Cours d’école doctorale
LJLL, Paris, Jan-Mar 2009

Défauts dans les cristaux et dans les cristaux liquides

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Plan of course

Lectures 1-3

Defects in solid crystals, arising from solid phase transformations.

Lectures 4-6

Defects in liquid crystals

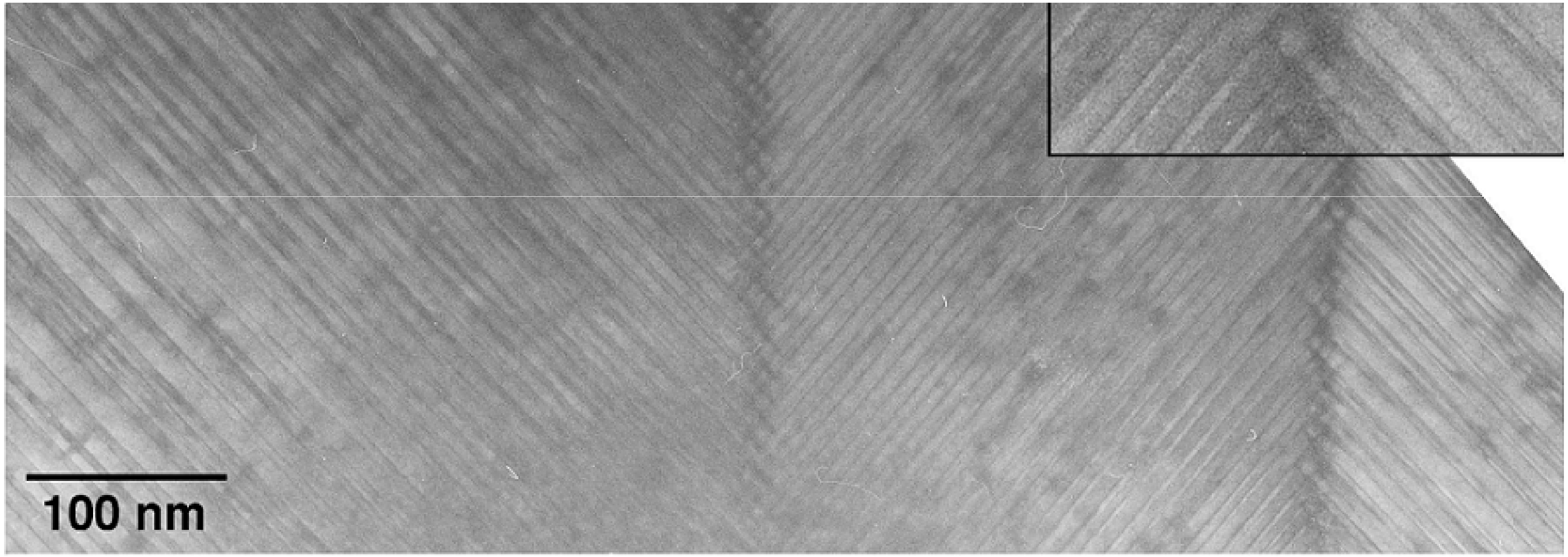
Plan for lectures 1-3

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

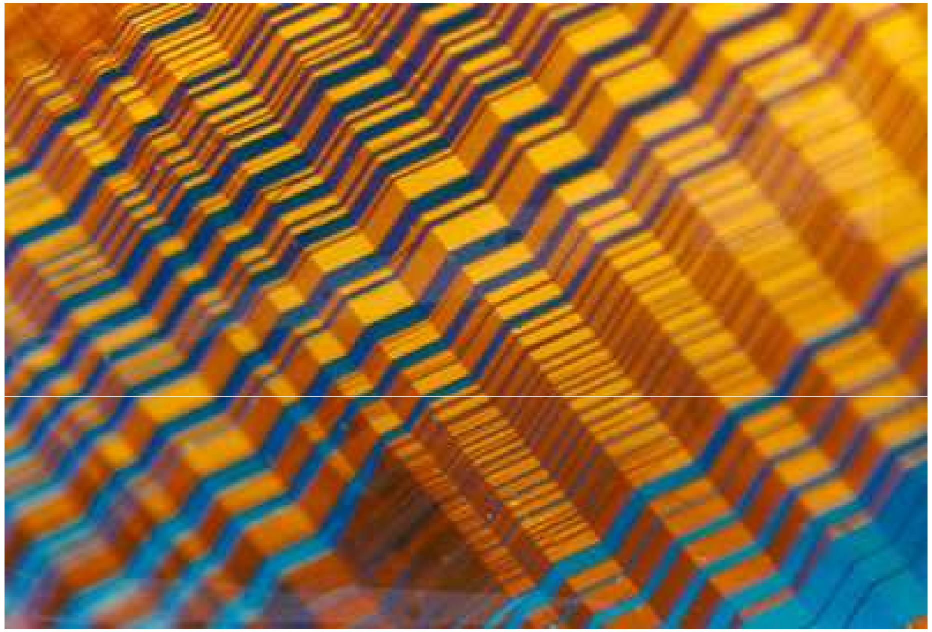
2. Macrotwins,
   Nonclassical austenite-martensite interfaces

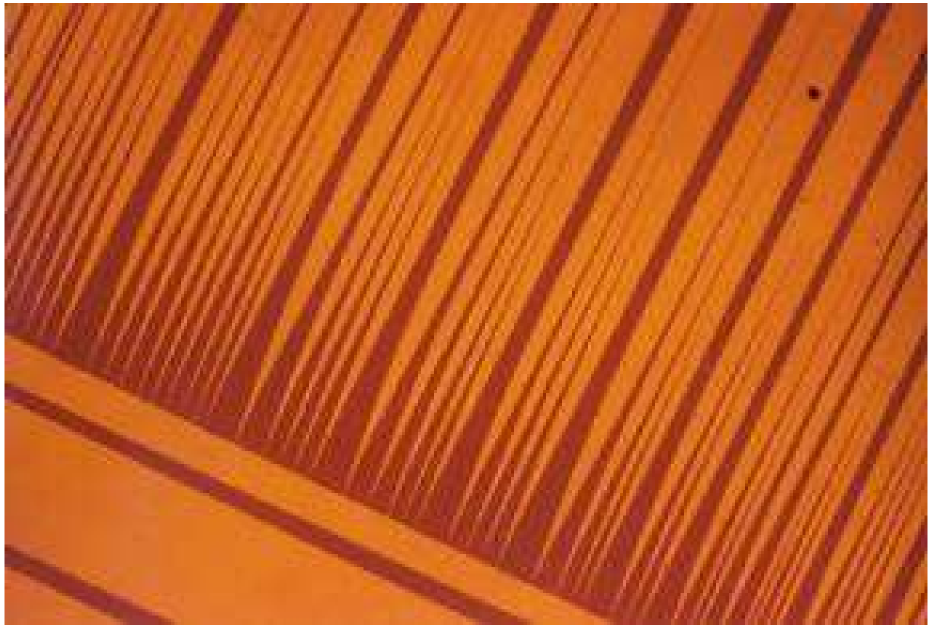
3. Incorporating interfacial energy.

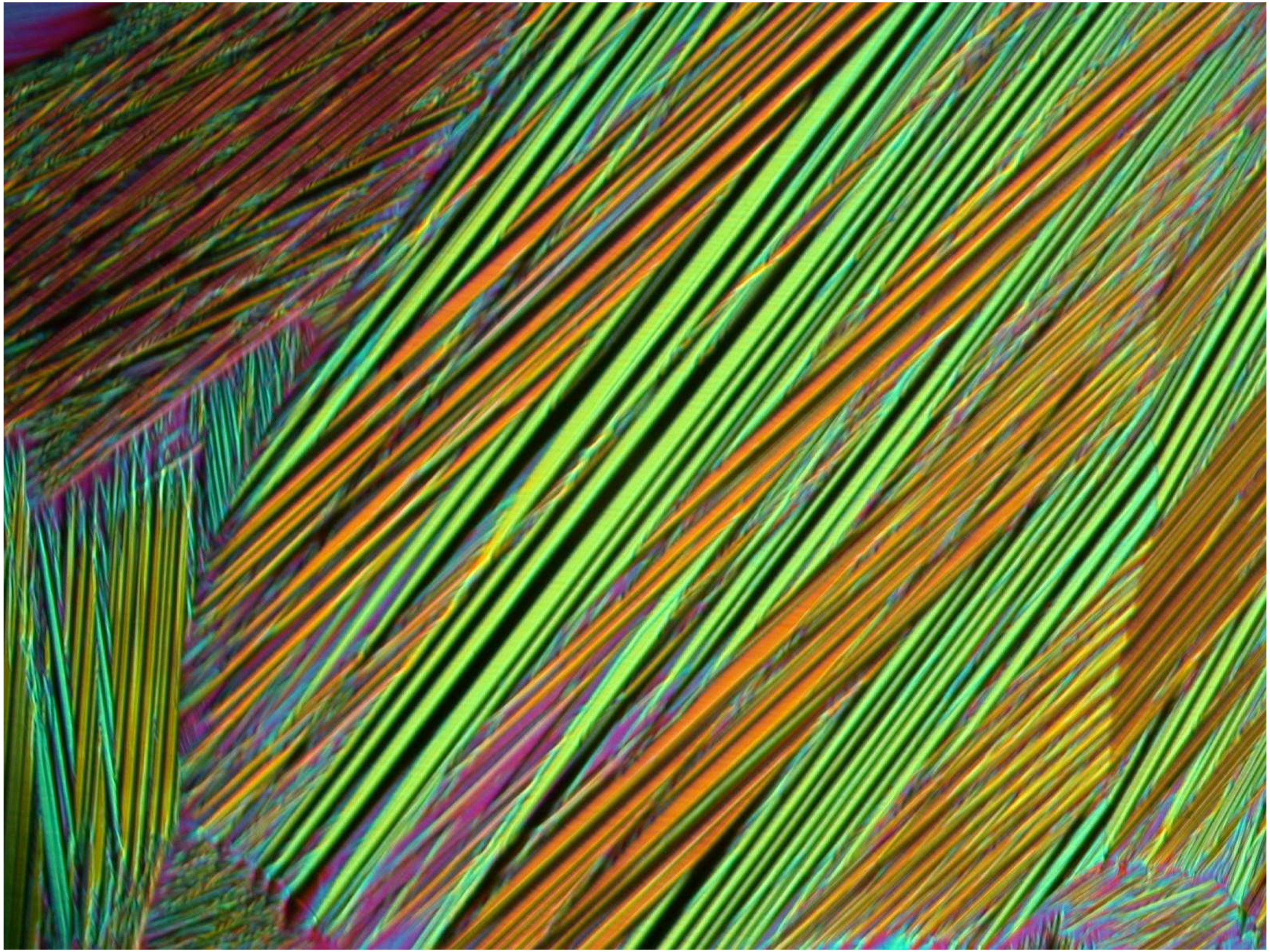
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



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.

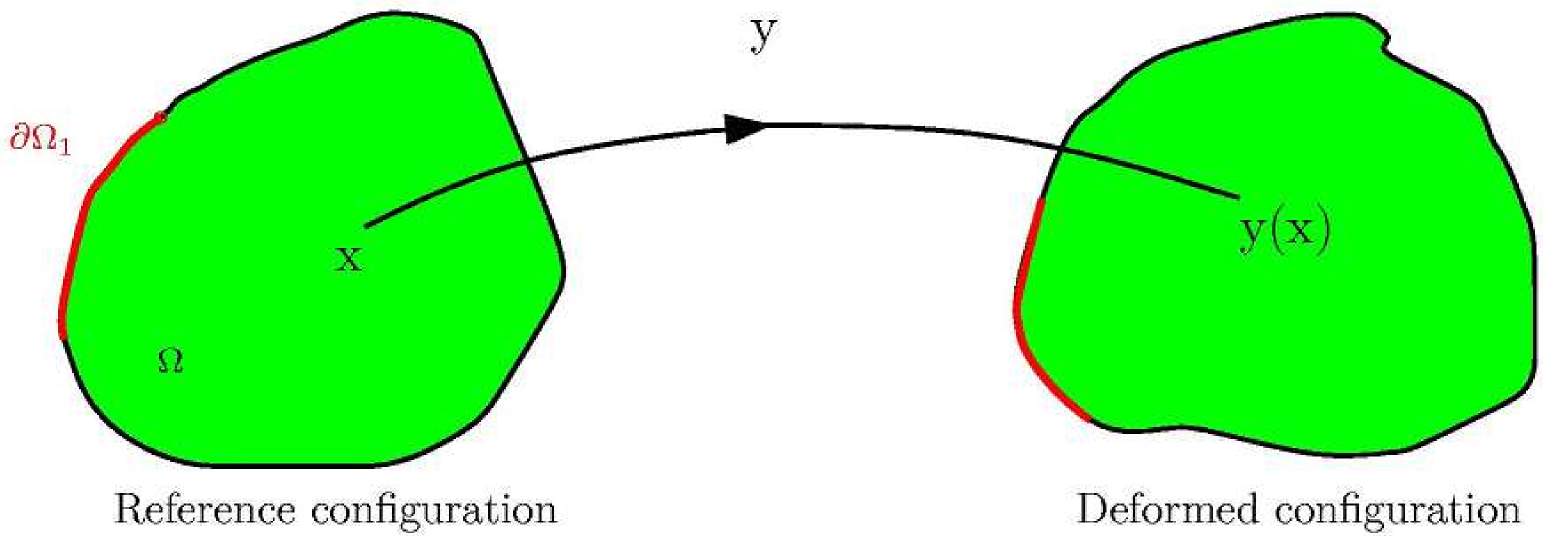
(a) what are appropriate dynamical equations?

(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

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

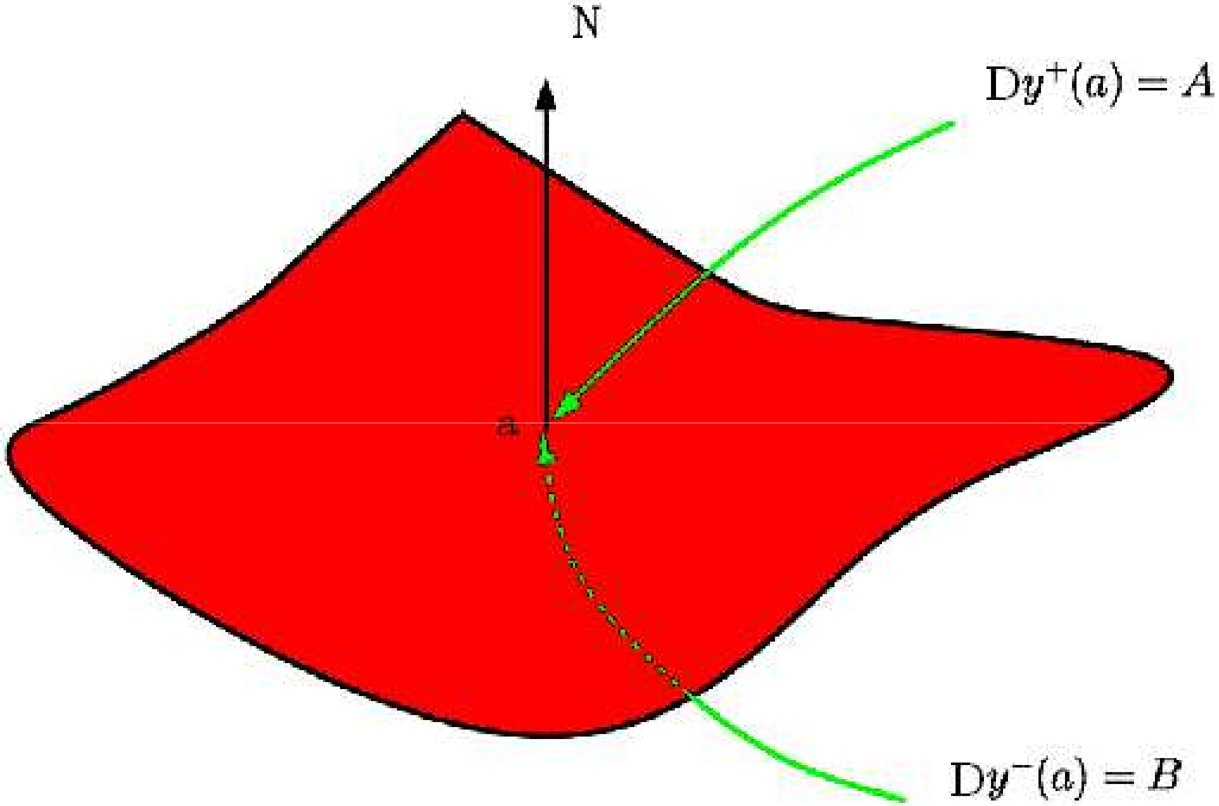
in the sense of distributions, i.e.

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

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

The condition is sufficient if Ω is simply connected.

Hadamard jump condition



y piecewise C^1

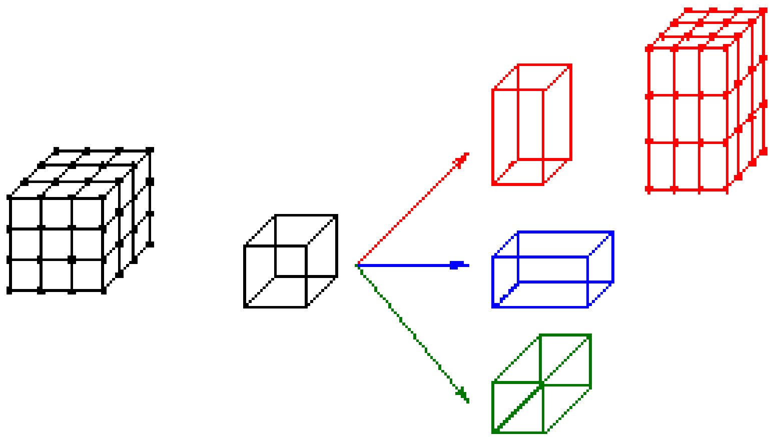
$$A - B = c \otimes N$$

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

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

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

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

austenite

Assume

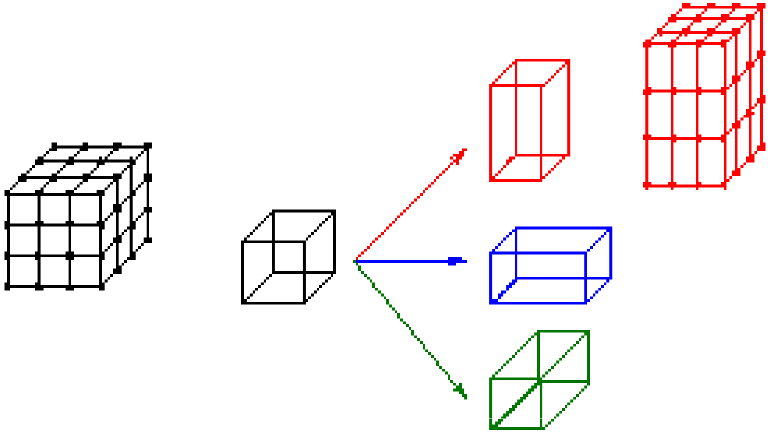
$$K(\theta) = \begin{cases} \alpha(\theta)\mathrm{SO}(3) & \theta > \theta_c \\ \mathrm{SO}(3) \cup \bigcup_{i=1}^N \mathrm{SO}(3)U_i(\theta_c) & \theta = \theta_c \\ \bigcup_{i=1}^N \mathrm{SO}(3)U_i(\theta) & \theta < \theta_c, \end{cases}$$

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

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 $Q \in P^{24}$.

