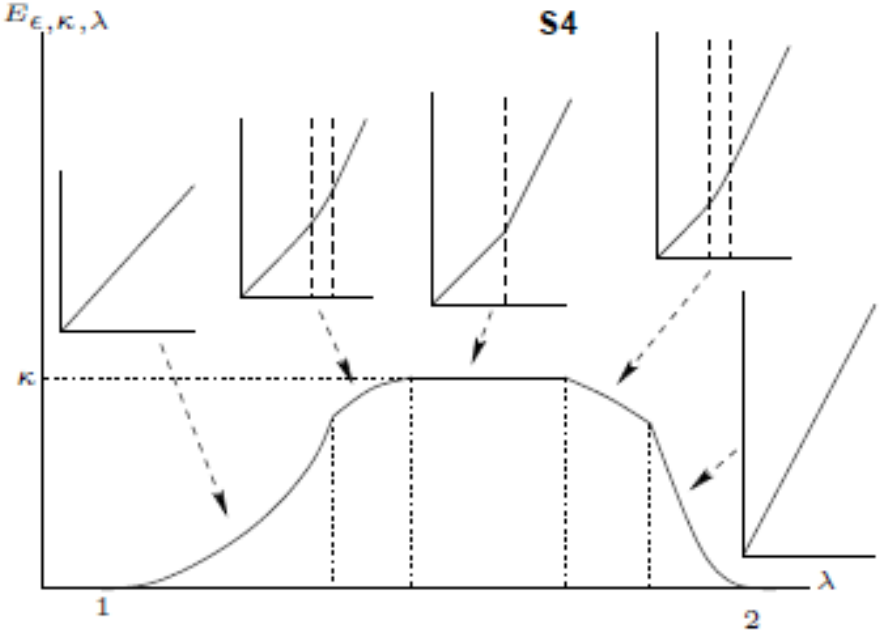

$E_{\epsilon,\kappa,\lambda}$
S4
κ
λ
1
2

More realistic 1D model

Minimize

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

in

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

We assume that ψ is continuous, even, of class C^1 on $(0,\infty)$, nondecreasing on $(0,\infty)$, and such that

$$\lim_{t\to 0}\frac{\psi(t)}{t}=\infty,\quad \psi(a+b)\le\psi(a)+\psi(b).$$

Typically $\psi(0)=0$ with ψ concave on $(0,\infty)$. For example

$$\psi(t)=\kappa|t|^{\alpha},\ \text{or}\ \psi(t)=\kappa|t|\log(1+\frac{1}{|t|}),$$

where $\alpha\in(0,1)$.

Theorem

Let $W : (0, \infty) \to [0, \infty)$ be C^1 and satisfy $\lim_{t \to 0^+} W(t) = \infty$ and suppose that there exist r_1, r_2 with $0 < r_1 < r_2$ such that $-\infty < \sup_{(0,r_i]} W' = \inf_{[r_i,\infty)} W' < \infty$ for $i \in \{1, 2\}$. Let $\lambda \in (r_1, r_2)$.

Then there exists a minimiser of the functional $I_{\varepsilon,\psi}$ in $\mathcal{A}_\lambda$. Moreover, if y is a minimizer then $u = y'$ satisfies:

(i) $u \in [r_1, r_2]$ a.e.

(ii) S_u is finite.

(iii) ∇u is continuous and in SBV,

$$W'(u) - 2\varepsilon^2 \nabla^2 u = c$$

for some constant $c \in \mathbf{R}$, $\nabla u(0) = \nabla u(1) = 0$ and $2\varepsilon^2 \nabla u(z) = \psi'([u](z))$ for all $z \in S_u$, $c = \int_0^1 W'(u)\, dx$ and

$$W(u) - \varepsilon^2 (\nabla u)^2 - cu = d,$$

for some constant $d \in \mathbf{R}$.

Remarks

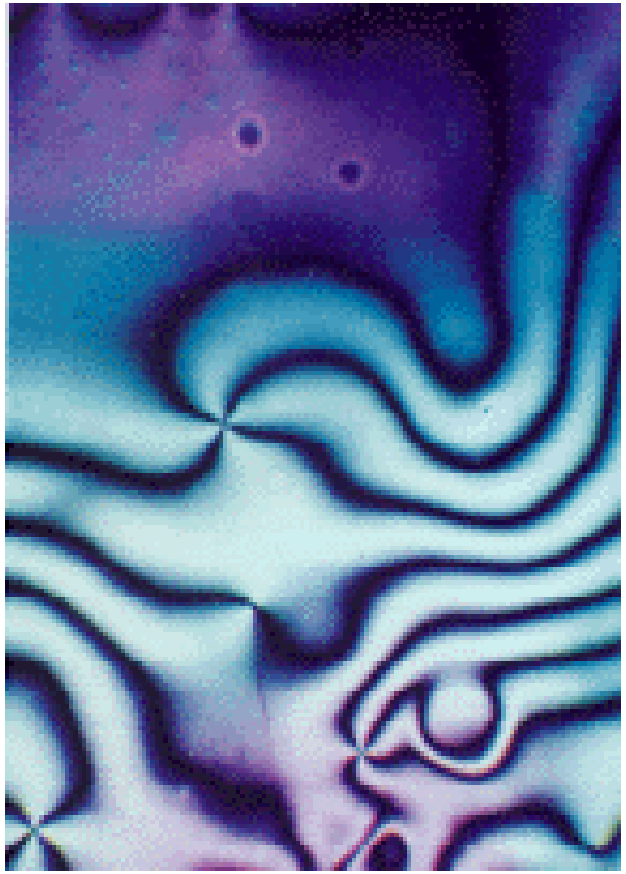
1. We cannot prove that there is at most one jump in y'.
2. The solution can be smooth or have a jump, but in general there are no piecewise affine solutions.

An introduction to the mathematics of liquid crystals

John Ball

Centre for Nonlinear PDE

University of Oxford



Liquid crystals

A multi-billion dollar industry.

An intermediate state of matter between liquids and solids.

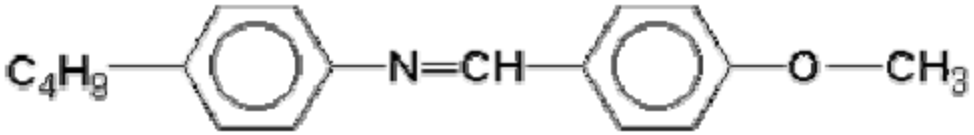
Liquid crystals flow like liquids, but the constituent molecules retain orientational order.

Classes of liquid crystals

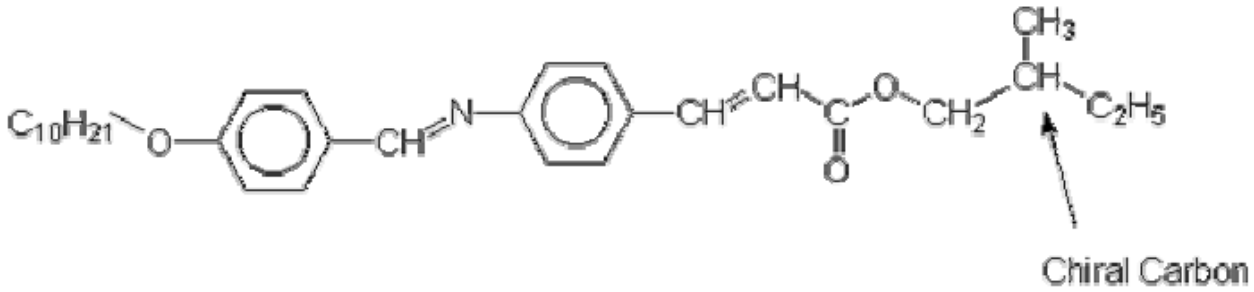
Liquid crystals are of many different types, three main classes being nematics, cholesterics and smectics.

Many liquid crystals consist of rod-like molecules.

Length 2-3 nm



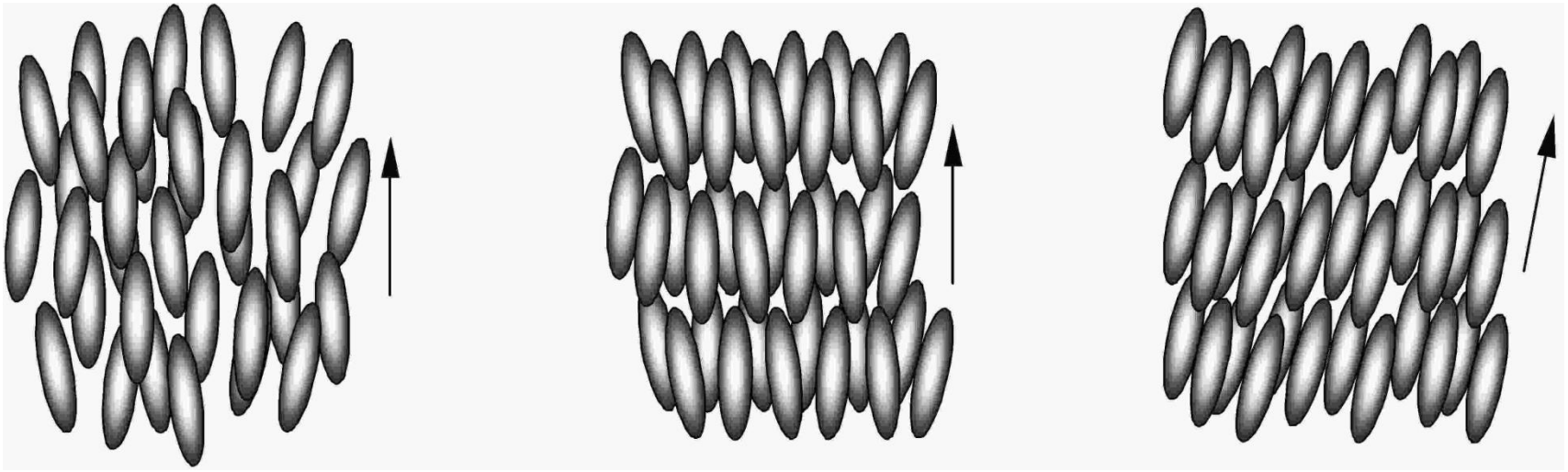
Methoxybenzilidene Butylanaline ("MBBA")



p-decyloxybenzylidene p'-amino 2-methylbutylcinnamate ("DOBAMBC")

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

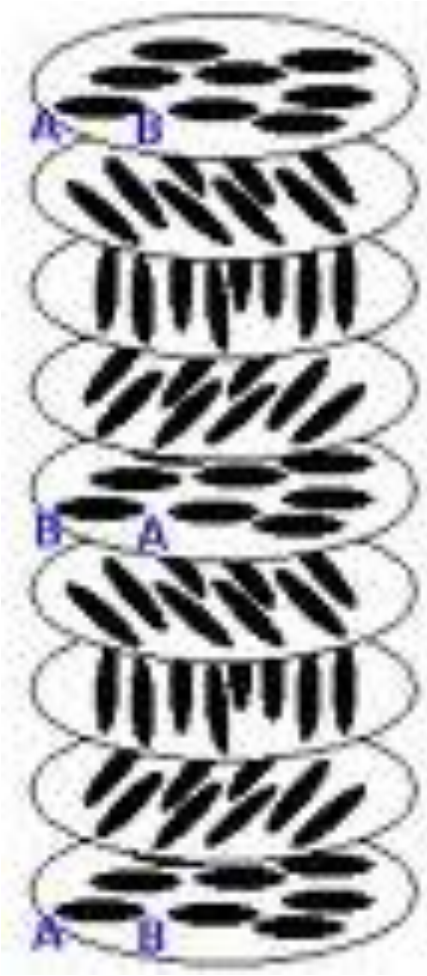
The molecules have time-varying orientations due to thermal motion.