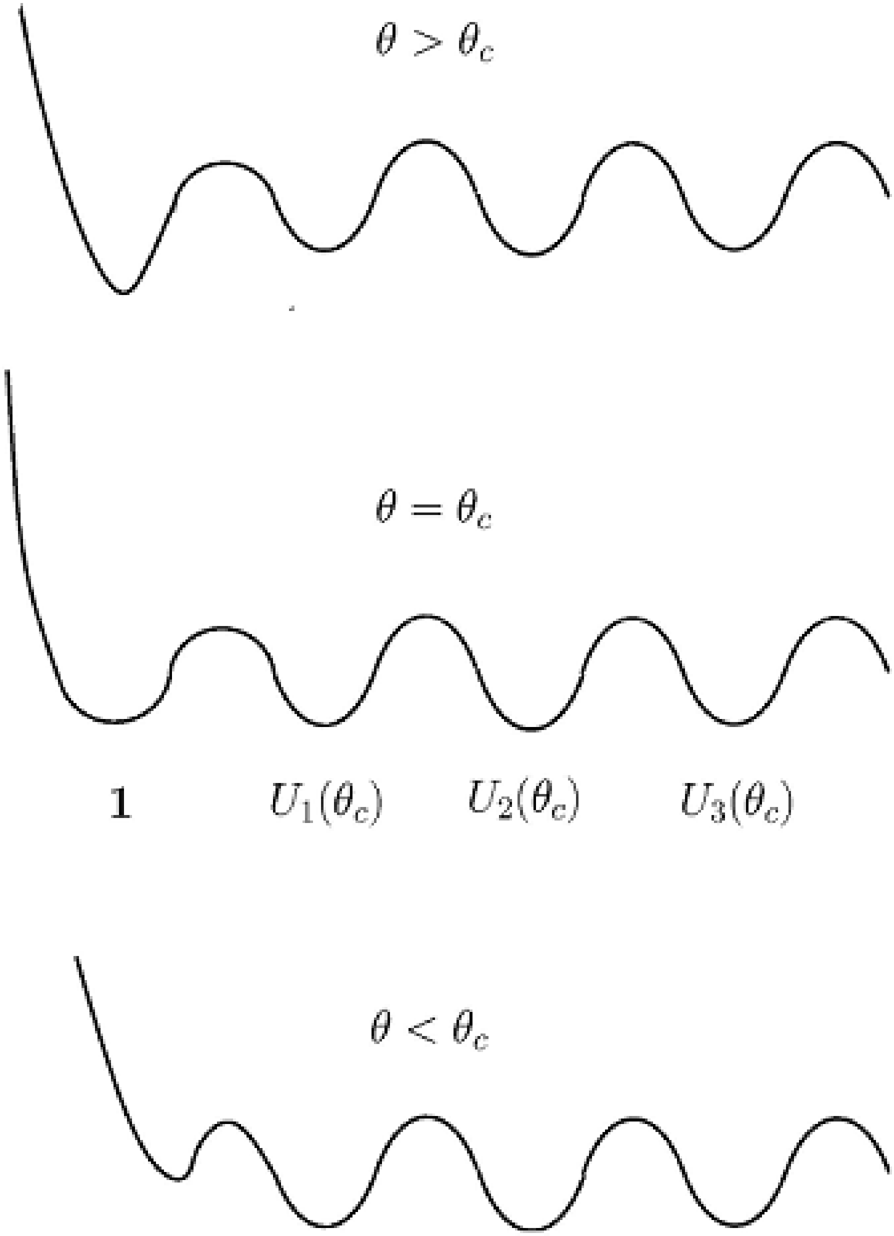
Cubic to tetragonal (e.g. $Ni_{65}Al_{35}$)



$$N = 3$$

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

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. $\lambda_1 = -\lambda_3$.*

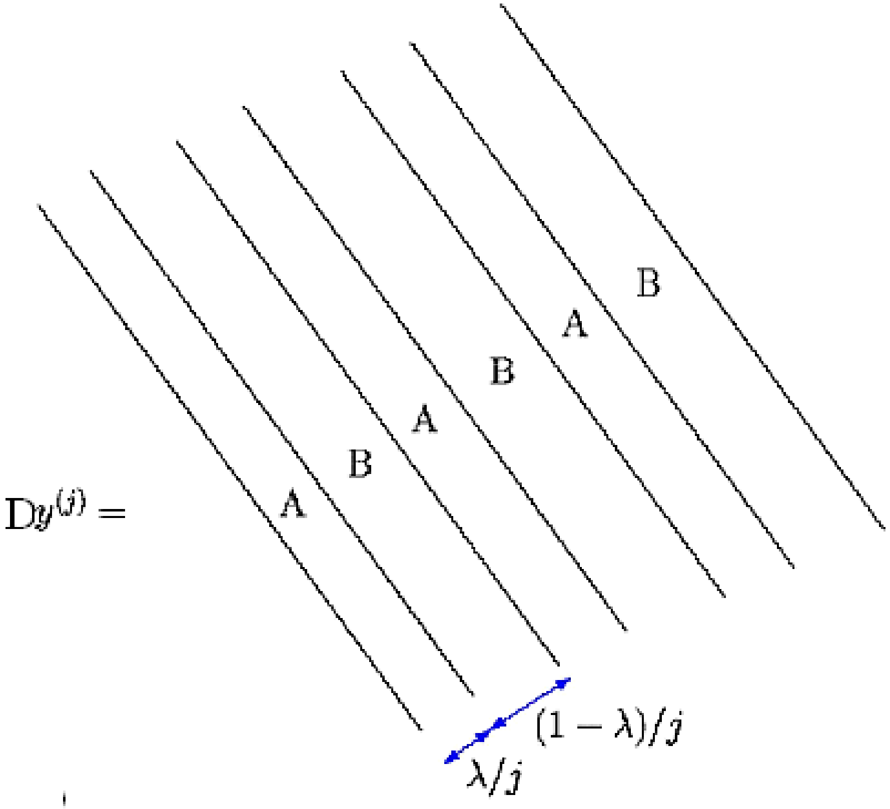
Twins

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

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

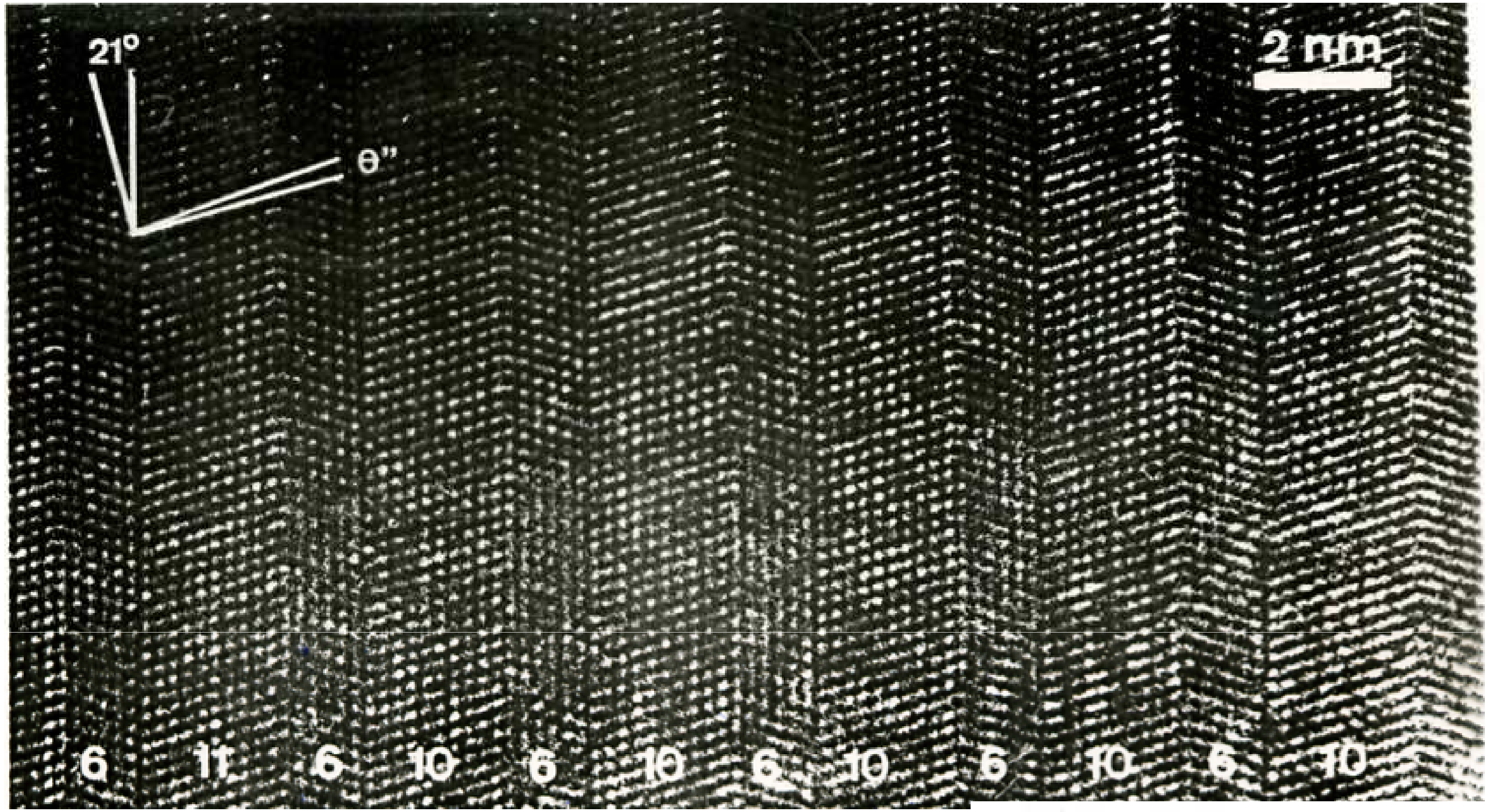
Weak convergence = convergence of averages



Simple laminate

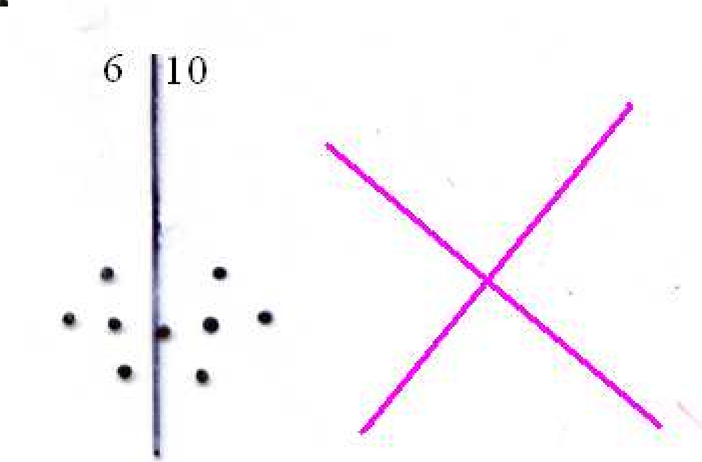
$$A - B = c \otimes N$$

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

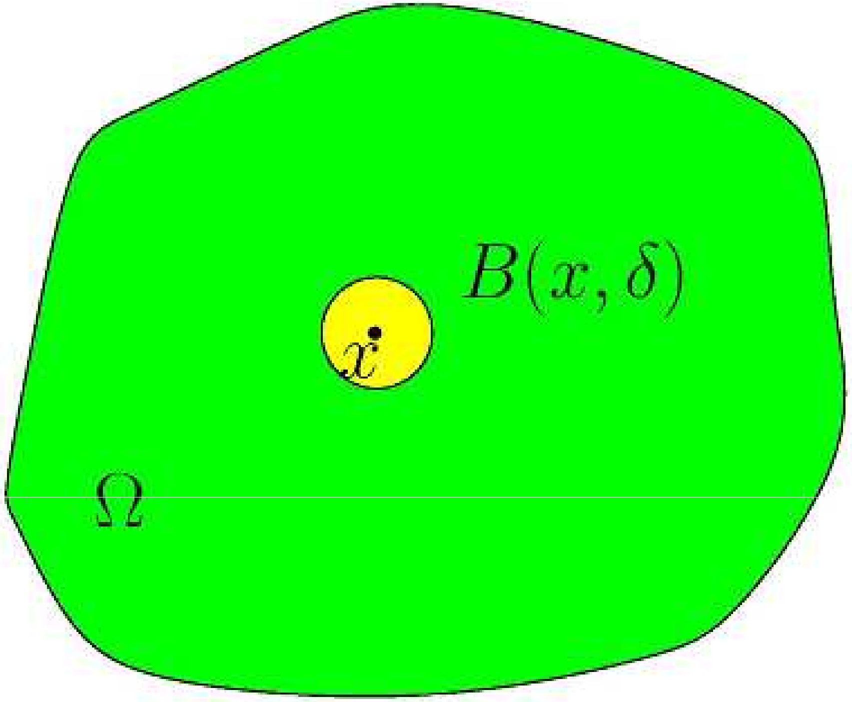


Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

Baele, van Tenderloo, Amelinckx



Gradient Young measures



Fix x, j, δ.

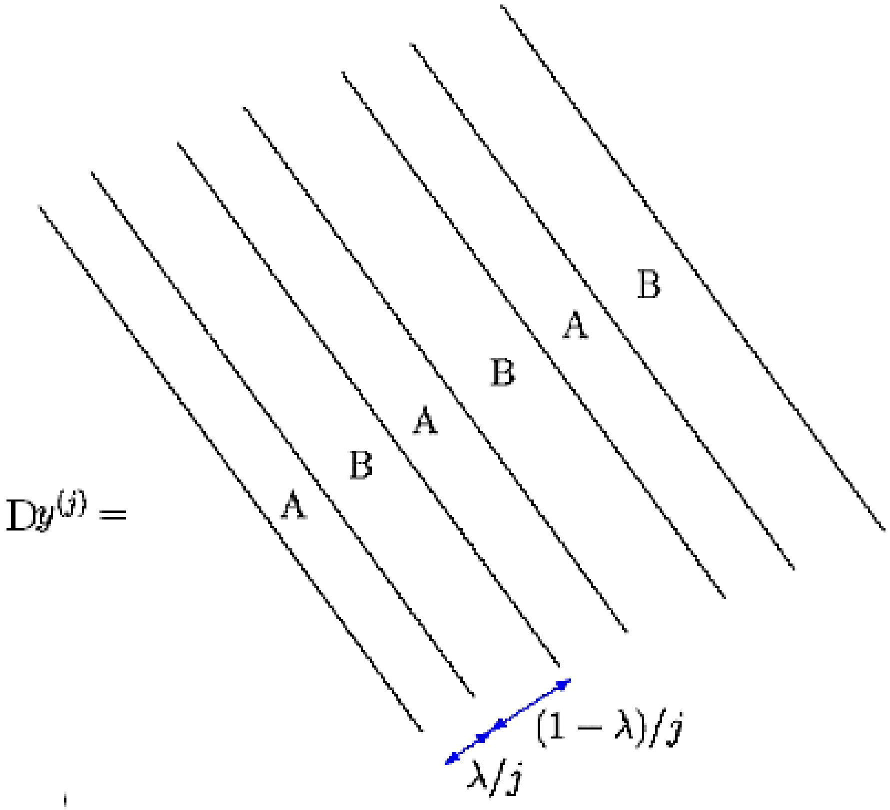
$$E \subset M^{m\times n}$$

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

$$\nu_x = \lim_{\delta\to 0} \lim_{k\to\infty} \nu_x^{j_k,\delta}$$

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

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

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

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

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

$K(\theta)^{\text{qc}}$ 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).

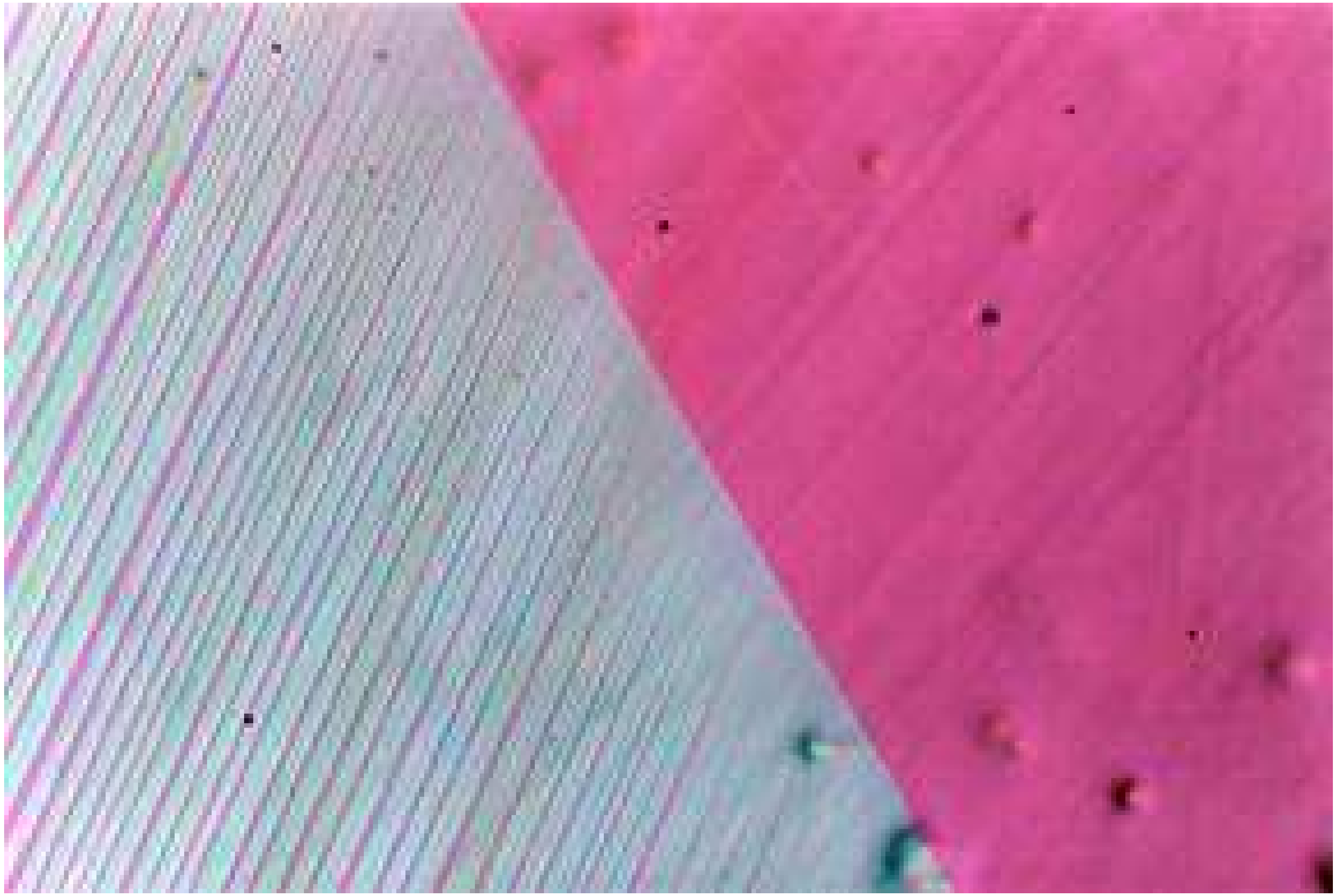
How does austenite transform to martensite as θ passes through θ_c?

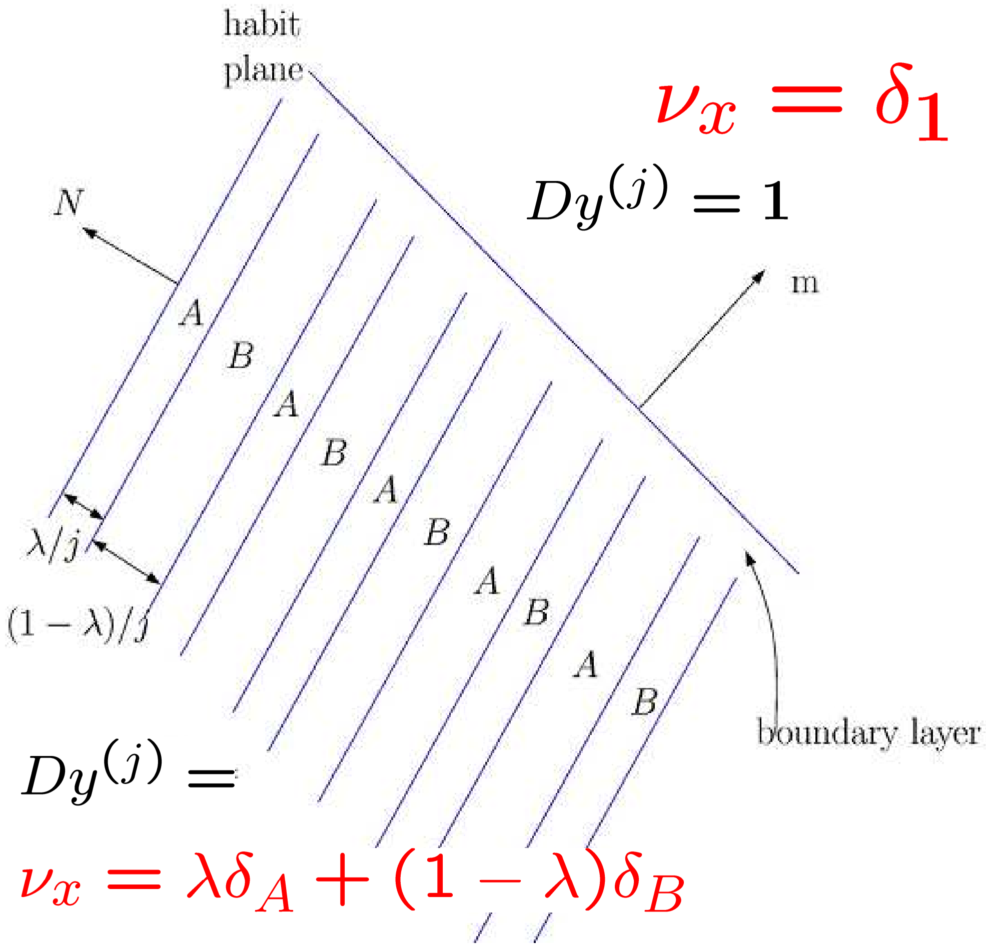
It cannot do this by means of an exact interface between austenite and martensite, because this requires the middle eigenvalue of U_i to be one, which in general is not the case (but see studies of James et al on low hysteresis alloys).

So what does it do?

(Classical) austenite-martensite interface in CuAlNi

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





$$\nu_x = \delta_1$$

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

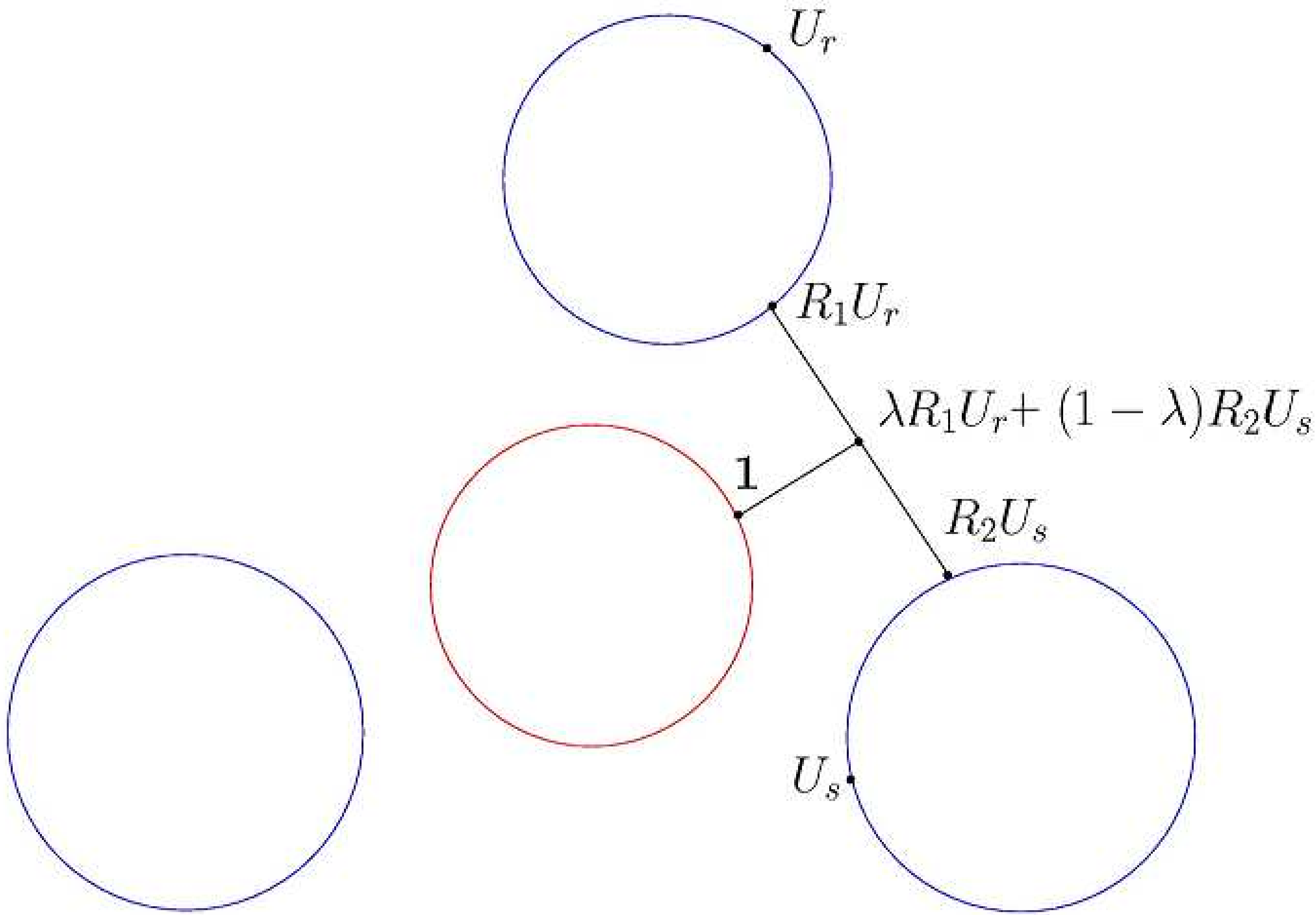
$$Dy^{(j)} =$$

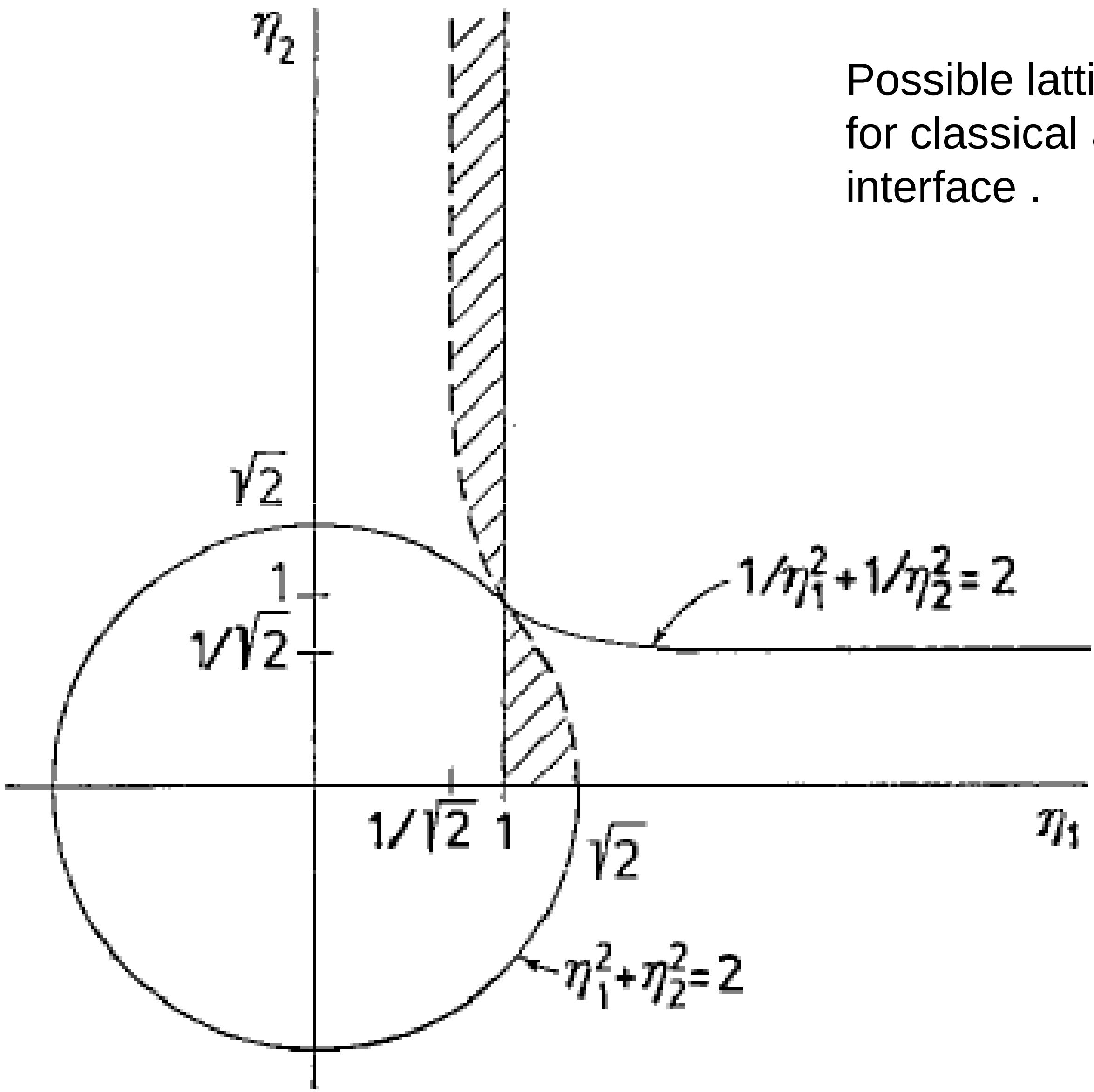
$$\nu_x = \lambda\delta_A + (1-\lambda)\delta_B$$

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

24 habit planes for cubic-to-tetragonal

Rank-one connections for A/M interface



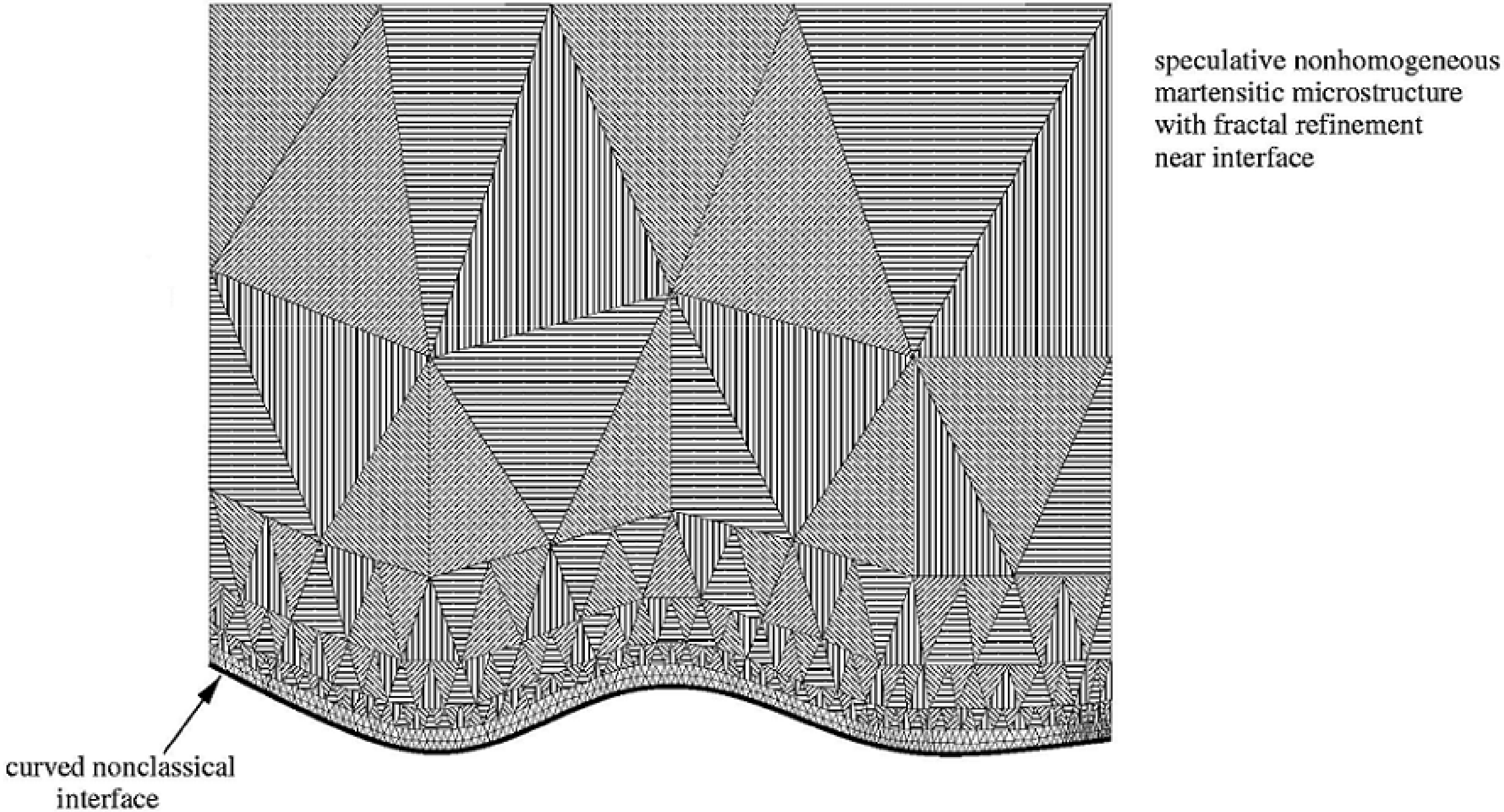


Possible lattice parameters
for classical austenite-martensite
interface .

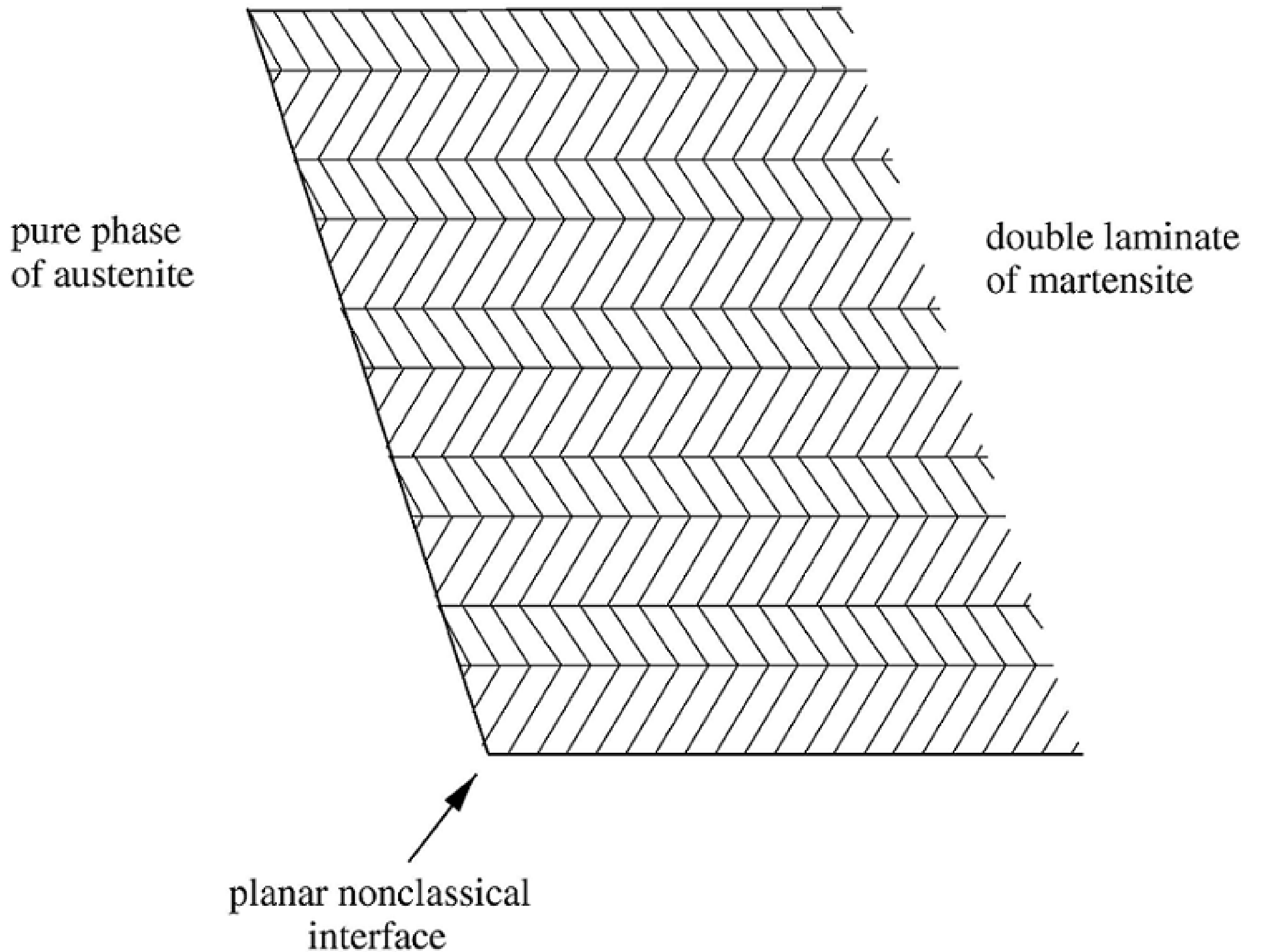
Nonclassical austenite-martensite interfaces