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.



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.

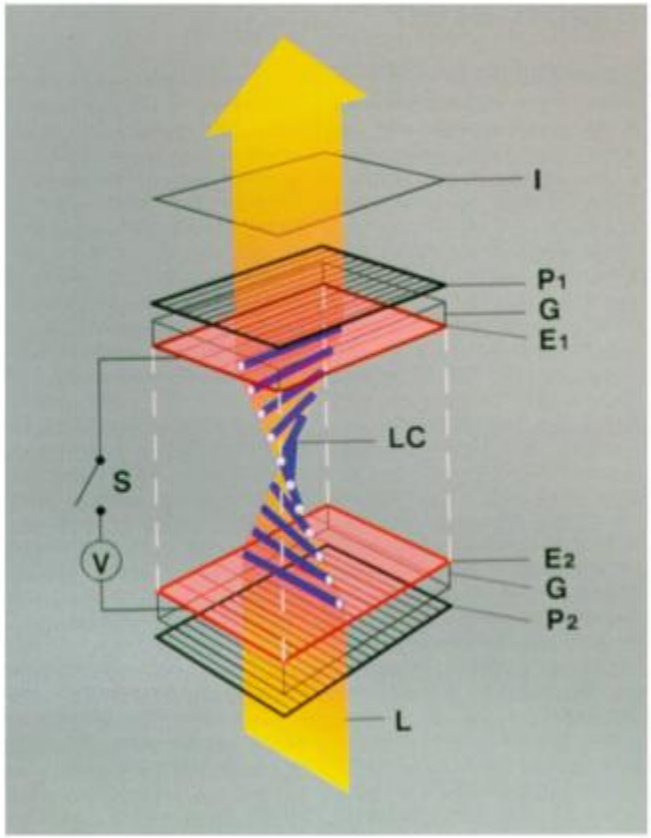
$\theta < \theta_m$
other LC or solid phase

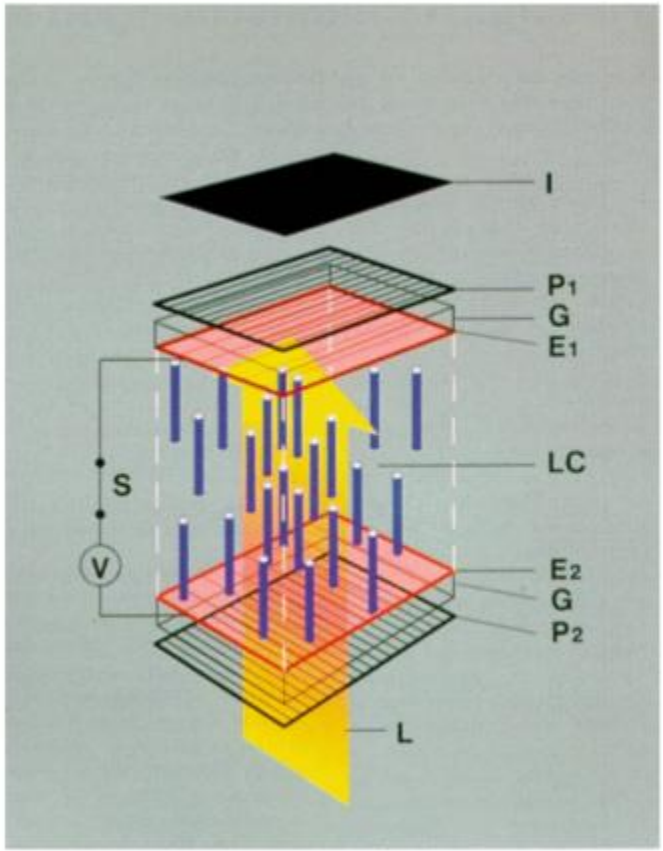
$\theta_m < \theta < \theta_c$
nematic

$\theta > \theta_c$
isotropic

DoITPoMS,
Cambridge

The twisted nematic display

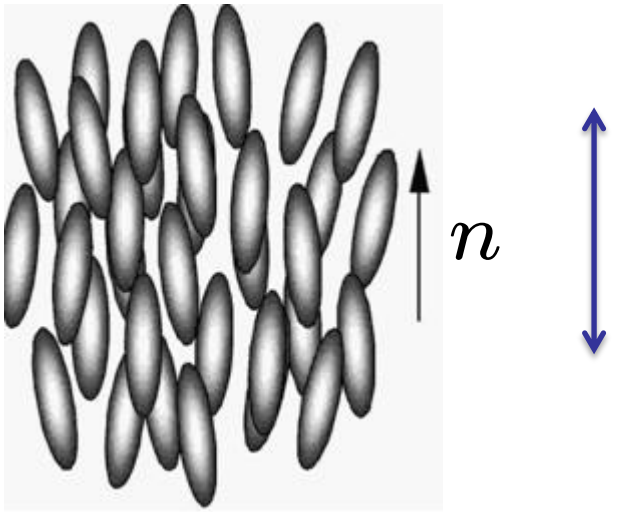




Wikipedia

The director

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



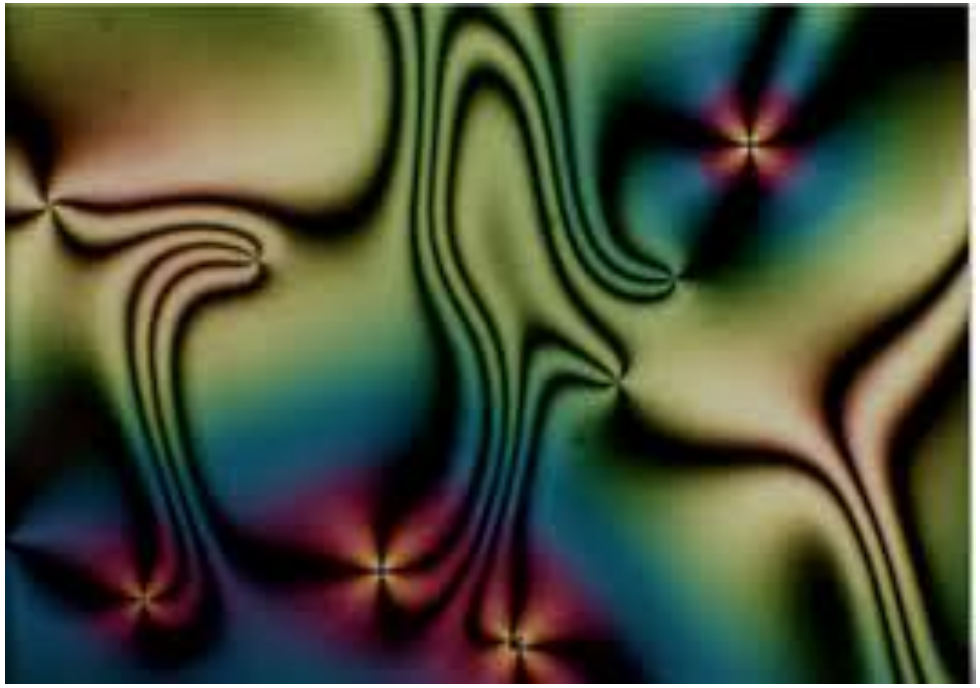
But note that for most liquid crystals n is equivalent to $-n$, so that a better description is via a *line field* in which we identify the mean orientation by the line through the origin parallel to it.

Such lines through the form the *real projective plane* $\mathbb{R}P^2$, and can be identified with 3×3 symmetric matrices of the form $n \otimes n$, where n is a unit vector, so that n belongs to the unit sphere S^2. Here

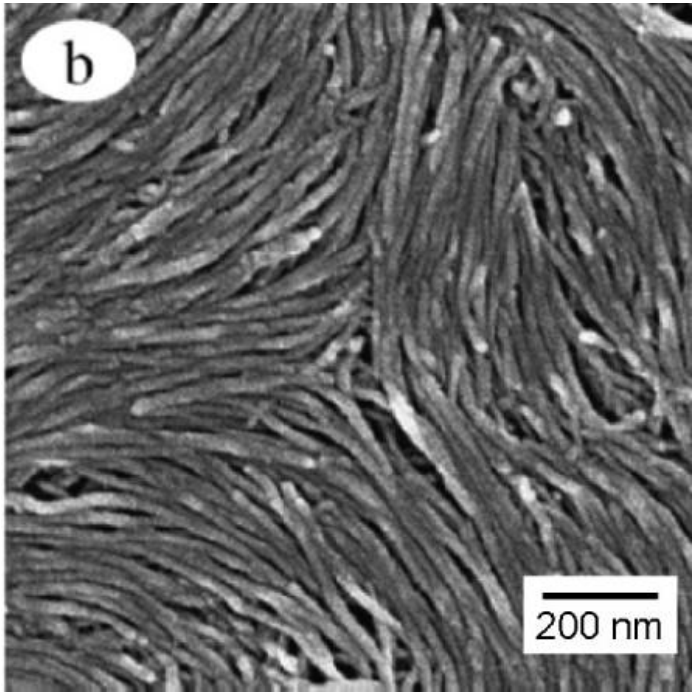
$$(n \otimes n)_{ij} = n_i n_j.$$

Defects

Roughly these can be thought of as (point or line) discontinuities in the director or line field.