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

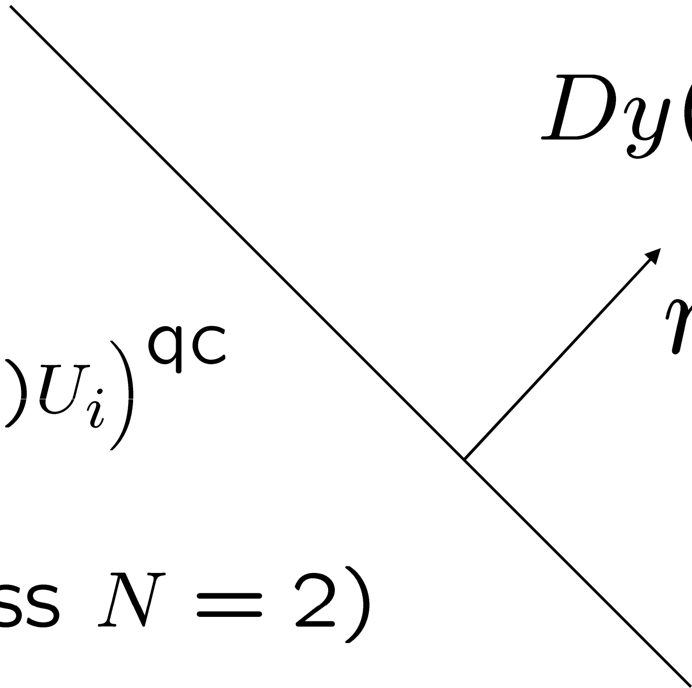
Nonclassical austenite-martensite interfaces (B/Carstensen 97)



Nonclassical interface with double laminate



Nonclassical interface calculation



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

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

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

(unknown unless $N = 2$)

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

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

More on quasiconvexifications

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

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

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.

$$\varphi \text{ polyconvex} \Rightarrow \varphi \text{ quasiconvex.}$$

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

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

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

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

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

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

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

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

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

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

Combining these inequalities we get that

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

For cubic to tetragonal we have that

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

and the necessary conditions become

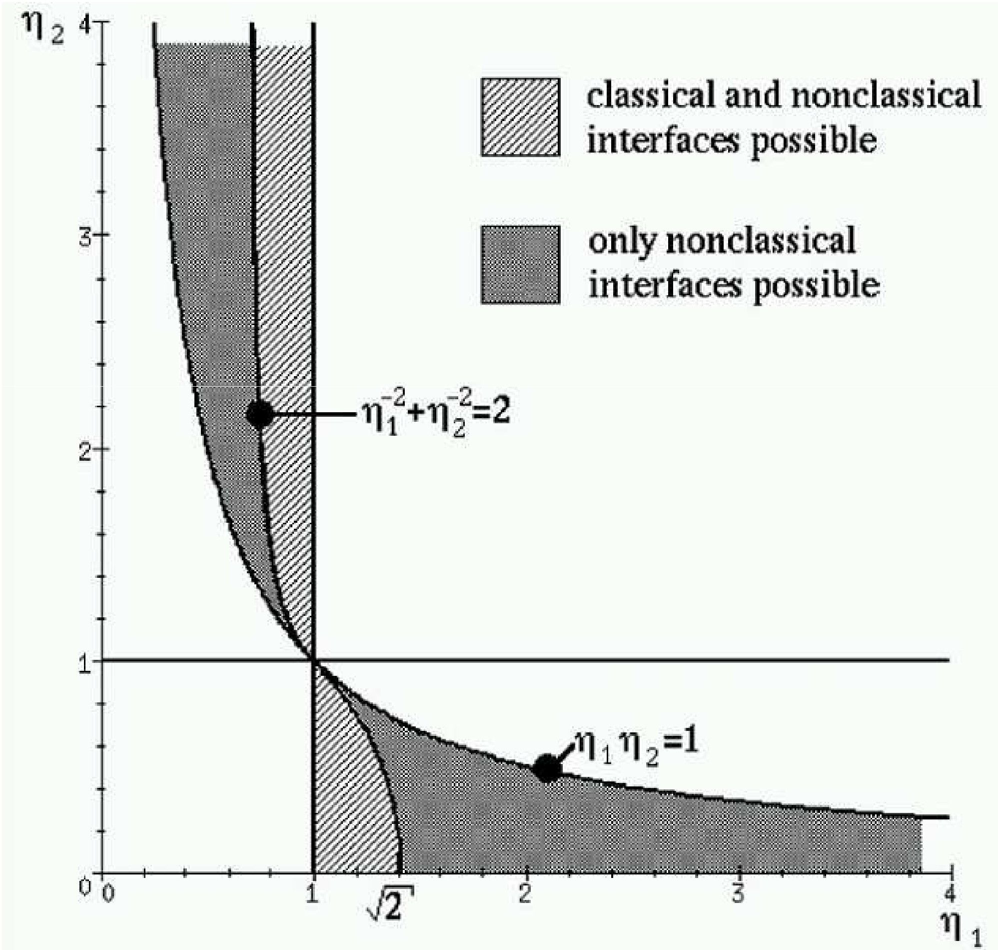
$$\eta_1 \le \eta_1^{-1} \le \eta_2 \text{ if } \eta_1 \le \eta_2,$$

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

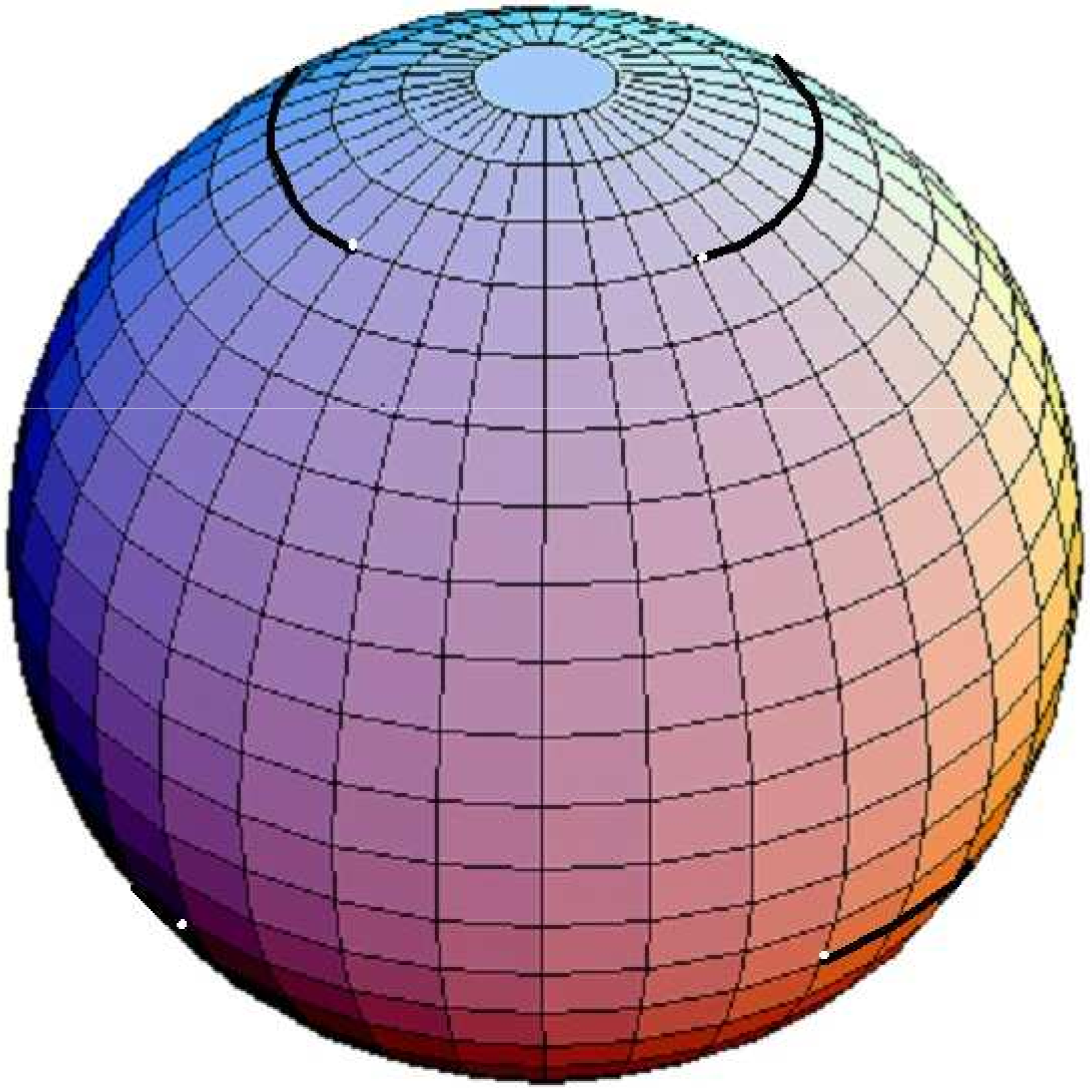
But these turn out to be exactly the conditions given by the two-well theorem to construct a rank-one connection from $(SO(3)U_1 \cup SO(3)U_2)^{qc}$ to the identity!

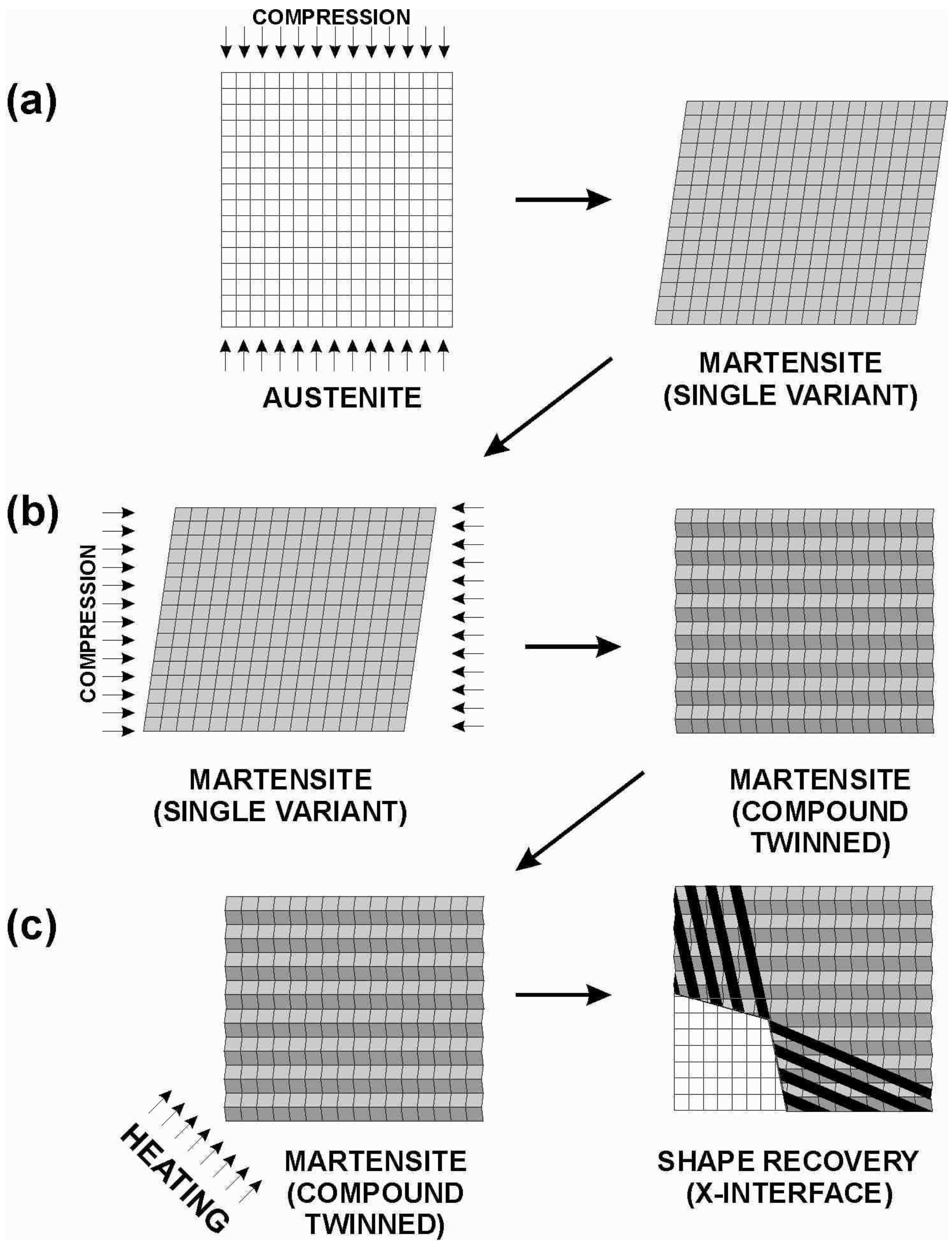
Hence the conditions are sufficient also.

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



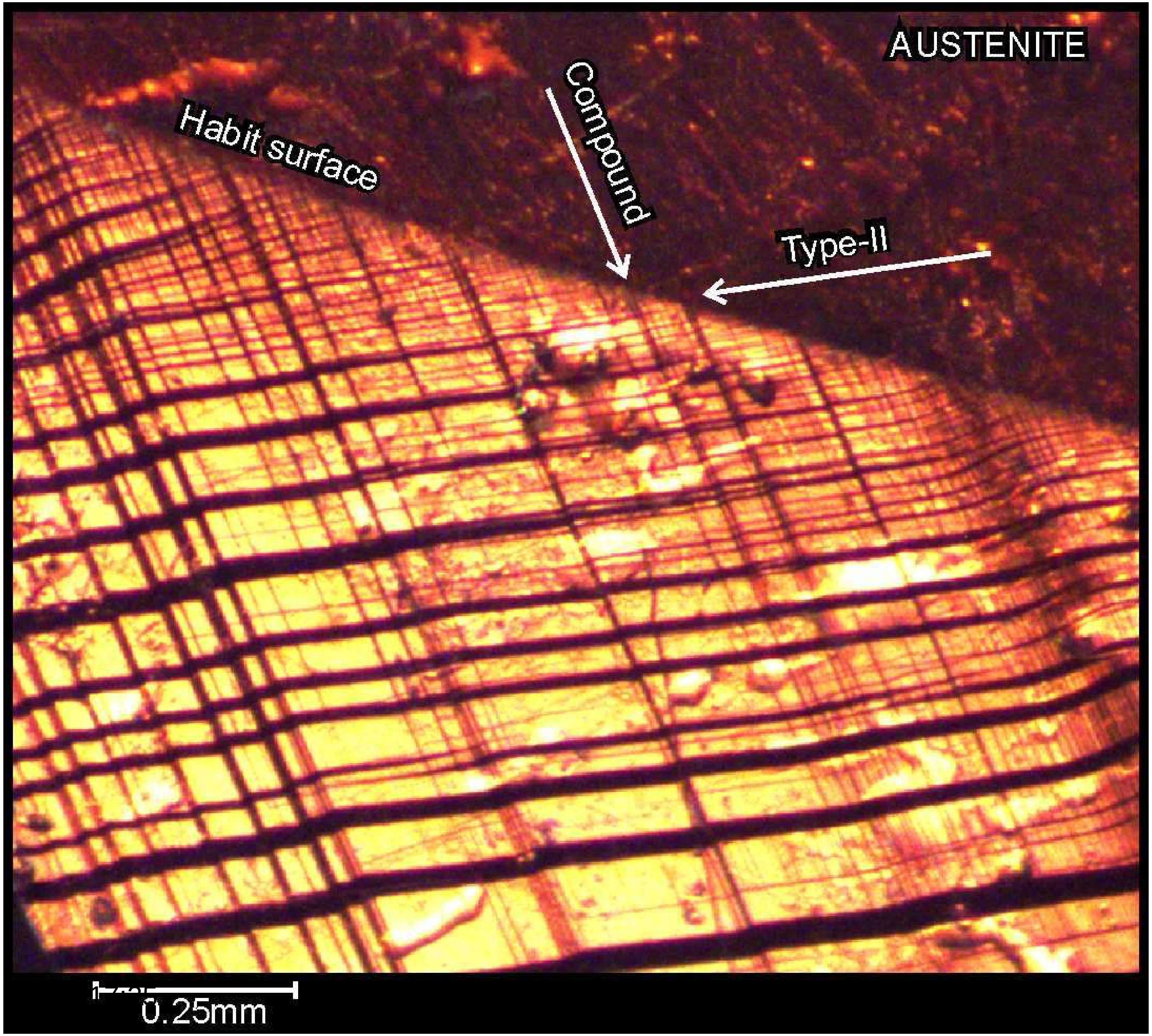
Interface normals



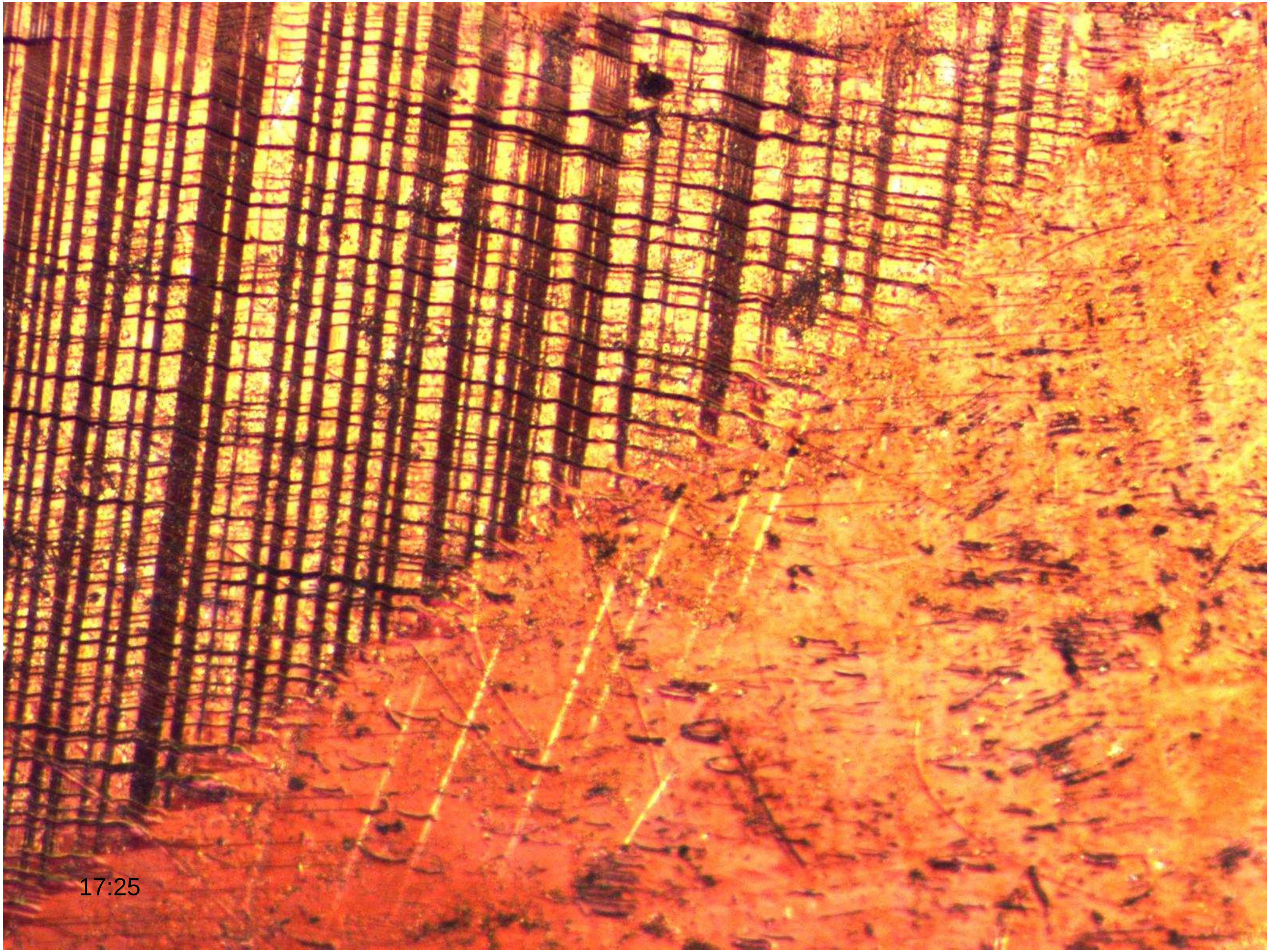


Experimental procedure (H. Seiner)

3.9×3.8×4.2mm CuAlNi single crystal



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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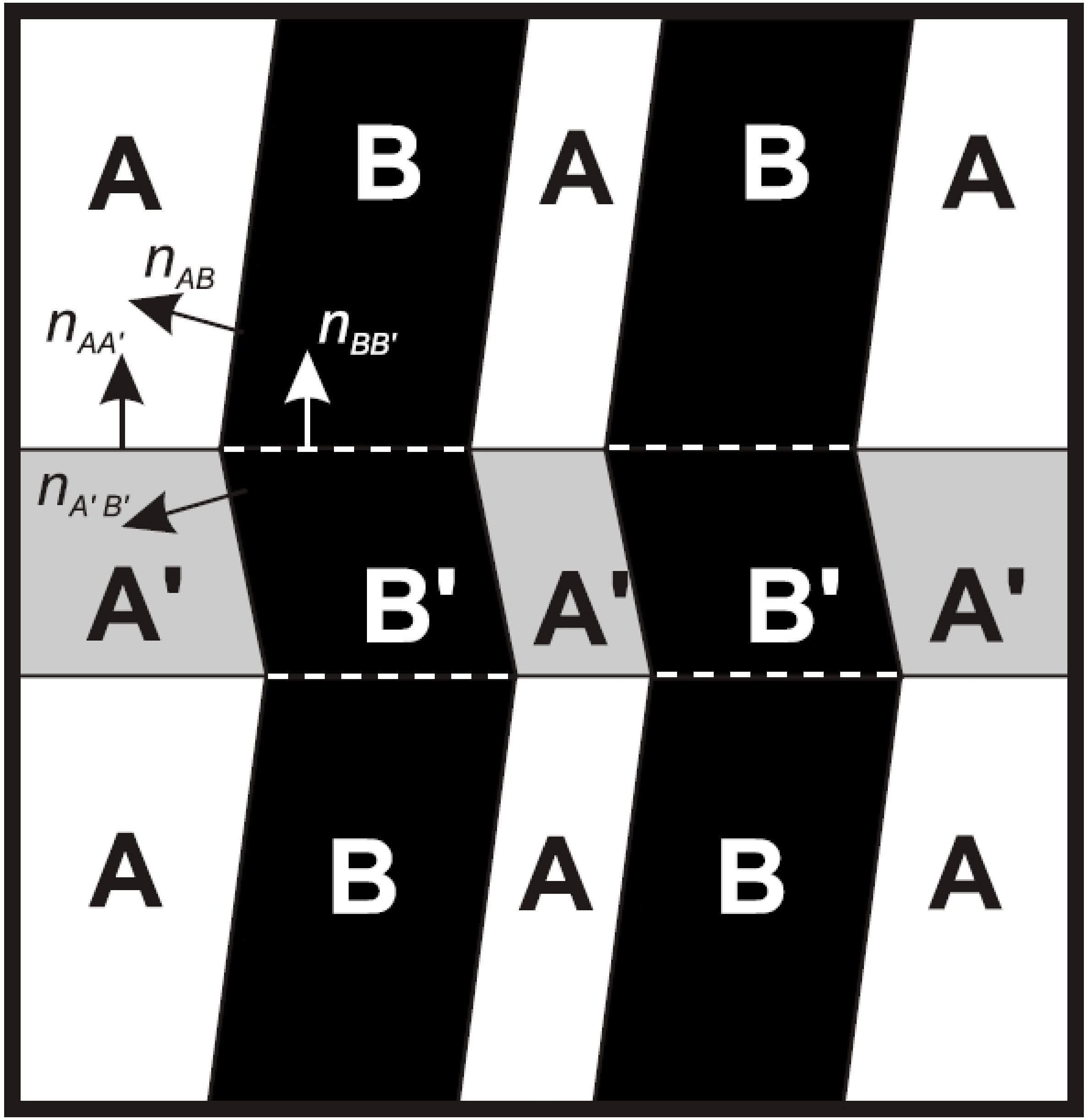


Twin crossing gradients

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

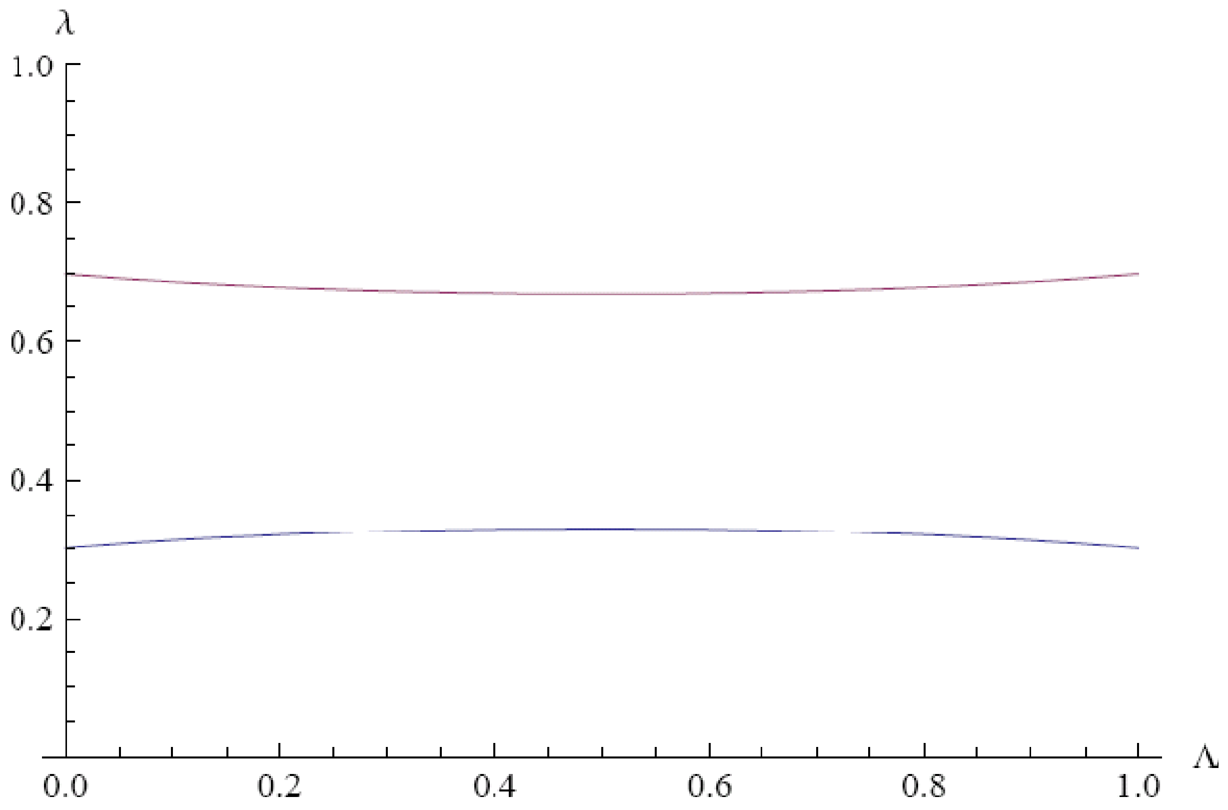
$$M = (1-\Lambda)M_{AB} + \Lambda R_{AA'}M_{A'B'}.$$

For compatibility with the austenite we need

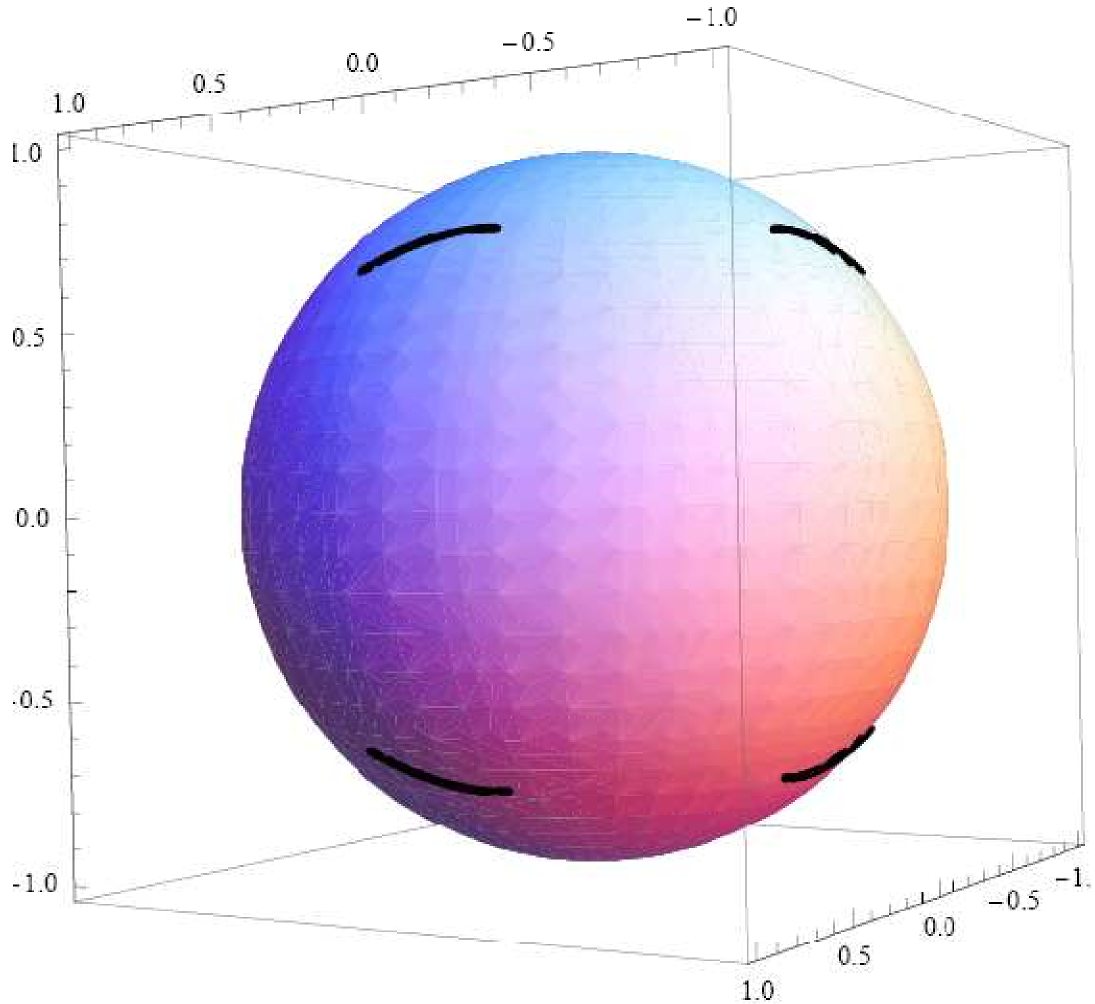
$$\lambda_{\mathsf{mid}}(M^T M) = 1$$

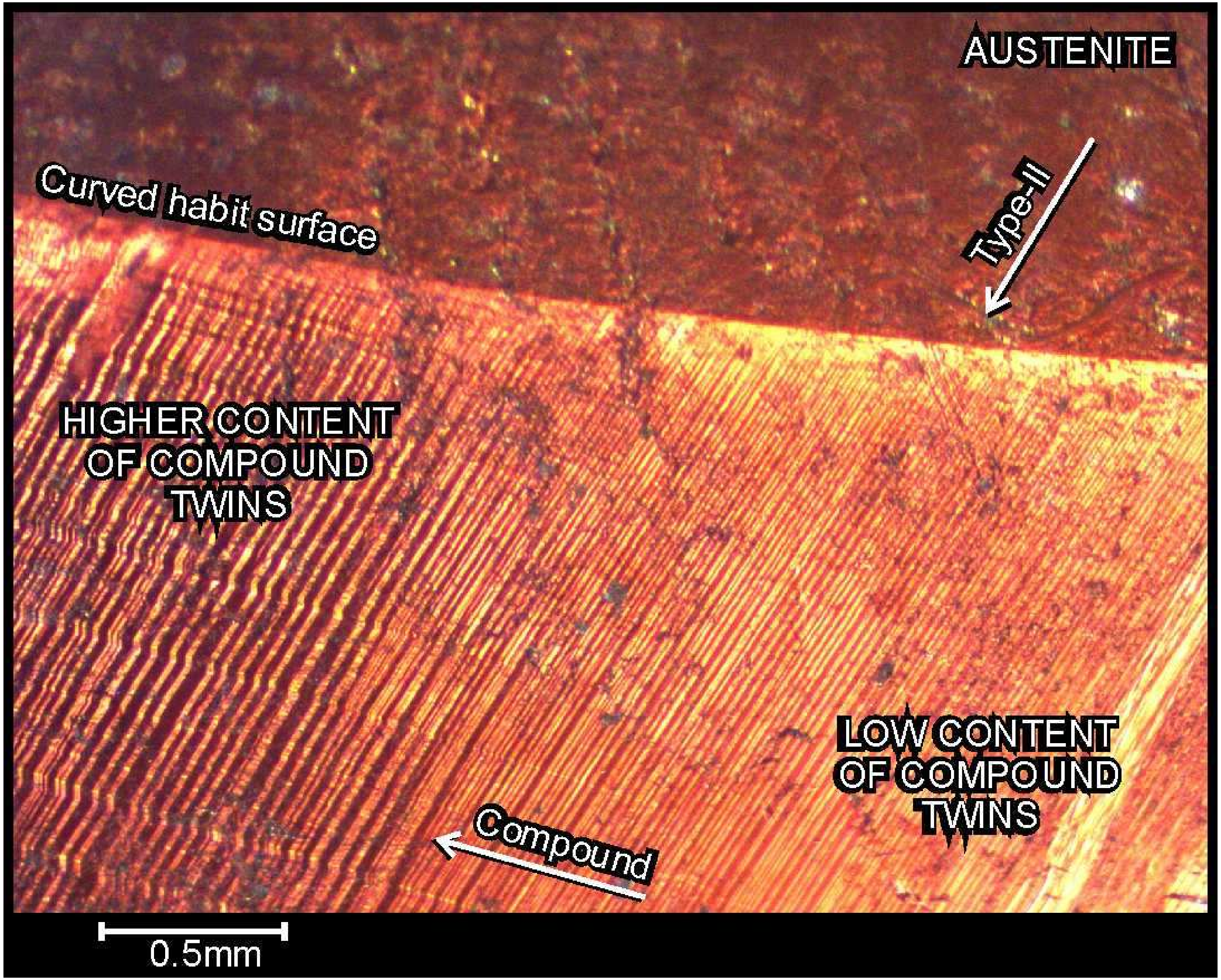
Possible volume fractions

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



Possible nonclassical interface normals



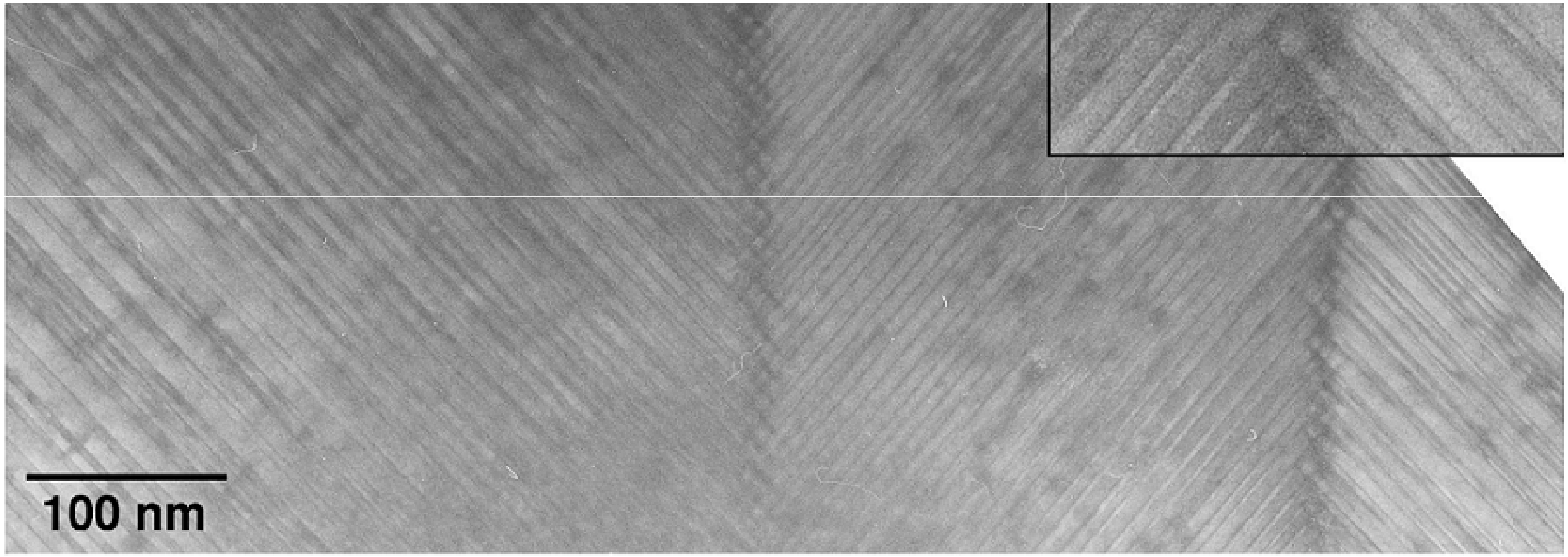


Curved interface between crossing twins and austenite resulting from the inhomogeneity of compound twinning. (Optical microscopy,H. Seiner)