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



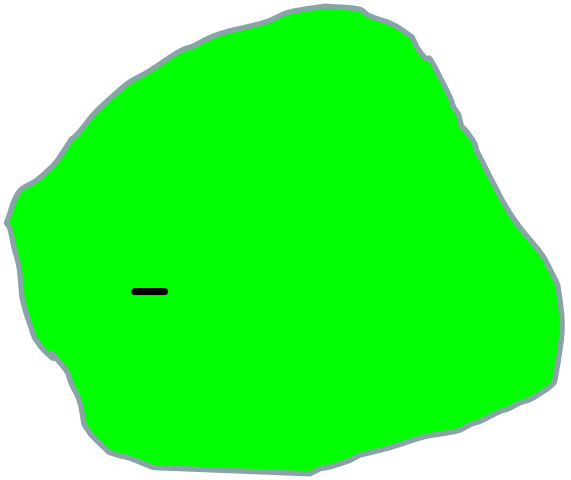
Zhang/Kumar 2007
Carbon nano-tubes as liquid crystals

Modelling via molecular dynamics

Twisted nematic display molecular simulation
M. Ricci, M. Mazzeo, R. Berardi, P. Pasini, C. Zannoni
(courtesy Claudio Zannoni)

Continuum models

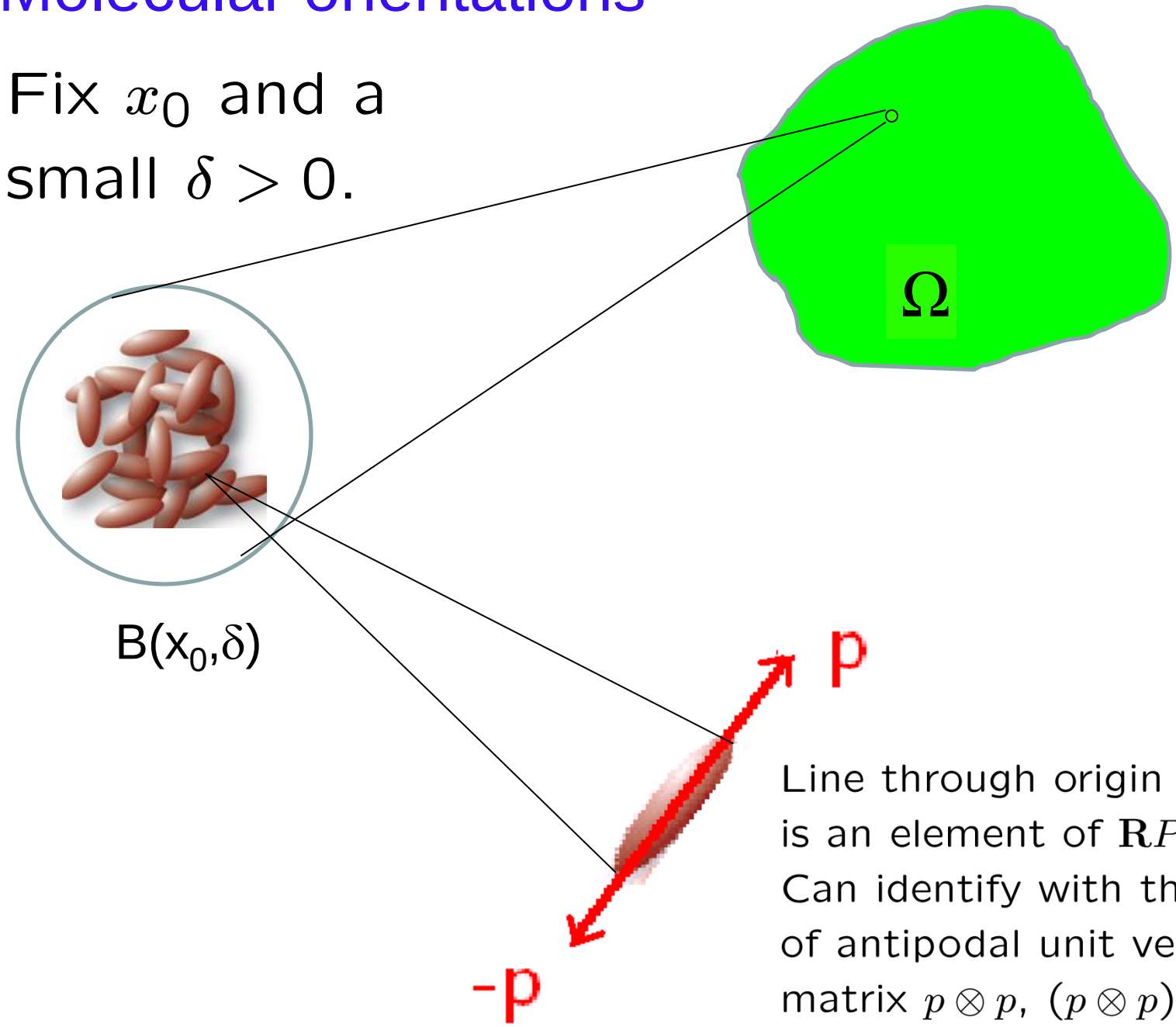
Consider a nematic liquid crystal filling a container $\Omega \subset \mathbb{R}^3$.



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

Molecular orientations

Fix x_0 and a small $\delta > 0$.



Line through origin parallel to p is an element of $\mathbf{R}P^2$.
Can identify with the pair $\{p, -p\}$ of antipodal unit vectors or the matrix $p \otimes p$, $(p \otimes p)_{ij} = p_i p_j$.

The distribution of orientations of molecules in $B(x_0, \delta)$ can be represented by a probability density function $\rho \geq 0, \int_{S^2} \rho(p)\, dp = 1$ on the unit sphere S^2 satisfying $\rho(p) = \rho(-p)$.

The first moment

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

The second moment

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

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

The *de Gennes* Q*-tensor*

$$Q = M - M_0$$

measures the deviation of M from its isotropic value $M_0 = \frac{1}{3}\mathbf{1}$, corresponding to the probability density function $\rho(p) = \frac{1}{4\pi}$.

Note that $Q = Q^T$, $\mathrm{tr}Q = 0$, $\frac{2}{3} \geq \lambda_i(Q) \geq -\frac{1}{3}$.

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

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

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

In practice Q is observed to be very nearly uniaxial except possibly very near defects, with a constant value of s (typical values being in the range $0.6 - 0.8$).

Landau – de Gennes free energy

At each point x we have a $Q-$tensor $Q(x)$.

We suppose that Q is obtained by minimizing the (free) energy

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

subject to suitable boundary conditions.

For simplicity we consider the special case when

$$\psi(Q,\nabla Q,\theta) = \underbrace{a(\theta)\mathrm{tr}\,Q^2 - \frac{2b}{3}\mathrm{tr}\,Q^3 + \frac{c}{2}\mathrm{tr}\,Q^4}_{\psi_B(Q,\theta)} + \underbrace{\varepsilon|\nabla Q|^2}_{\psi_E(\nabla Q)}$$

where θ is the temperature, $b > 0, c > 0, a(\theta) = \alpha(\theta - \theta^*), \alpha > 0, \varepsilon > 0$ and

$$|\nabla Q|^2 = \sum_{i,j,k=1}^{3} \left(\frac{\partial Q_{ij}}{\partial x_k}\right)^2,$$

so that we have to minimize

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

If

$$\theta > \theta_{\mathrm{NI}} = \theta^* + \frac{2b^2}{27\alpha c}$$

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

Thus this model predicts that there is a phase transformation from an isotropic fluid to a uniaxial nematic phase at the critical temperature θ_{NI}.

Possible defects in constrained theory

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

Hedgehog $\quad n(x) = \dfrac{x}{|x|}$

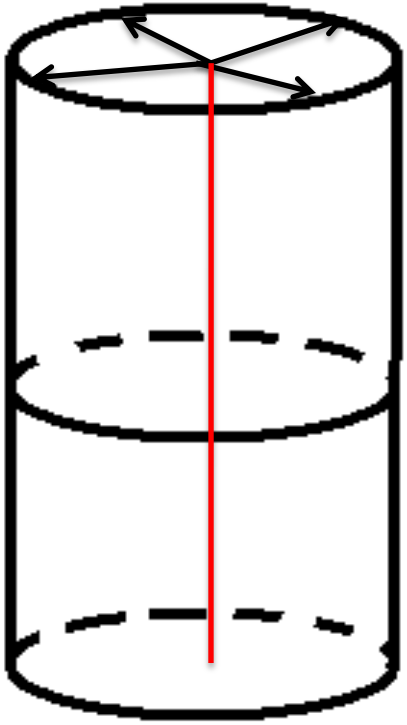
$$\nabla n(x) = \frac{1}{|x|}(\mathbf{1} - n \otimes n)$$

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

$$\int_0^1 r^{-2} r^2 dr < \infty$$

Finite energy

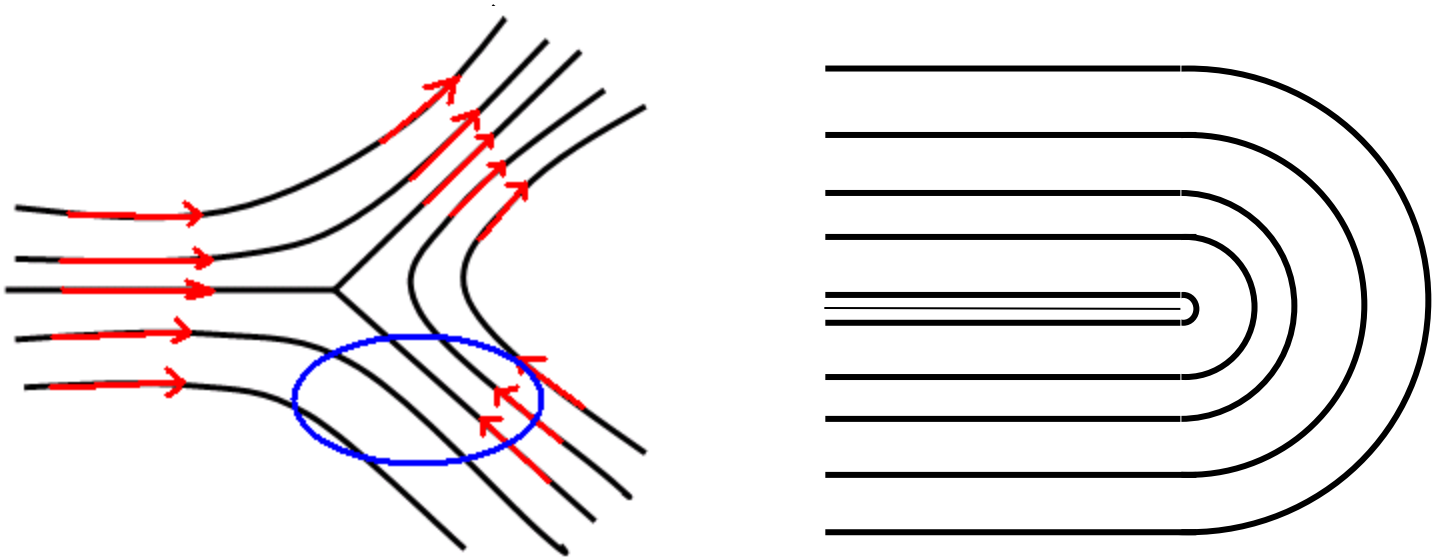
Disclinations



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

infinite energy

Index one half singularities



These are nonorientable and of infinite energy.

Mathematical challenges

1. Give a rigorous derivation of a continuum model from a molecular one. What forms should the bulk and elastic energies have, is it reasonable to use second moments, boundary conditions ...?)

2. What is the best way to describe defects? (For example, are there useful asymptotics as $\varepsilon \to 0$ in the Landau - de Gennes theory?)

The eigenvalue constraints

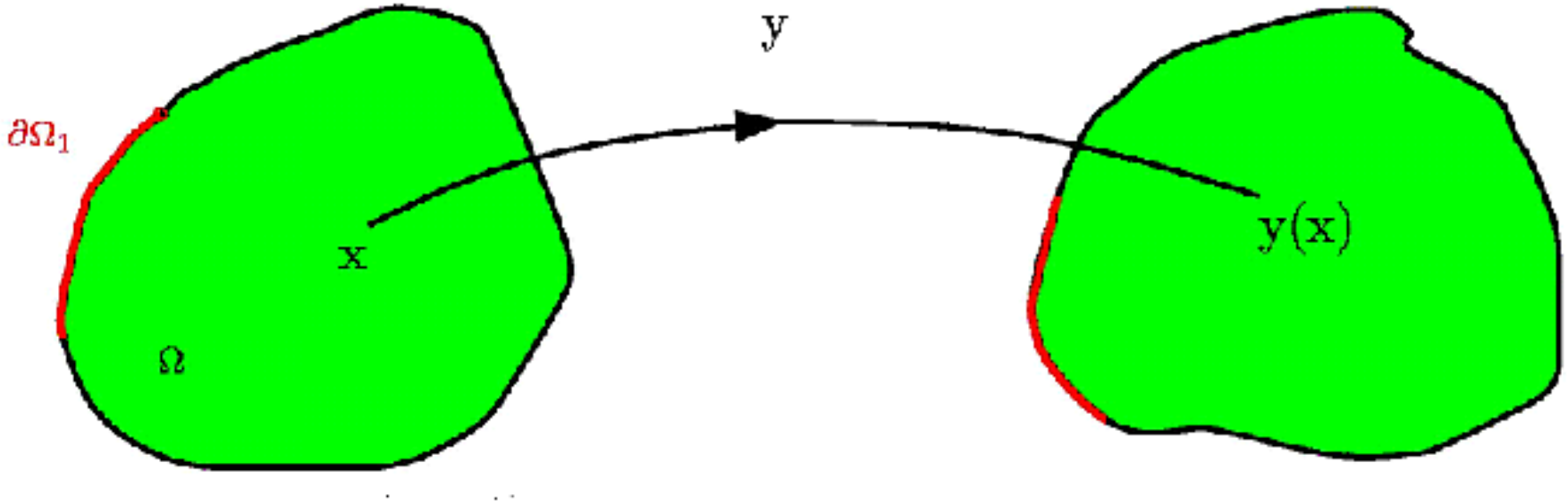
Question: how are the eigenvalue constraints

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}$$

maintained in the theory?

B/Majumdar

Nonlinear elasticity



Minimize

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

subject to suitable boundary conditions, e.g. $y|_{\partial\Omega_1} = \bar{y}$.

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

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

To ensure this we assume 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 Onsager model

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

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

With the Maier-Saupe molecular interaction, the internal energy is given by

$$U(\rho) \;=\; \kappa \int_{S^2} \int_{S^2} [\tfrac{1}{3} - (p \cdot q)^2] \rho(p) \rho(q)\, dp\, dq$$

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

Denoting by

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

the corresponding Q-tensor, a short calculation shows that

$$U(\rho) = -\kappa |Q(\rho)|^2.$$

Hence

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

Given Q we define

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

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

Theorem

$$\psi_B(Q,\theta) \geq c_0 - \frac{\theta}{2}\ln(\lambda_{\min}(Q) + \frac{1}{3}),$$

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

Remarks

1. The blow-up corresponds to a perfectly aligned state having entropy $-\infty$.

2. All critical points of ψ_B are uniaxial. Phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

Given appropriate boundary conditions, do minimizers of

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

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

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

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

Example (B & Mizel)

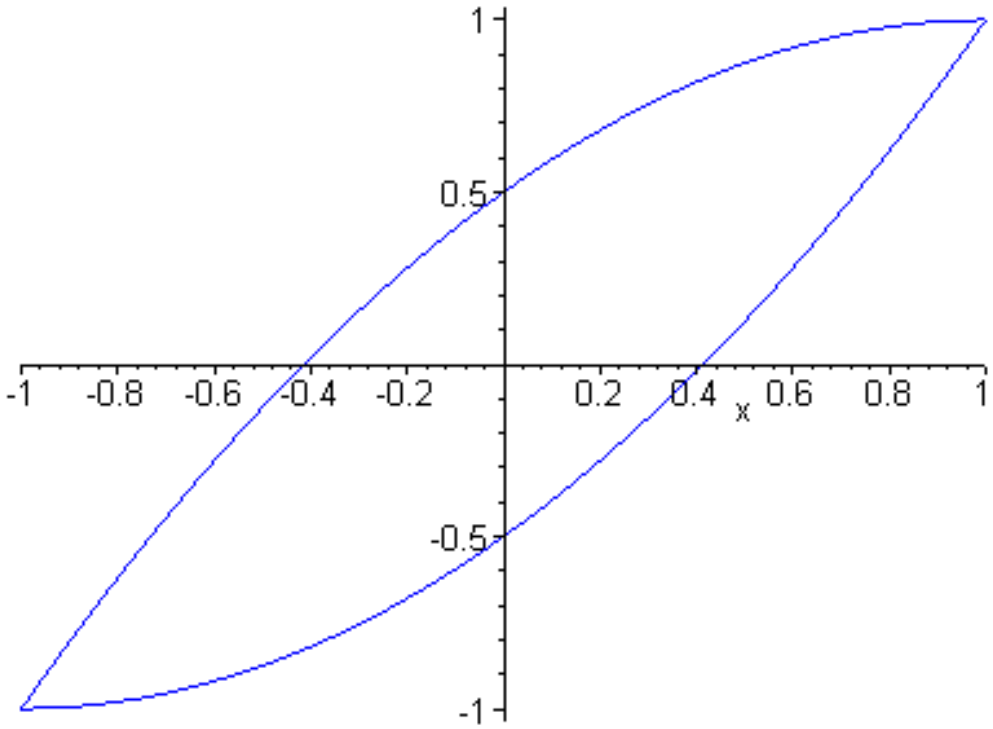
Minimize

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

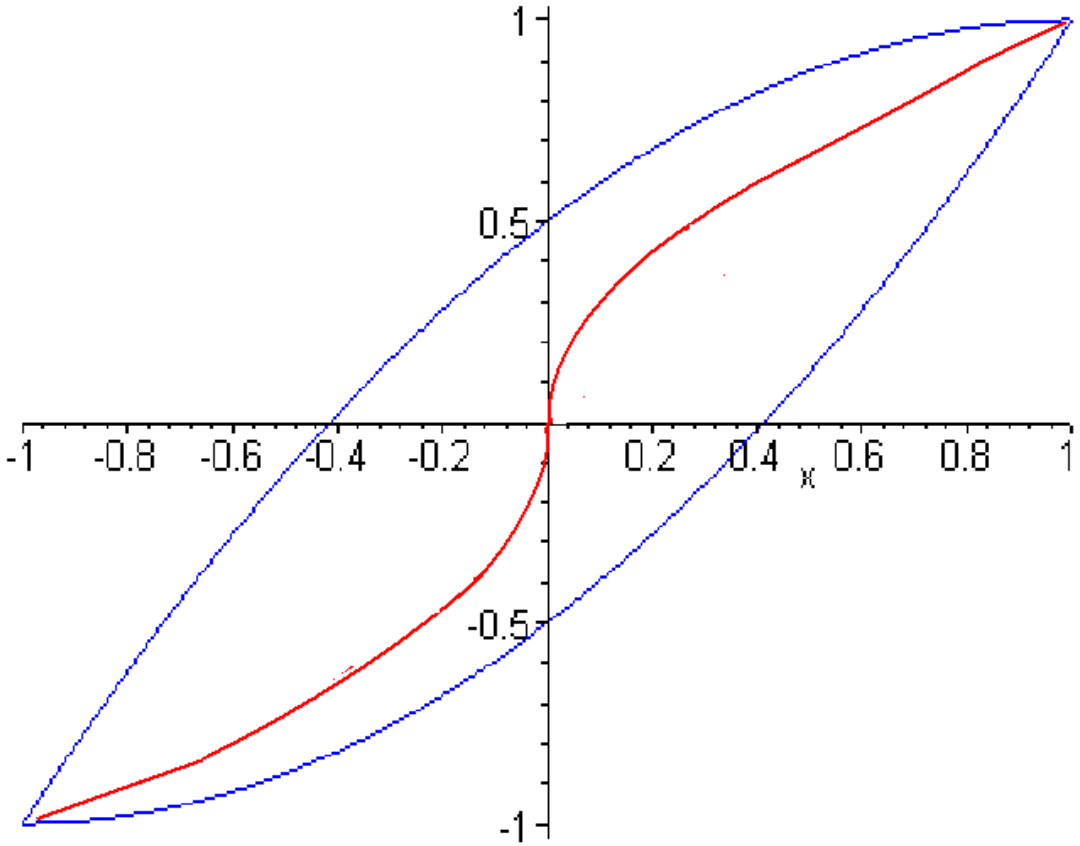
subject to

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

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 y^*, which has a singularity

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

Theorem

Let Q minimize

$$I(Q) = \int_\Omega [\psi_B(Q) + \varepsilon |\nabla Q|^2] \, dx,$$

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

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

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

Nonlinear elasticity problem: Do minimizers for suitable boundary conditions of

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

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

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

for some $\varepsilon > 0$?

This seems to be very difficult.

Recall the definition of the Q-tensor for nematics, namely

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

and that $Q = Q^T, \operatorname{tr} Q = 0, -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}$.

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 if and only if

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

Proof. The characteristic equation of Q is

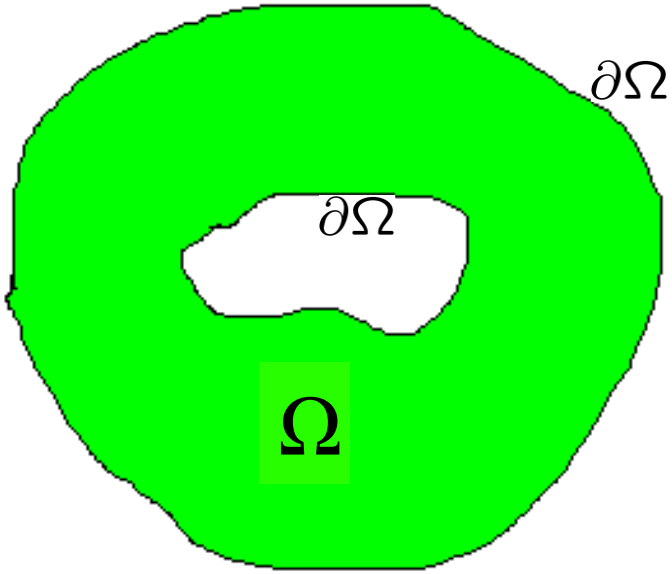
$$\det(Q - \lambda \mathbf{1}) = \det Q - \lambda \operatorname{tr} \operatorname{cof} Q + 0\lambda^2 - \lambda^3.$$

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 $4p^3 = 27q^2$.

Energetics



Consider a liquid crystal material filling a container $\Omega \subset \mathbf{R}^3$. We suppose that the material is incompressible, homogeneous (same material at every point) and that the temperature is constant.

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 $\psi(Q, \nabla Q)$, so that the total free energy is given by

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

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

The domain of ψ

For what Q, D should $\psi(Q, D)$ 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 $\psi : \operatorname{dom}\psi \to \mathbf{R}$, 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 ψ to all of $M^{3\times 3}\times$(3rd order tensors). To do this first set $\psi(Q, D) = \infty$ if $(Q, D) \in \mathcal{E} \times \mathcal{D}$ with some $\lambda_i(Q) \leq -\frac{1}{3}$.

Then note that

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

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

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

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

Thus we can assume that ψ satisfies for $(Q, D) \in \operatorname{dom}\psi$

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

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

Frame-indifference

Fix $\bar{x} \in \Omega$, 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 $R \in SO(3)$. We require that both observers see the same free-energy density, that is

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

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

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

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

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

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

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

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

Material symmetry

The requirement that

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

when $z = \bar{x} + \hat{R}(x - \bar{x})$, where $\hat{R} = -\mathbf{1} + 2e \quad e$, $|e| = 1$, 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

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

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

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

Thus, putting $D = 0$,

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

which holds if and only if ψ_B is a function of the principal invariants of Q, that is, since $\operatorname{tr} Q = 0$,

$$\psi_B(Q) = \bar{\psi}_B(|Q|^2, \det Q).$$

Examples of isotropic functions quadratic in ∇Q :

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

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

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

where the L_i are material constants.