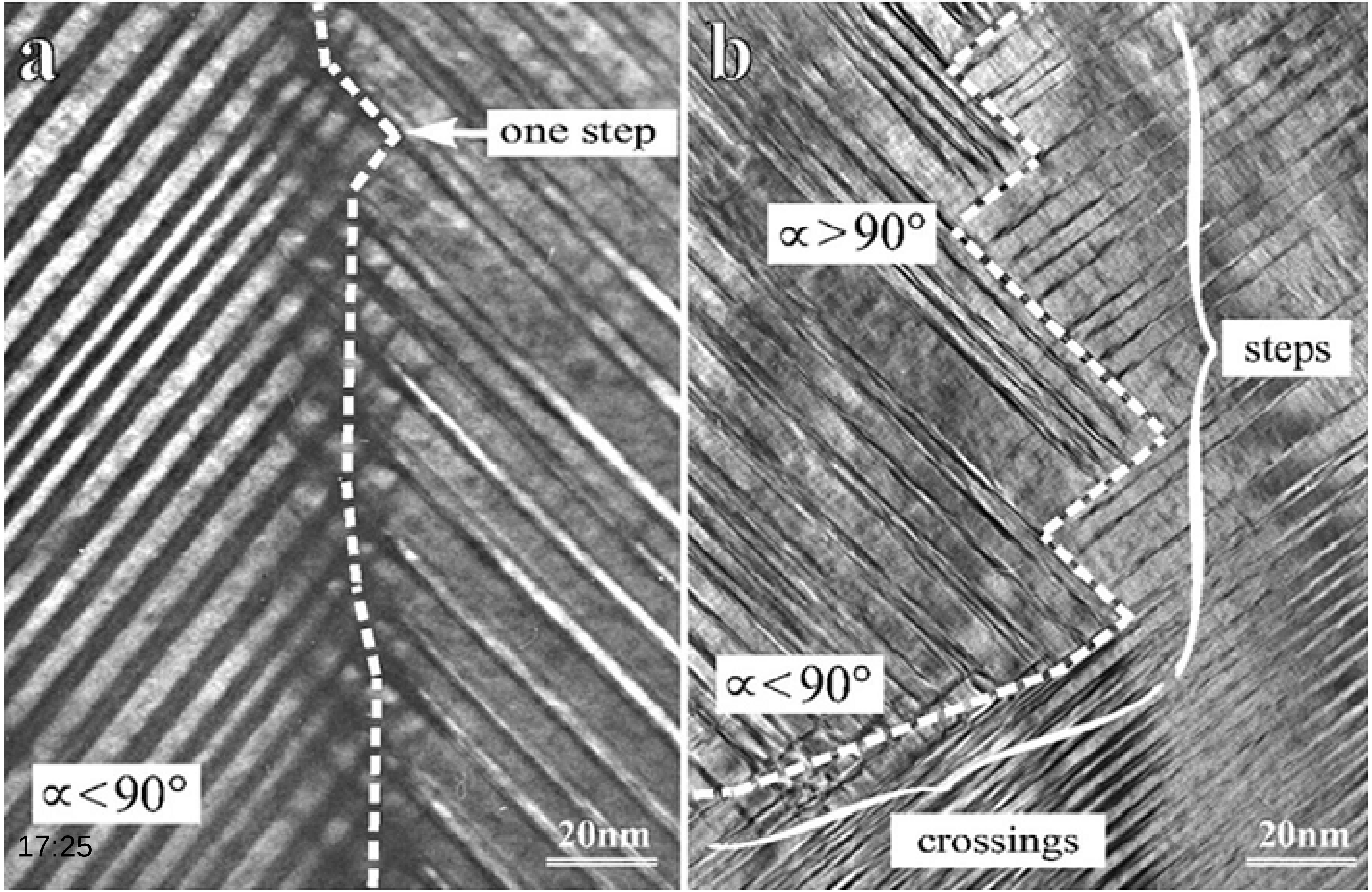
Macrotwins in $Ni_{65}Al_{35}$

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

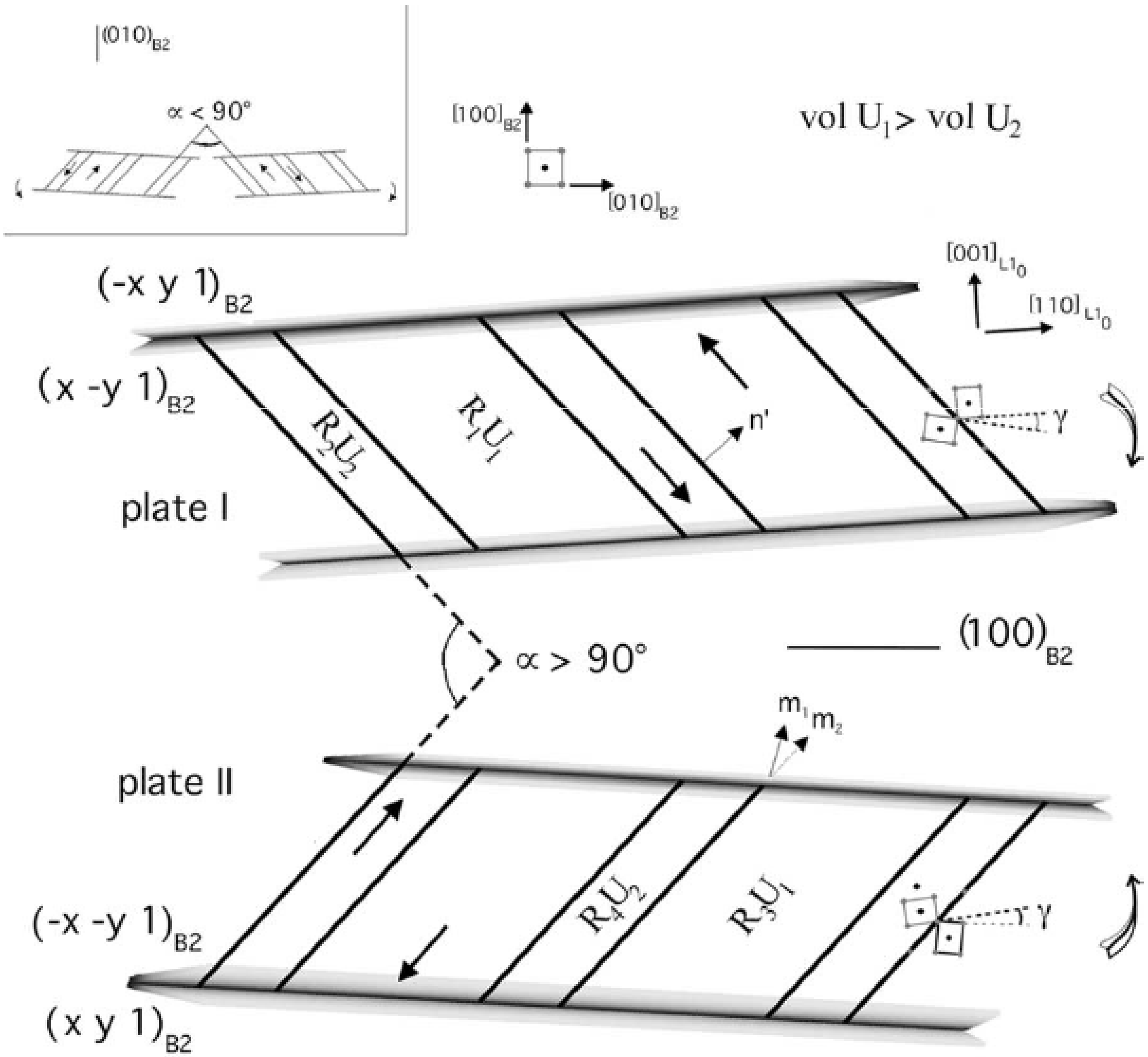
Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



Crossings and steps



Macrotwin formation



Macroscopic deformation gradient in martensitic plate is

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

B/Schryvers

Different martensitic plates never compatible (Bhattacharya)

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

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

:y with Plate I ($\kappa_1 = \chi_1 = \nu_1 = 1$) and rotation is that of a right-handed screw 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)

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

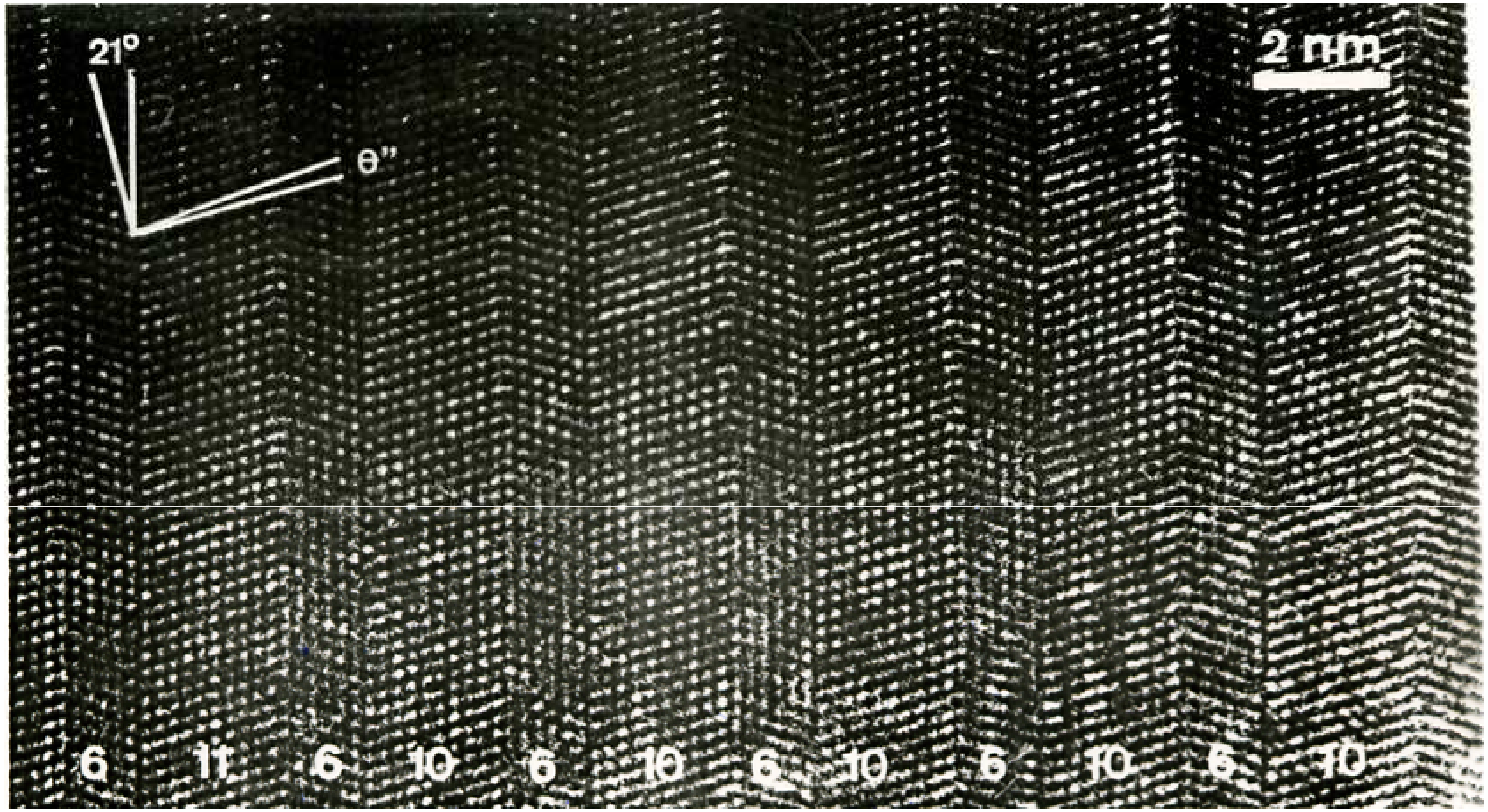
(a) because real microstructures are not infinitely fine, and have characteristic length-scales,

(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.

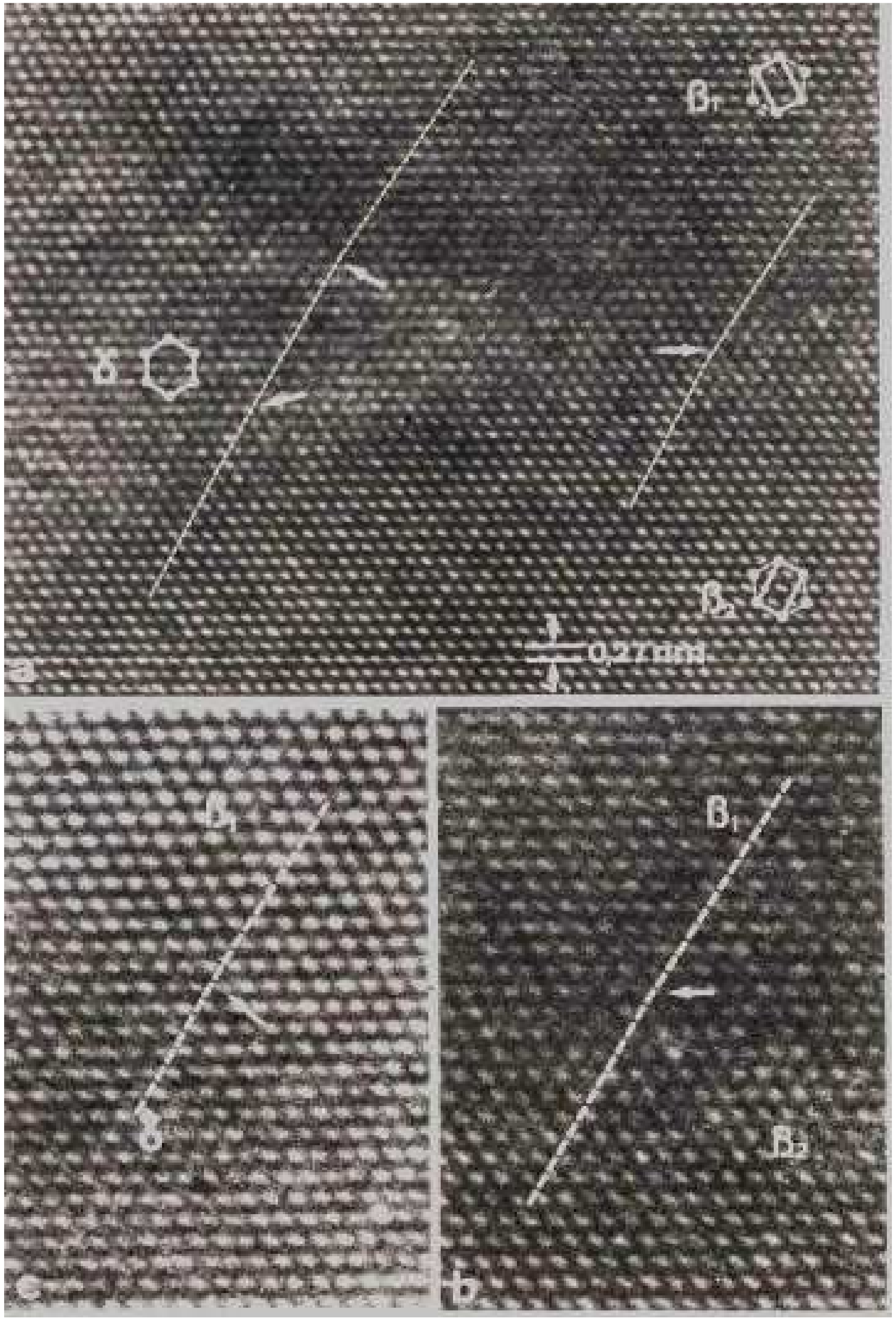
The natural way to try to understand what form the interfacial energy should take is via passage from an atomistic to a continuum model, but there is some confusion as to how this should be done.

Some interfaces are atomistically sharp



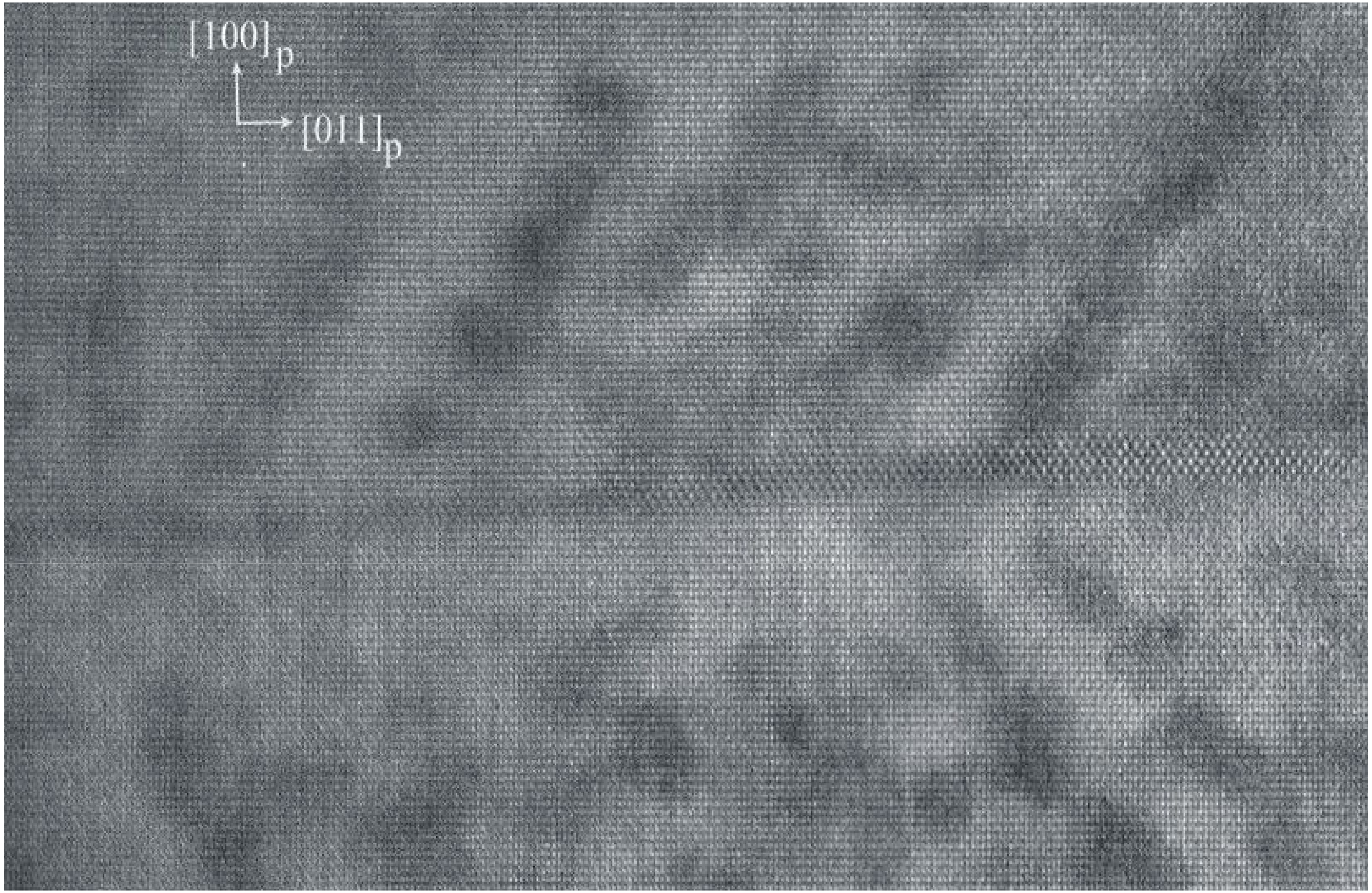
NiMn   Baele, van Tenderloo, Amelinckx

while others are diffuse …



Diffuse (smooth) interfaces in $Pb_3V_2O_8$

Manolikas, van Tendeloo, Amelinckx

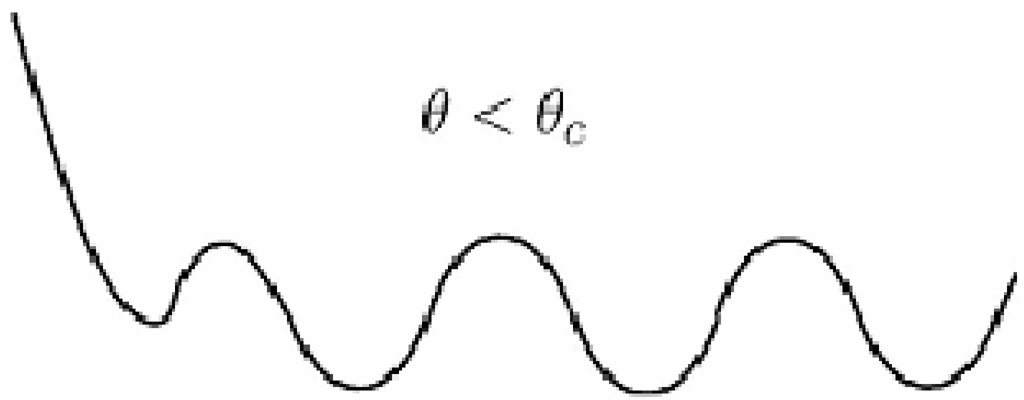


Diffuse interface in perovskite (courtesy Ekhard Salje)

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?



$\alpha(\theta)\mathbf{1}$ $U_1(\theta)$ $U_2(\theta)$ $U_3(\theta)$

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).

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.

Hypotheses

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

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

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

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

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

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

Remark.

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

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

by Friesecke, James, Müller Rigidity Theorem

Idea of proof

Reduce to problem of local minimizers for

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

studied by Taheri (2002), using

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

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

Smoothing of twin boundaries

Seek solution to equilibrium equations for

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

such that

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

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

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

Lemma

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

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

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

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

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

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

In particular

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

The ansatz

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

leads to the 1D integral

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

For cubic $\to$ tetragonal or orthorhombic (and probably in general) 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 to appear) we get a solution.

Remarks

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

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

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 (Bilbao)

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

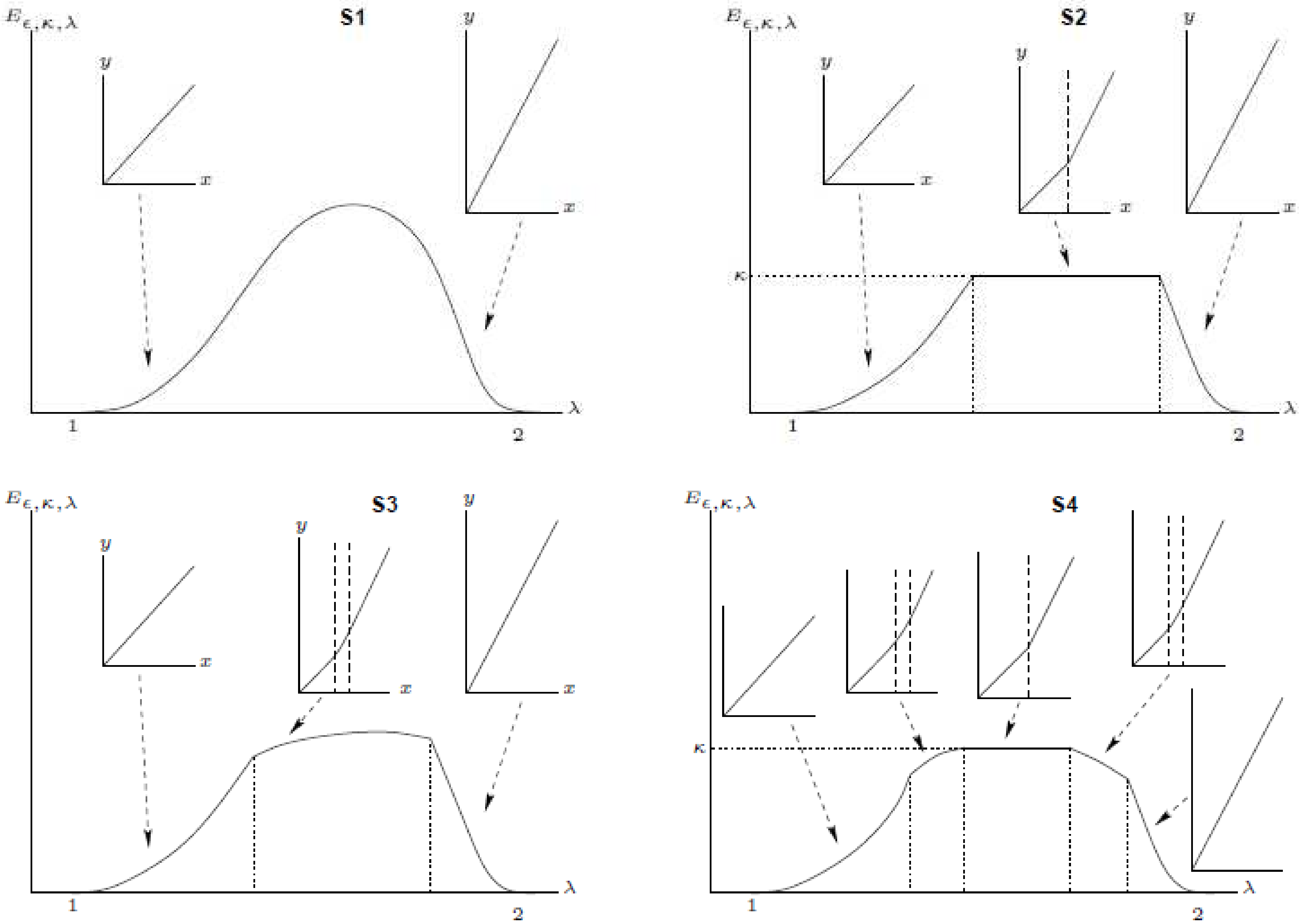
$$I_{\varepsilon,\kappa}(y) = \int_0^1 (W(y') + \varepsilon^2 |\nabla^2 y|^2)\, dx + \kappa \mathcal{H}^0(S_{y'})$$

in

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

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

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



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

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

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

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

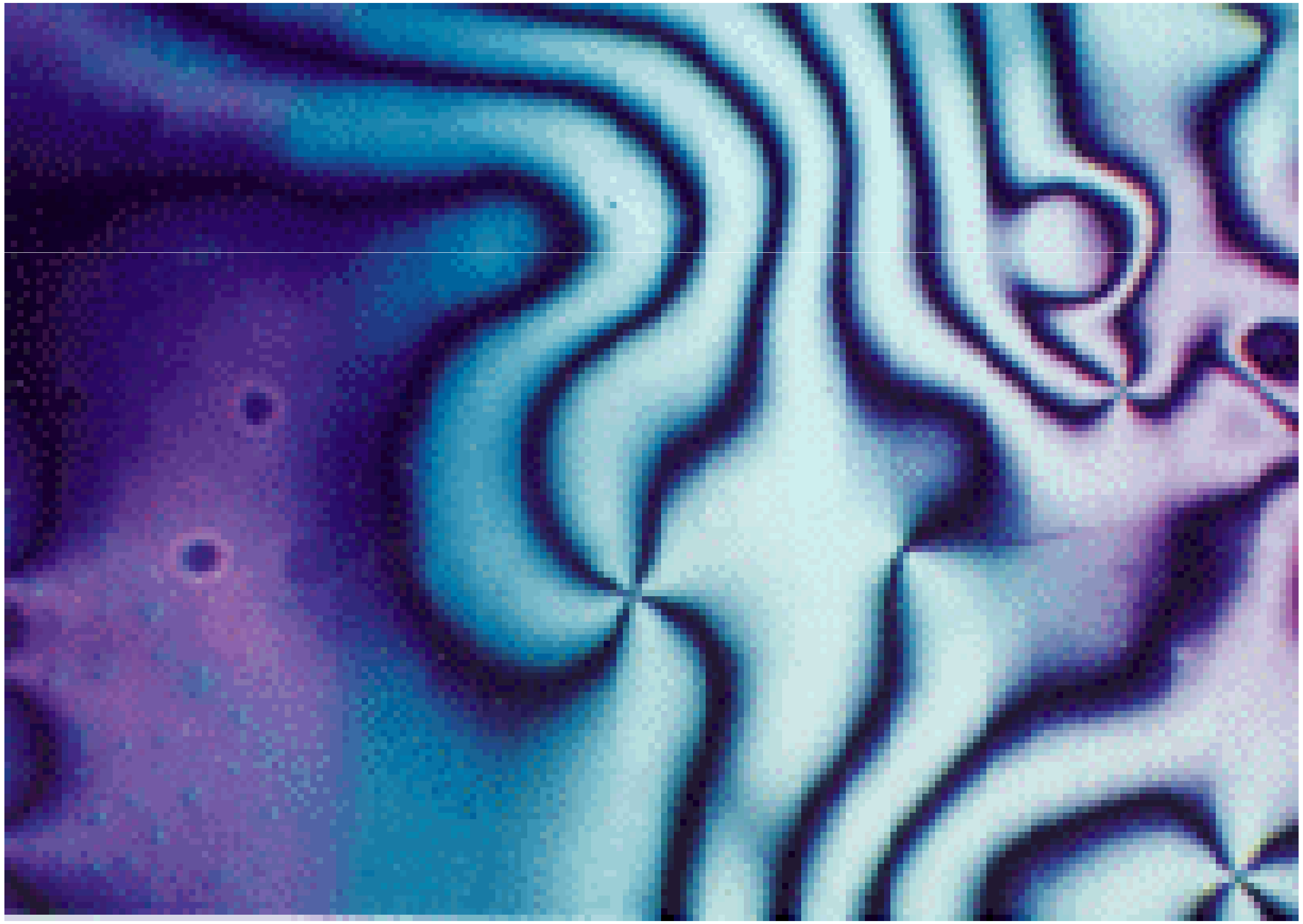
for some constant $d \in \mathbf{R}$.

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.

Defects in liquid crystals



Overview

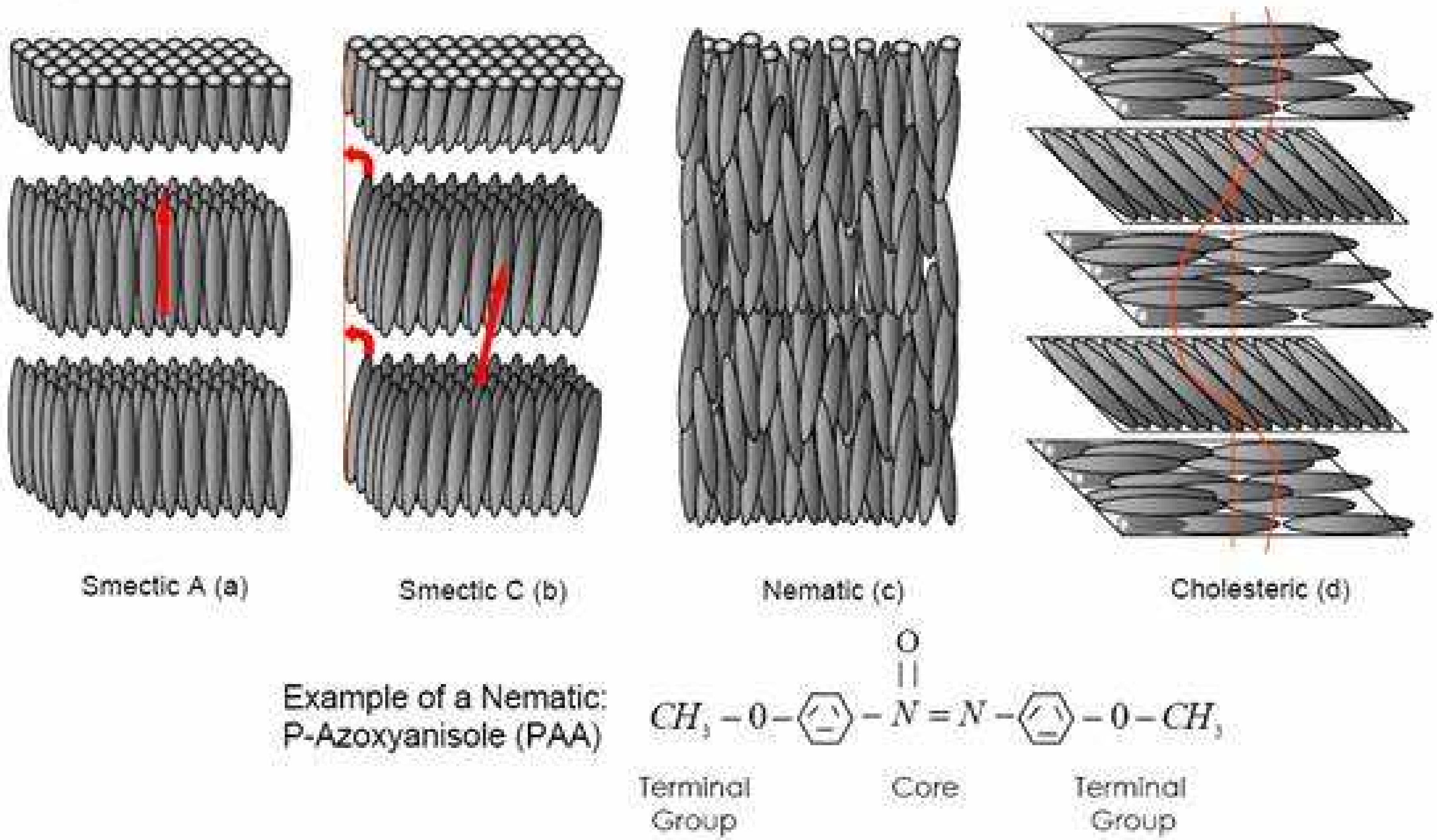
We consider various theories of static configurations of nematic liquid crystals (de Gennes, Oseen-Frank, Onsager / Maier-Saupe), and relations between them.

Liquid crystals can be of different types. Nematics are the simplest (others are cholesterics, smectics ...) and consist of rod-like molecules which are ordered so that they have a locally preferred orientation. Liquid crystals are the basis of a multi-billion dollar display technology industry.

The mathematics of liquid crystals involves modelling, variational methods, PDE, algebra, topology, probability ...

Plan

1. Introduction to liquid crystals. The de Gennes and Oseen-Frank energies.
2. Relations between the theories. Orientability of the director field.
3. The Onsager/Maier-Saupe theory and eigenvalue constraints.



http://www.laynetworks.com/Molecular-Orientation-in-Liquid-Crystal-Phases.htm

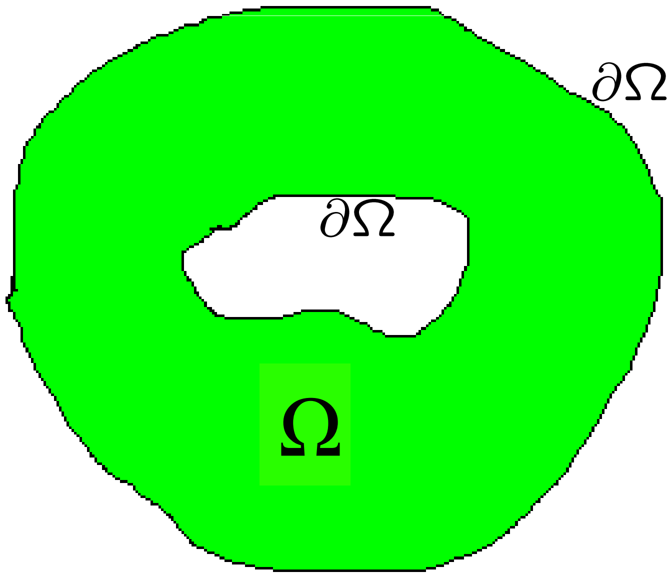
Electron micrograph
of nematic phase

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

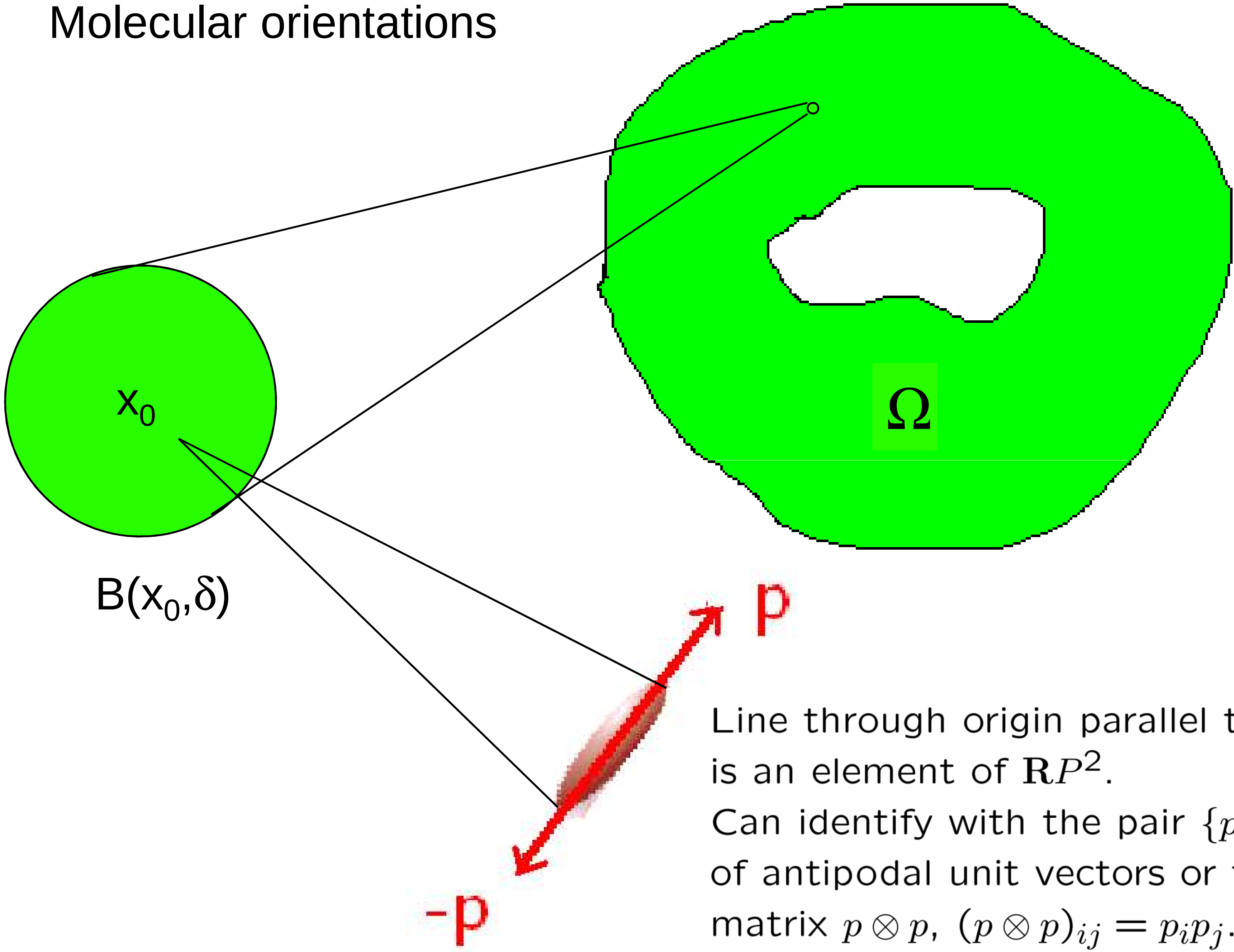
Review of Q-tensor theory

Consider a nematic liquid crystal filling a container $\Omega \subset \mathbf{R}^3$, where Ω is connected with Lipschitz boundary $\partial\Omega$.