The constrained theory

If the L_i are small , it is reasonable to consider the *constrained theory* in which Q is required to be uniaxial with a constant scalar order parameter $s > 0$, so that

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

(For recent rigorous work justifying this see Majumdar & Zarnescu, Nguyen & Zarnescu.) In this theory the bulk energy is constant and so we only have to consider the elastic energy

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

Oseen-Frank energy

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

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

where

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

$K_2 = 2L_1 s^2 - \frac{2}{3} L_4 s^3,$

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

$K_4 = L_3 s^2.$

Function Spaces (part of the mathematical model)

Unconstrained theory.

We are interested in equilibrium configurations of finite energy

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

We use the Sobolev space $W^{1,p}(\Omega; M^{3\times 3})$. Since usually we assume

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

$$I_1 = Q_{ij,j} Q_{ik,k},\ I_2 = Q_{ik,j} Q_{ij,k},$$

$$I_3 = Q_{ij,k} Q_{ij,k},\ I_4 = Q_{lk} Q_{ij,l} Q_{ij,k},$$

we typically take $p = 2$.

Constrained theory.

For $1 \leq p < \infty$ the Sobolev space $W^{1,p}(\Omega, \mathbf{R}P^2)$ is the set of $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$ with weak derivative ∇Q satisfying $\int_\Omega |\nabla Q(x)|^p dx < \infty$.

Thus for the Landau - de Gennes energy density, the space of Q with finite elastic energy is $W^{1,2}(\Omega, \mathbf{R}P^2)$.

Existence of minimizers in the constrained theory

Immediate in $W^{1,2}(\Omega, \mathbf{R}P^2)$, for a variety of boundary conditions, under suitable inequalities on the L_i, since ψ_E is then convex in ∇Q and coercive and the uniaxiality contraint is weakly closed.

The equilibrium equations (JB/Majumdar)

Let Q be a minimizer of

$$I(Q) = \int_\Omega \psi_E(Q, \nabla Q)\, dx$$

subject to $Q \in K = \{s(n \otimes n - \frac{1}{3}\mathbf{1}) : n \in S^2\}$.
Considering a variation

$$Q_\varepsilon = s\left(\frac{[n + \varepsilon a \wedge n] \otimes [n + \varepsilon a \wedge n]}{|n + \varepsilon a \wedge n|^2} - \frac{1}{3}\mathbf{1}\right),$$

with a smooth and of compact support, we get the weak form of the equilibrium equations

$$ZQ = QZ,$$

where $Z_{ij} = \frac{\partial \psi_E}{\partial Q_{ij}} - \frac{\partial}{\partial x_k}\frac{\partial \psi_E}{\partial D_{ijk}}$ (ψ_E symmetrized).

Can we orient the director? (JB/Zarnescu)

We say that $Q = Q(x)$ is *orientable* if we can write

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

where $n \in W^{1,p}(\Omega, S^2)$.

This means that for each x we can make a choice of the unit vector $n(x) = \pm\tilde{n}(x) \in S^2$ so that $n(\cdot)$ has some reasonable regularity, sufficient to have a well-defined gradient ∇n (in topological jargon such a choice is called a *lifting*).

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 $W^{1,p}(\Omega; \mathbf{R}P^2)$ 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 1

An orientable Q has exactly two orientations.

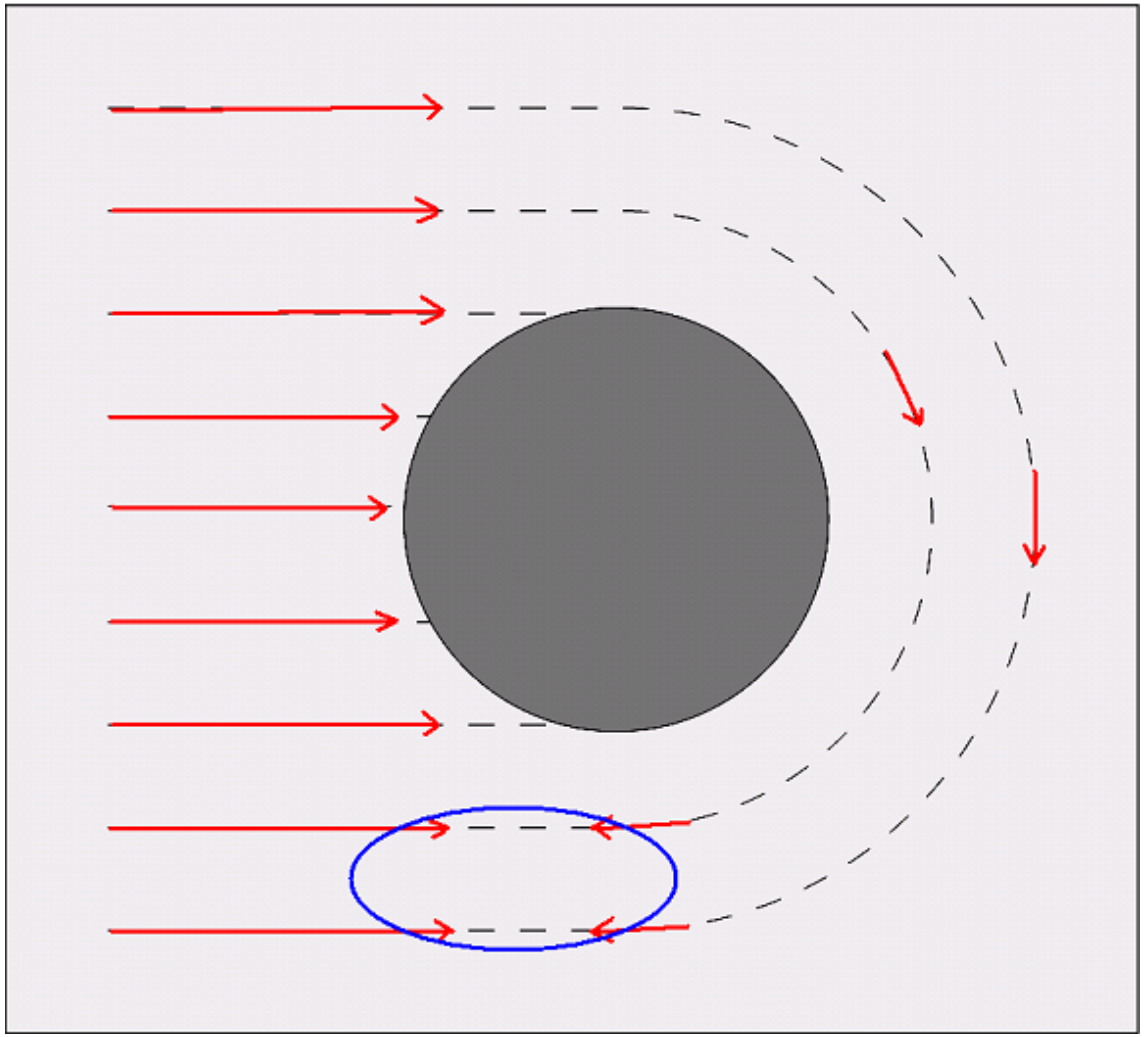
Proof

Suppose that n and τn both generate Q and belong to $W^{1,1}(\Omega, S^2)$, where $\tau^2(x) = 1$ a.e.. For a.e. x_2, x_3, both $n(x)$ and $\tau(x)n(x)$ are absolutely continuous in x_1. Hence

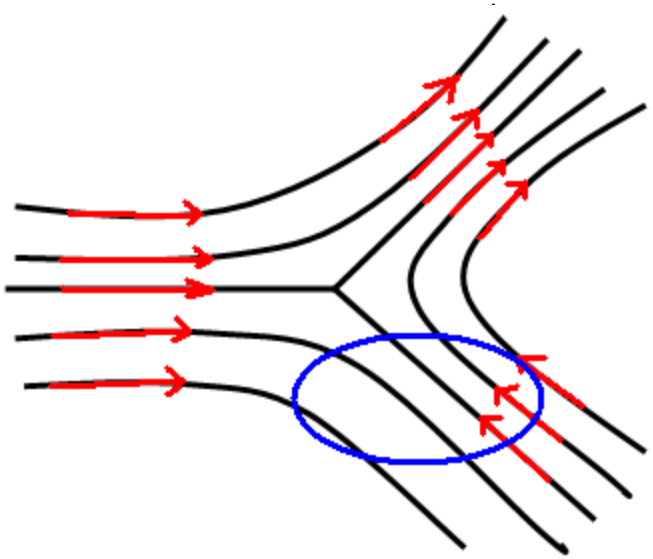
$$\tau(x)n(x) \cdot n(x) = \tau(x)$$

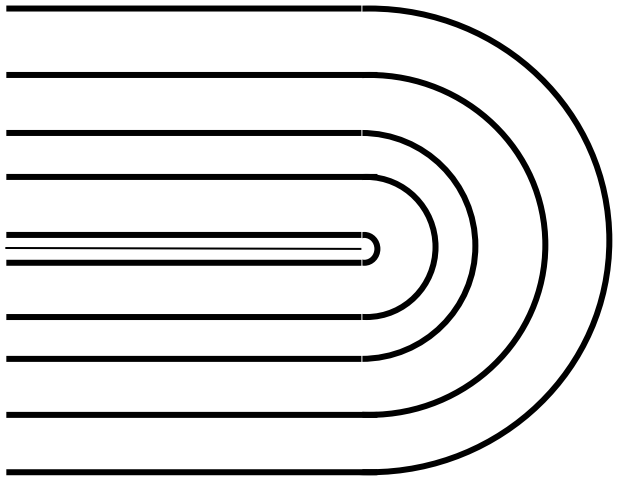
is continuous in x_1. Hence the weak partial derivative $\tau_{,1}$ exists and is zero. Similarly $\tau_{,2}, \tau_{,3}$ exist and are zero. Thus $\nabla\tau = 0$ a.e. in Ω. Hence $\tau = 1$ a.e. or $\tau = -1$ a.e..

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



The index one half singularities are non-orientable



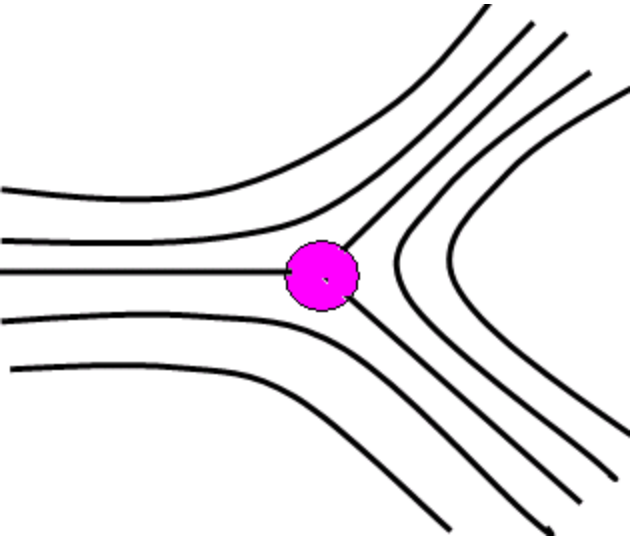


Theorem 2

If Ω is simply-connected and $Q \in W^{1,p}$, $p \geq 2$, then Q is orientable.

(See also a recent topologically more general lifting result of Bethuel and Chiron for maps u:$\Omega \rightarrow$N.)

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



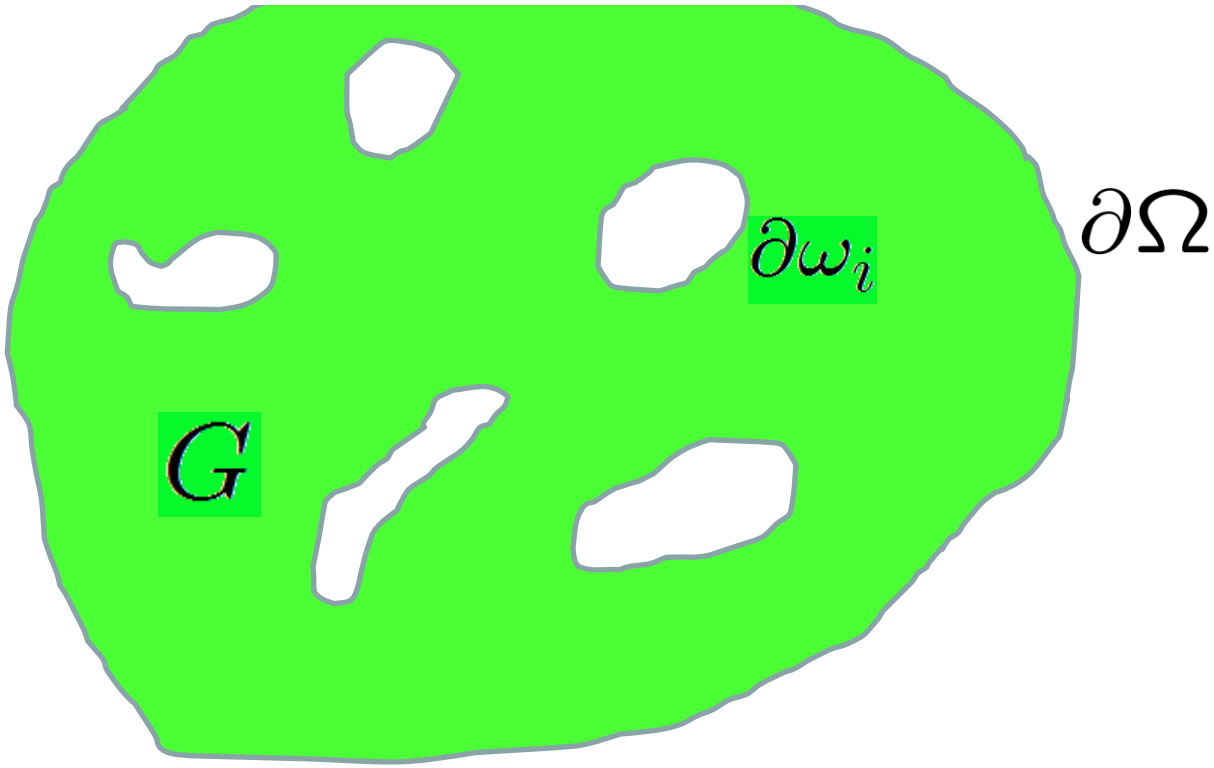
Another consequence is that it is impossible to modify this Q-tensor field in a core around the singular line so that it has finite Landau-de Gennes energy.

Ingredients of Proof of Theorem 2

- Lifting possible if Q is smooth and Ω simply-connected
- Pakzad-Rivière theorem (2003) implies that if $\partial\Omega$ is smooth, then there is a sequence of smooth $Q^{(j)}$ converging weakly to Q in $W^{1,2}$
- We can approximate a simply-connected domain with boundary of class C by ones that are simply-connected with smooth boundary
- The Proposition implies that orientability is preserved under weak convergence

2D examples and results for non simply-connected regions

Let $\Omega \subset \mathbb{R}^2$, $\omega_i \subset \mathbb{R}^2, i = 1, \ldots, n$ be bounded, open and simply connected, with C^1 boundary, such that $\bar{\omega}_i \subset \Omega$, $\bar{\omega}_i \cap \bar{\omega}_j \neq \emptyset$ for $i \neq j$, and set $G = \Omega \backslash \bigcup_{i=1}^{n} \bar{\omega}_i$.



$$\mathcal{Q}_2 = \{Q = s(n \otimes n - \frac{1}{3}\mathbf{1}) : n = (n_1, n_2, 0)\}$$

Given $Q \in W^{1,2}(G; \mathcal{Q}_2)$ define the auxiliary complex-valued map

$$A(Q) = \frac{2}{s}Q_{11} - \frac{1}{3} + i\frac{2}{s}Q_{12}.$$

Then $A(Q) = Z(n)^2$,
where $Z(n) = n_1 + in_2$.

$$A : Q_2 \to S^1.$$

Let $C = \{C(s) : 0 \leq s \leq 1\}$ be a smooth Jordan curve in $\mathbb{R}^2 \simeq \mathbb{C}$.

If $Z : C \to S^1$ is smooth then the degree of Z is the integer

$$\deg(Z, C) = \frac{1}{2\pi i} \int_C \frac{Z_s}{Z} ds.$$

Writing $Z(s) = e^{i\theta(s)}$ we have that

$$\deg(Z, C) = \frac{1}{2\pi i} \int_0^1 i\theta_s ds = \frac{\theta(1) - \theta(0)}{2\pi}.$$

If $Z \in H^{\frac{1}{2}}(C; S^1)$ then the degree may be defined by the same formula

$$\deg(Z, C) = \frac{1}{2\pi i} \int_C \frac{Z_s}{Z} ds.$$

interpreted in the sense of distributions (L. Boutet de Monvel).

Theorem

Let $Q \in W^{1,2}(G; Q_2)$. The following are equivalent:

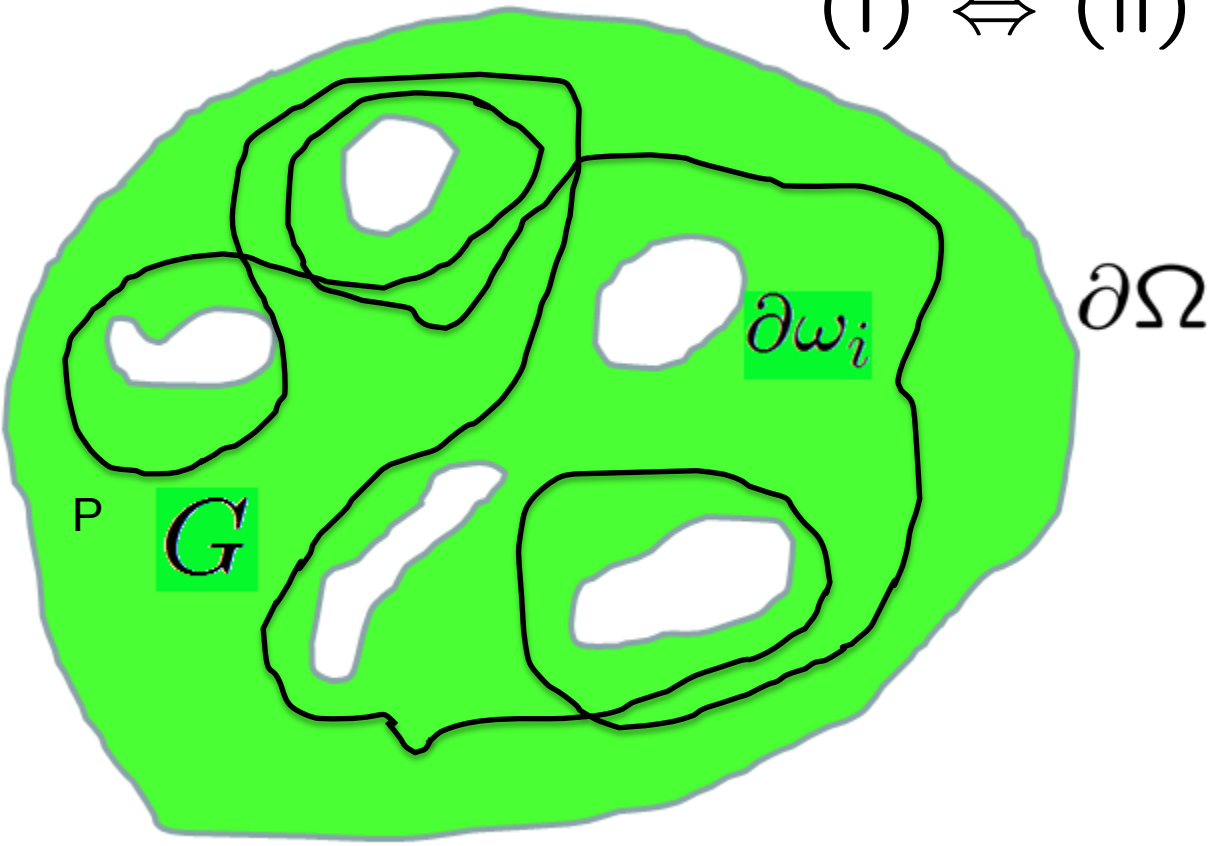
(i) Q is orientable.

(ii) $\operatorname{Tr} Q \in H^{\frac{1}{2}}(C; Q_2)$ is orientable for every component C of ∂G.

(iii) $\deg(A(\operatorname{Tr} Q), C) \in 2\mathbb{Z}$ for each component C of ∂G.

We sketch the proof, which is technical.

(i) $\Leftrightarrow$ (ii) for continuous Q



The orientation at the beginning and end of the loop are the same since we can pass the loop through the holes using orientability on the boundary.

(ii) $\Leftrightarrow$ (iii). If $\mathrm{Tr}\, Q$ is orientable on C then

$$\begin{aligned}
\deg\left(A(\mathrm{Tr}\, Q), C\right) &= \deg\left(Z^2(n), C\right) \\
&= \frac{1}{2\pi i}\int_C \frac{(Z^2)_s}{Z^2} ds \\
&= \frac{1}{2\pi i}\int_C 2\frac{Z_s}{Z} ds \\
&= 2\deg\left(Z(n), C\right)
\end{aligned}$$

Conversely, if $A(\mathrm{Tr}\, Q(s)) = e^{i\theta(s)}$ and

$$\deg(A(\mathrm{Tr}\, Q), C) = \frac{\theta(1) - \theta(0)}{2\pi} \in 2\mathbb{Z}$$

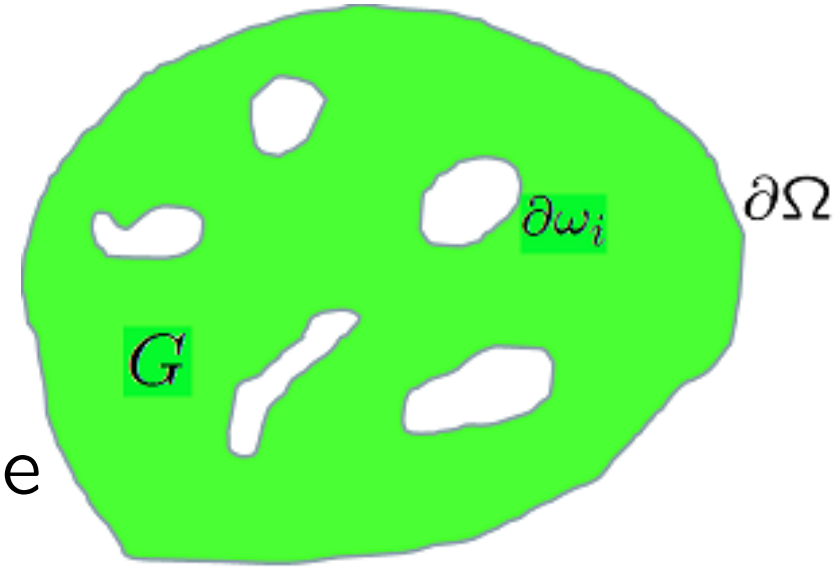
then $Z(s) = e^{\frac{i\theta(s)}{2}} \in H^{\frac{1}{2}}(C, S^1)$ and so $\mathrm{Tr}\, Q$ is orientable.

We have seen that the (constrained) Landau-de Gennes and Oseen-Frank theories are equivalent in a simply-connected domain. Is this true in 2D for domains with holes?

If we specify Q on each boundary component then by the Theorem either all Q satisfying the boundary data are orientable (so that the theories are equivalent), or no such Q are orientable, so that the Oseen Frank theory cannot apply and the Landau- de Gennes theory must be used.

More interesting is to apply boundary conditions which allow both the Landau - de Gennes and Oseen-Frank theories to be used and compete energetically.

$$G = \Omega \setminus \bigcup_{i=1}^{n} \bar{\omega}_i$$



So we consider the problem of minimizing

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

subject to $Q|_{\partial\Omega} = g$ orientable with the boundaries $\partial\omega_i$ free.

Since A is bijective and

$$I(Q) = \frac{2}{s^2} \int_G |\nabla A(Q)|^2 dx$$

our minimization problem is equivalent to min-
imizing

$$\hat{I}(m) = \frac{2}{s^2} \int_G |\nabla m|^2 dx$$

in $W^{1,2}_{A(g)}(G; S^1) =$

$$\{m \in W^{1,2}(G; S^1) : m|_{\partial_-} = A(g)\}.$$

In order that Q is orientable on $\partial\Omega$ we need that

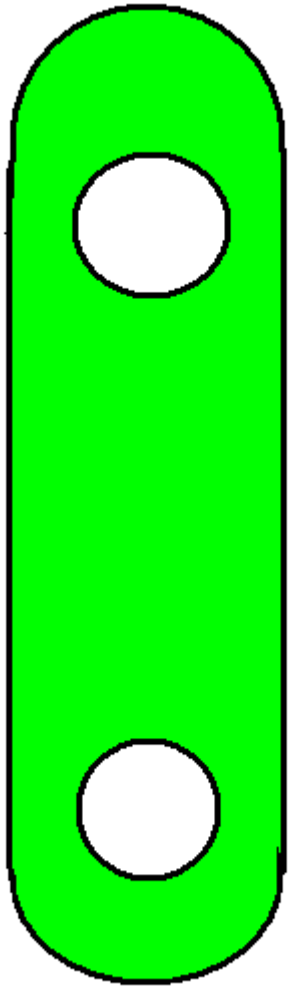
$$\deg(m, \partial\Omega) \in 2\mathbb{Z}.$$

We always have that

$$\deg(m, \partial\Omega) = \sum_{i=1}^{n} \deg(m, \partial\omega_i).$$

Hence if there is only one hole ($n = 1$) then $\deg(m, \partial\omega_1)$ is even and so every Q is orientable.

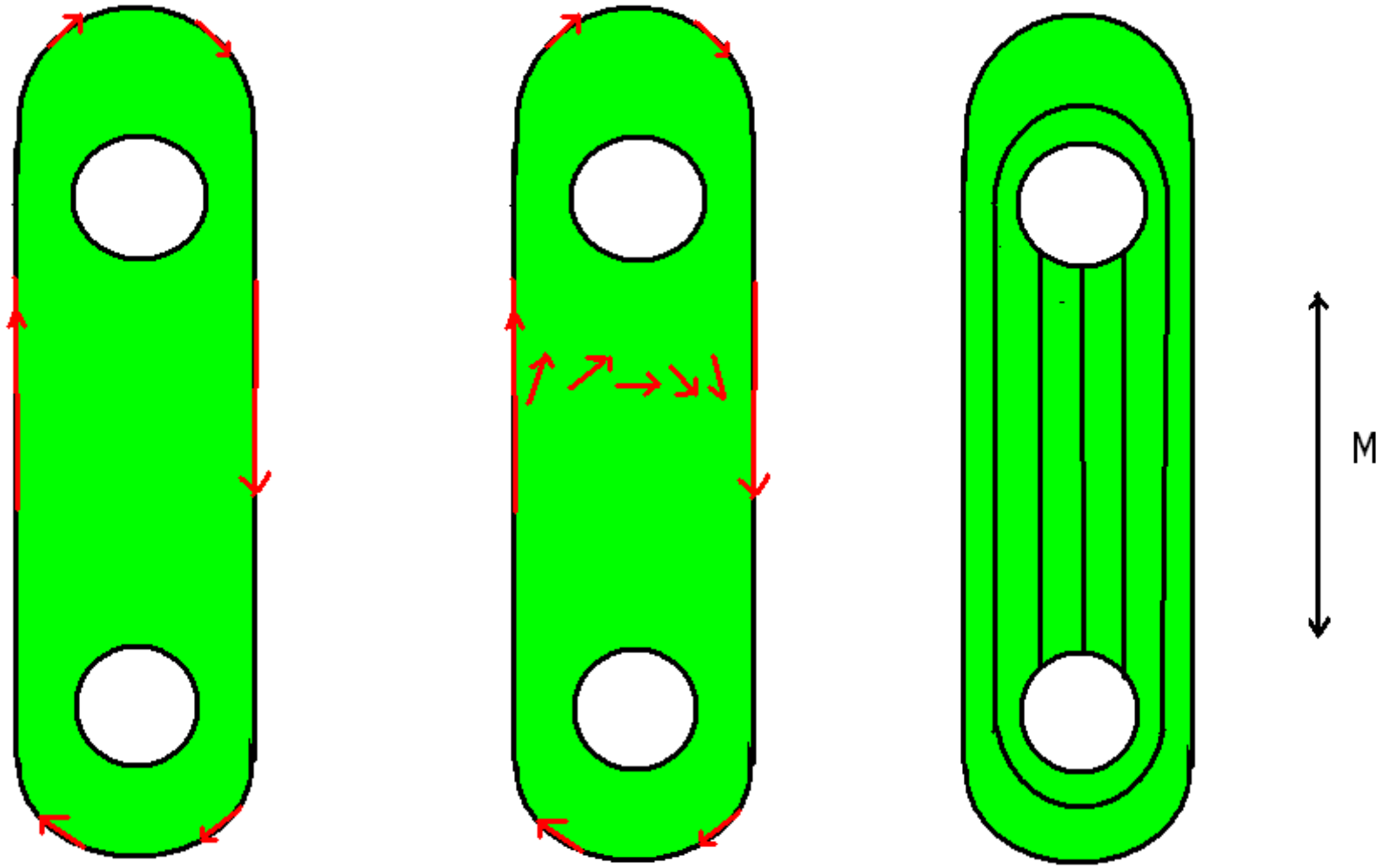
So to have both orientable and non-orientable Q we need at least two holes.



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

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

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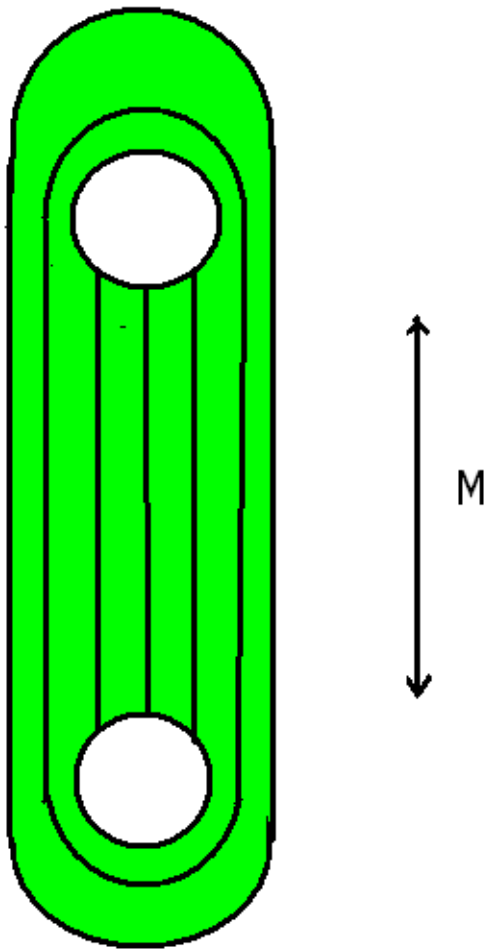


For M large enough the minimum energy configuration is unoriented, even though there is a minimizer among oriented maps.

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

The general case of two holes ($n = 2$).

Let $h(g)$ be the solution of the problem

$$\begin{aligned} \Delta h(g) &= 0 \text{ in } G \\ \frac{\partial h(g)}{\partial \nu} &= A(g) \times \frac{\partial A(g)}{\partial \tau} \text{ on } \partial\text{-} \\ h(g) &= 0 \text{ on } \partial\omega_1 \cup \partial\omega_2, \end{aligned}$$

where $\frac{\partial}{\partial \tau}$ is the tangential derivative on the boundary (cf Bethuel, Brezis, Helein).

Let $J(g) = (J(g)^1, J(g)^2)$, where $J(g)^i = \frac{1}{2\pi} \int_{\partial\omega_i} \frac{\partial h(g)}{\partial \nu} ds$.

Theorem

All global minimizers are nonorientable iff

$$\text{dist}(J(g)^1, \mathbb{Z}) < \text{dist}(J(g)^1, 2\mathbb{Z})$$

and all are orientable iff

$$\text{dist}(J(g)^1, 2\mathbb{Z}) < \text{dist}(J(g)^1, 2\mathbb{Z}+1)$$

In the stadium example we can show that the first condition holds whatever the distance between the holes, so that the minimizer is always non-orientable.

Existence for full Q-tensor theory

We have to minimize

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

subject to suitable boundary conditions.

Suppose we take $\psi_B : \mathcal{E} \to \mathbf{R}$ to be continuous and bounded below, $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$, (e.g. of the quartic form considered previously) and

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

which is the simplest form that reduces to Oseen-Frank in the constrained case.

Theorem (Davis & Gartland 1998)

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with smooth boundary $\partial\Omega$. Let $L_4 = 0$ 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

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

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.

Proposition. For any boundary conditions, if $L_4 \neq 0$ then

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

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

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

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

Choose

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

where $r = |x|$. Then

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

and

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

Hence

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

where C is a constant.

Provided θ is bounded, all the terms are bounded except

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

Choose

$$\theta(r) = \begin{cases} \theta_0(2 + \sin kr) & 0 < r < \frac{1}{2} \\ 2\theta_0(2 + \sin \frac{k}{2})(1 - r) & \frac{1}{2} < r < 1 \end{cases}$$

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

$$4\pi \int_0^{\frac{1}{2}} r^2 \left(\frac{2}{3} C + \frac{4}{9} L_4 \theta_0 (2 + \sin kr) \right) \theta_0^2 k^2 \cos^2 kr \, dr,$$

which tends to $-\infty$ if $L_4\theta_0$ is sufficiently negative.

The Onsager model (joint work with Apala Majumdar)

In the Onsager model 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

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

With the Maier-Saupe molecular interaction, the internal energy is given by

$$U(\rho) \;=\; \kappa \int_{S^2}\int_{S^2} [\tfrac{1}{3} - (p\cdot q)^2]\rho(p)\rho(q)\,dp\,dq$$

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

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 $U(\rho) = -\kappa|Q(\rho)|^2$ and

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

Given Q we define

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

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

Let

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

Given Q with $Q = Q^T, \operatorname{tr} Q = 0$ and satisfying $\lambda_i(Q) > -1/3$ we seek to minimize J on the set of admissible ρ

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

Remark: We do not impose the condition $\rho(p) = \rho(-p)$, since it turns out that the minimizer in $\mathcal{A}_Q$ satisfies this condition.

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

(Remark: this is not true if we allow some $\lambda_i = -1/3$.)

Proof. A singular measure μ satisfying the constraints is

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

and a $\rho \in \mathcal{A}_Q$ can be obtained by approximating this.

For $\varepsilon > 0$ sufficiently small and $i = 1, 2, 3$ let

$$\varphi_i^\varepsilon = \begin{cases} 0 & \text{if } |p \cdot e_i| < 1 - \varepsilon \\ \frac{1}{4\pi\varepsilon} & \text{if } |p \cdot e_i| \geq 1 - \varepsilon \end{cases}$$

Then

$$\rho(p) = \frac{1}{(1 - \frac{1}{2}\varepsilon)(1 - \varepsilon)} \sum_{i=1}^{3} [\lambda_i + \frac{1}{3} - \frac{\varepsilon}{2} + \frac{\varepsilon^2}{6}] \varphi_{e_i}^\varepsilon(p)$$

works. $\square$

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

Proof. By the direct method, using the facts that $\rho \ln \rho$ is strictly convex and grows superlinearly in ρ, while $\mathcal{A}_Q$ is sequentially weakly closed in $L^1(S^2)$. $\square$

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

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

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

The Euler-Lagrange equation for J

Theorem. Let $Q = \mathrm{diag}\,(\lambda_1, \lambda_2, \lambda_3)$. 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 solve the equations

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

and are unique up to adding a constant to each μ_i.

Proof. We need to show that ρ_Q satisfies the Euler-Lagrange equation. There is a small difficulty due to the constraint $\rho \geq 0$. For $\tau > 0$ let $S_\tau = \{p \in S^2 : \rho_Q(p) > \tau\}$, and let $z \in L^\infty(S^2)$ be zero outside S_τ and such that

$$\int_{S_\tau} (p \otimes p - \frac{1}{3}\mathbf{1}) z(p)\, dp = 0, \quad \int_{S_\tau} z(p)\, dp = 0.$$

Then $\rho_\varepsilon := \rho_Q + \varepsilon z \in \mathcal{A}_Q$ for all $\varepsilon > 0$ sufficiently small. Hence

$$\frac{d}{d\varepsilon} J(\rho_\varepsilon)|_{\varepsilon=0} = \int_{S_\tau} [1 + \ln \rho_Q] z(p)\, dp = 0.$$

So by Hahn-Banach

$$1 + \ln \rho_Q = \sum_{i,j=1}^{3} C_{ij}[p_i p_j - \frac{1}{3}] + C$$

for constants $C_{ij}(\tau), C(\tau)$. Since S_τ increases as τ decreases the constants are independent of τ, and hence

$$\rho_Q(p) = A \exp\left(\sum_{i,j=1}^{3} C_{ij} p_i p_j\right) \text{ if } \rho_Q(p) > 0.$$

Suppose for contradiction that

$$E = \{p \in S^2 : \rho_Q(p) = 0\}$$

is such that $\mathcal{H}^2(E) > 0$. Note that since $\int_{S^2} \rho_Q dp = 1$ we also have that $\mathcal{H}^2(S^2 \backslash E) > 0$. There exists $z \in L^\infty(S^2)$ such that

$$\int_{\{\rho_Q > 0\}} (p \;\; p - \frac{1}{3}\mathbf{1}) z(p)\, dp = 0, \; \int_{\{\rho_Q > 0\}} z(p)\, dp = 4\pi.$$

Indeed if this were not true then by Hahn-Banach we would have

$$1 = \sum_{i,j=1}^{3} D_{ij}(p_i p_j - \frac{1}{3}\delta_{ij}) \text{ on } S^2 \backslash E$$

for a constant matrix $D = (D_{ij})$.
Changing coordinates we can assume that $D = \sum_{i=1}^{3} \mu_i e_i \quad e_i$ and so $1 = \sum_{i=1}^{3} \mu_i (p_i^2 - \frac{1}{3})$ on $S^2 \backslash E$ for constants μ_i. If the μ_i are equal then the right-hand side is zero, a contradiction, while if the μ_i are not all zero it is easily shown that the intersection of S^2 with the set of such p has 2D measure zero.

Define for $\varepsilon > 0$ sufficiently small

$$\rho_\varepsilon = \rho_Q + \varepsilon - \varepsilon z.$$

Then $\rho_\varepsilon \in \mathcal{A}_Q$, since $\int_{S^2}(p \otimes p - \frac{1}{3}1)\, dp = 0$.
Hence, since ρ_Q is the unique minimizer,

$$\int_E \varepsilon \ln \varepsilon + \int_{\{\rho_Q > 0\}} [(\rho_Q + \varepsilon - \varepsilon z) \ln(\rho_Q + \varepsilon - \varepsilon z) - \rho_Q \ln \rho_Q]\, dp > 0.$$

This is impossible since the second integral is of order ε.
Hence we have proved that

$$\rho_Q(p) = A \exp(\sum_{i,j=1}^{3} C_{ij} p_i p_j), \text{a.e. } p \in S^2.$$

Lemma. Let $R^T Q R = Q$ for some $R \in O(3)$. Then $\rho_Q(Rp) = \rho_Q(p)$ for all $p \in S^2$.

Proof.

$$\begin{aligned}
&\int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1}) \rho_Q(Rp)\, dp \\
&\qquad = \quad \int_{S^2} (R^T q \otimes R^T q - \frac{1}{3}\mathbf{1}) \rho_Q(q)\, dq \\
&\qquad = \quad R^T Q R = Q,
\end{aligned}$$

and ρ_Q is unique. $\square$

Applying the lemma with $Re_i = -e_i$, $Re_j = e_j$ for $j \neq i$, we deduce that for $Q = \mathrm{diag}\,(\lambda_1, \lambda_2, \lambda_3)$,

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

where

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

as claimed.

Finally

$$\begin{aligned}\frac{\partial \ln Z}{\partial \mu_i} &= Z^{-1} \int_{S^2} p_i^2 \exp(\sum_{j=1}^{3} \mu_j p_j^2)\, dp \\ &= \lambda_i + \frac{1}{3},\end{aligned}$$

and the uniqueness of the μ_i up to adding a constant to each follows from the uniqueness of ρ_Q. $\square$

Hence the bulk free energy has the form

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

Remarks

1. $c_0 - \frac{1}{2}\ln(\lambda_{\min}(Q) + \frac{1}{3}) \leq \frac{1}{\theta}\psi_B \leq c_1 - \ln(\lambda_{\min}(Q) + \frac{1}{3})$.

2. All critical points of ψ_B are uniaxial. Phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

3. Minimizers ρ^* of $I_\theta(\rho)$ correspond to minimizers over Q of $\psi_B(Q)$. These ρ^* were calculated and shown to be uniaxial by Fatkullin and Slastikov (2005), Liu, H. Zhang and P. Zhang (2005).

Now consider the problem of minimizing

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

subject to, for example,

$$Q(x)|_{\partial\Omega} = Q_0(x).$$

Since $\psi_B(Q) \to \infty$ when $\lambda_{\mathsf{min}}(Q) \to -1/3$ the difficult term I_4 can be absorbed into I_3, since

$$I_3 + 3I_4 = (\delta_{kl} + 3Q_{kl})Q_{ij,k}Q_{ij,l} \geq 0$$

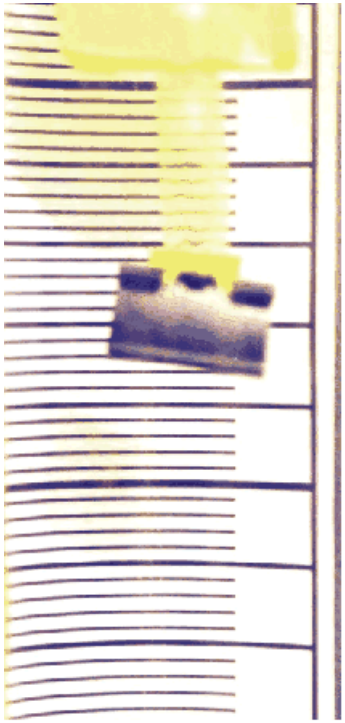
and the existence of a minimizer follows under appropriate conditions (c.f. Gartland & Davis) on the L_i, even when $L_4 \neq 0$.

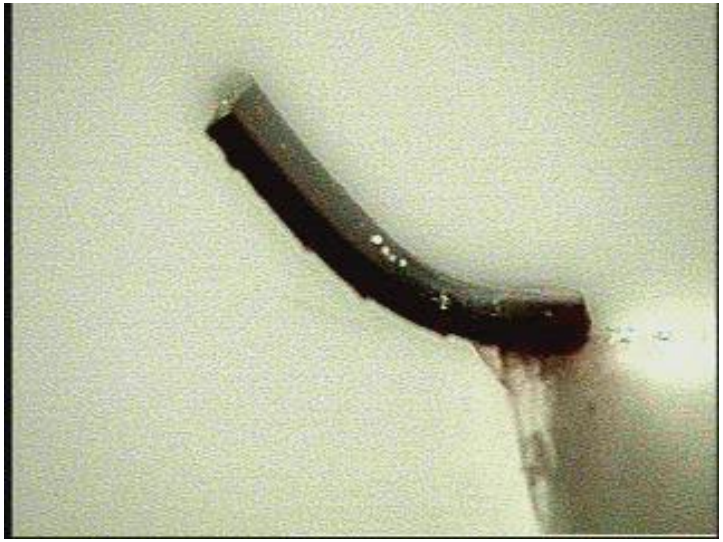
Liquid crystal elastomers

These are polymers for which the long chain molecules are liquid crystals.

Actuation by
hot and cold air
(E. Terentyev)

Courtesy M. Warner





Thermo-optical actuation
(P. Palffy-Muhoray)

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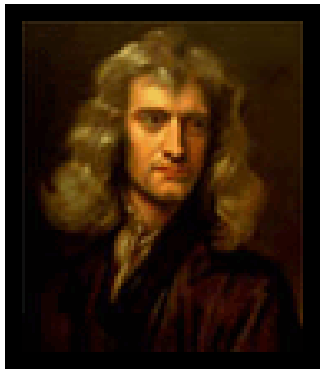

The Mathematics of Liquid Crystals

7 January - 5 July 2013

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Organisers:

John Ball
David Chillingworth
Mikhail Osipov
Peter Palffy-Muhoray
Mark Warner