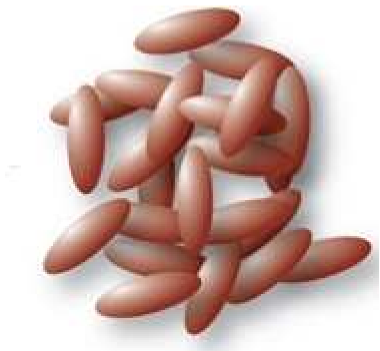
The topology of the container can play a role.



Molecular orientations



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 measure on $\mathbf{R}P^2$, that is by a probability measure μ on the unit sphere S^2 satisfying $\mu(E) = \mu(-E)$ for $E \subset S^2$.

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

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

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

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

Let $e \in S^2$. Then

$$
\begin{aligned}
e \cdot Me &= \int_{S^2} (e \cdot p)^2 d\mu(p) \\
&= \langle \cos^2 \theta \rangle,
\end{aligned}
$$

where θ is the angle between p and e.

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

$$d\mu_0(p) = \frac{1}{4\pi} dS.$$

The corresponding second moment tensor is

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

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

The *de Gennes Q-tensor*

$$Q = M - M_0$$

measures the deviation of M from its isotropic value.

Note that

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

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

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

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

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

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

where $\{n_i\}$ is an orthonormal basis of eigenvectors of Q with corresponding eigenvalues $\lambda_1, \lambda_2, \lambda_3$ with

$$\lambda_1 + \lambda_2 + \lambda_3 = 0.$$

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

Conversely, if $-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}$ then M is the second moment tensor for some μ, e.g. for

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

If the eigenvalues λ_i of Q are distinct then Q is said to be *biaxial*, and if two λ_i are equal *uniaxial*.

In the uniaxial case we can suppose $\lambda_1 = \lambda_2 = -\frac{s}{3}$, $\lambda_3 = \frac{2s}{3}$, and setting $n_3 = n$ we get

$$Q = -\frac{s}{3}(\mathbf{1} - n \otimes n) + \frac{2s}{3} n \otimes n.$$

Thus

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

where $-\frac{1}{2} \leq s \leq 1$.

Note that

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

where θ is the angle between p and n. Hence

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

$$s = -\frac{1}{2} \;\Leftrightarrow\; \int_{S^2} (p \cdot n)^2 d\mu(p) = 0$$

(all molecules perpendicular to n).

$$s = 0 \;\Leftrightarrow\; Q = 0$$

(which occurs when μ is isotropic).

$$s = 1 \;\Leftrightarrow\; \int_{S^2} (p \cdot n)^2 d\mu(p) = 1$$

$$\Leftrightarrow\; \mu = \frac{1}{2}(\delta_n + \delta_{-n})$$

(perfect ordering parallel to n).

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

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

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 measure μ_x and 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 $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \mathrm{tr}\, Q = 0\}$
$\mathcal{D} = \{D = (D_{ijk}) : D_{ijk} = D_{jik}, D_{kki} = 0\}$.
We suppose that $\psi : \mathrm{dom}\, \psi \to \mathbf{R}$, where

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

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

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

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

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

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

Thus we can assume that ψ satisfies

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

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

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.

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

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

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

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

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 $D=0$,

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

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

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

Following de Gennes, Schophol & Sluckin PRL 59(1987), Mottram & Newton, Introduction to Q-tensor theory, we consider the example

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

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

Then

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

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

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

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

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

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

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 (in comparison to the steepness of the potential well about the minimum of ψ_B), 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

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

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, ∇n we obtain the Oseen-Frank energy functional

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

where

$$K_1 = 2L_1s^2 + L_2s^2 + L_3s^2 - \tfrac{2}{3}L_4s^3,$$
$$K_2 = 2L_1s^2 - \tfrac{2}{3}L_4s^3,$$
$$K_3 = 2L_1s^2 + L_2s^2 + L_3s^2 + \tfrac{4}{3}L_4s^3,$$
$$K_4 = L_3s^2.$$

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 $W^{1,p}(\Omega; M^{3\times3})$. Since usually we assume

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

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

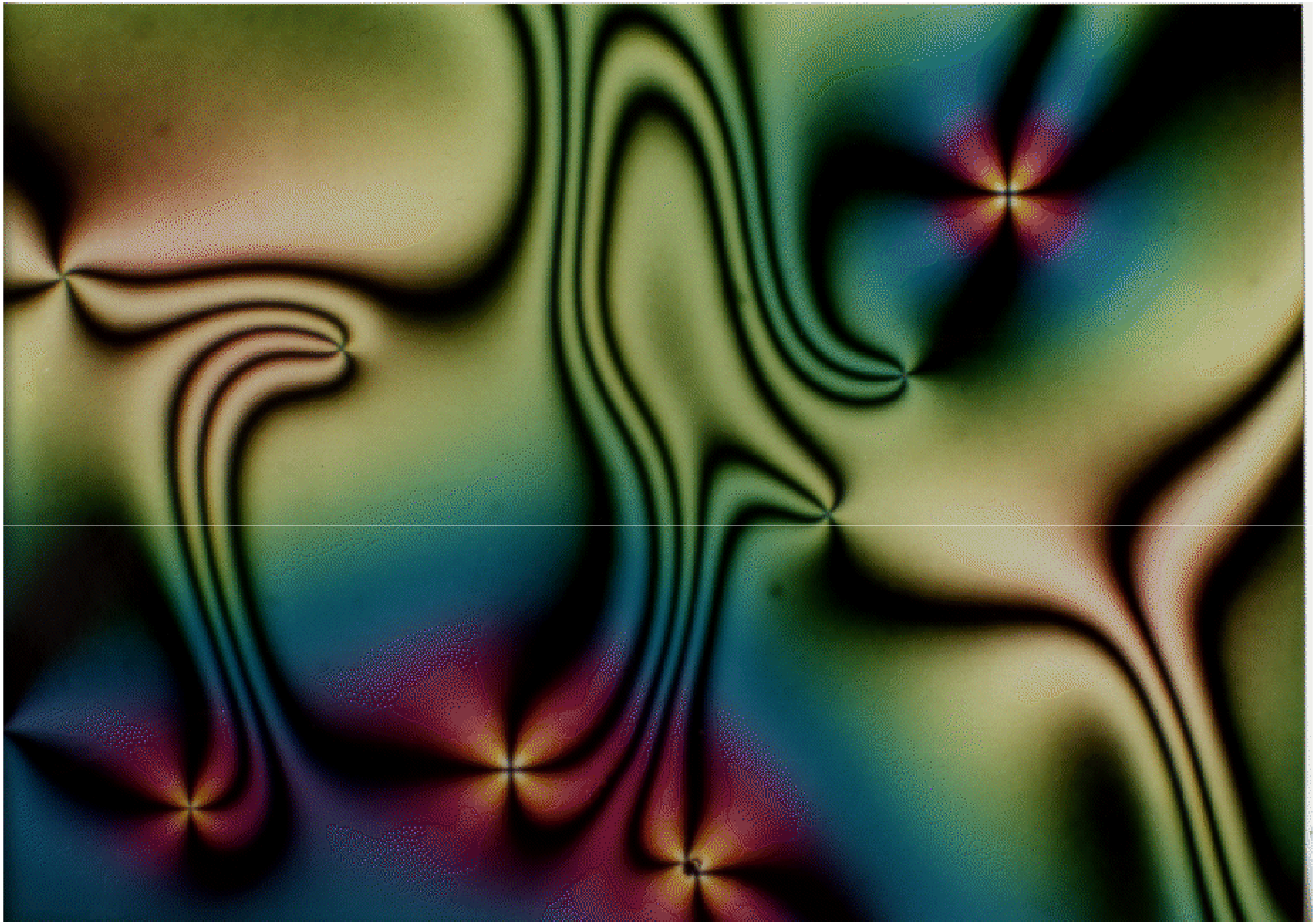
$$I_3 = Q_{ij,k}Q_{ij,k},\ I_4 = Q_{lk}Q_{ij,l}Q_{ij,k},$$

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



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

Possible defects in constrained theory

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

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

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

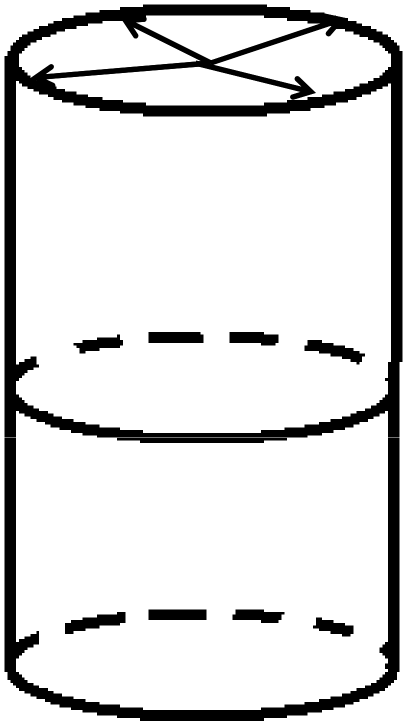
$$|\nabla n(x)|^2 = \frac{2}{|x|^2}$$

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

$Q, n \in W^{1,p},\ 1 \le p < 3$

Finite energy

Disclinations



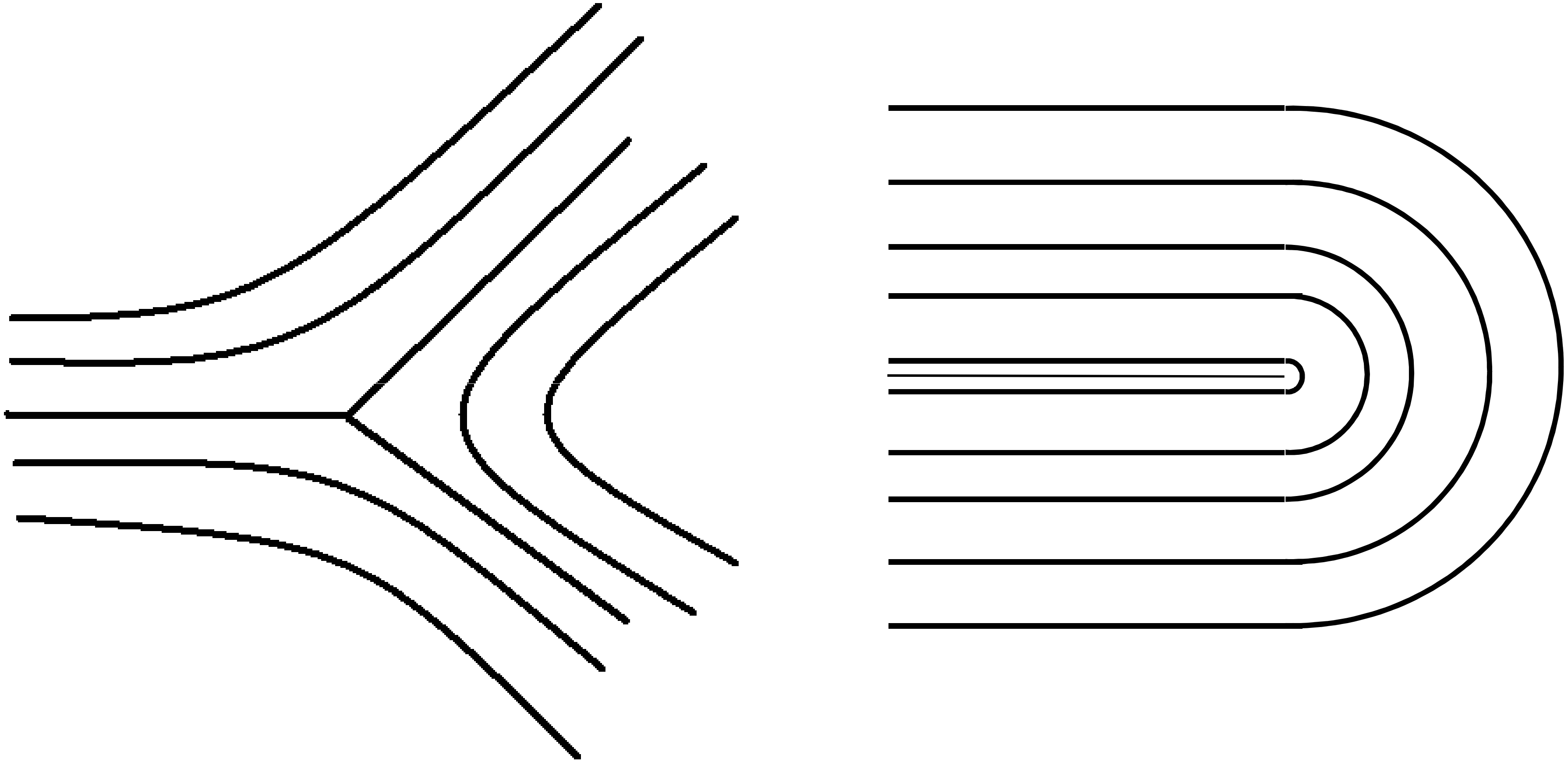
$$n(x) = (\tfrac{x_1}{r}, \tfrac{x_2}{r}, 0) \quad r = \sqrt{x_1^2 + x_2^2}$$

$$|\nabla n(x)|^2 = \tfrac{1}{r^2}$$

$$n, Q \in W^{1,p} \Leftrightarrow 1 \leq p < 2$$

infinite energy for quadratic models

Index one half singularities



$$Q \notin W^{1,2}$$

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

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

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.

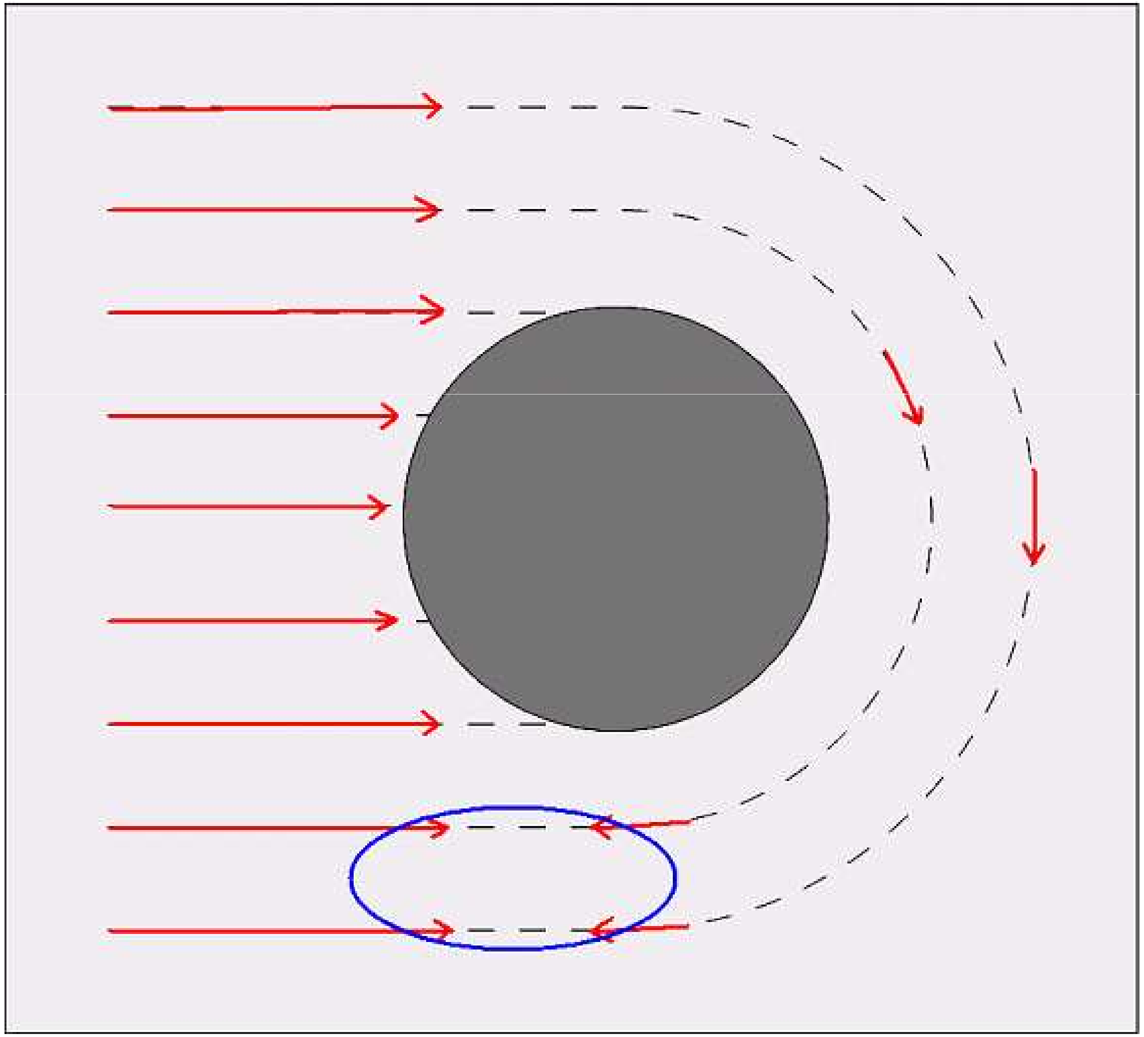
Proof

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

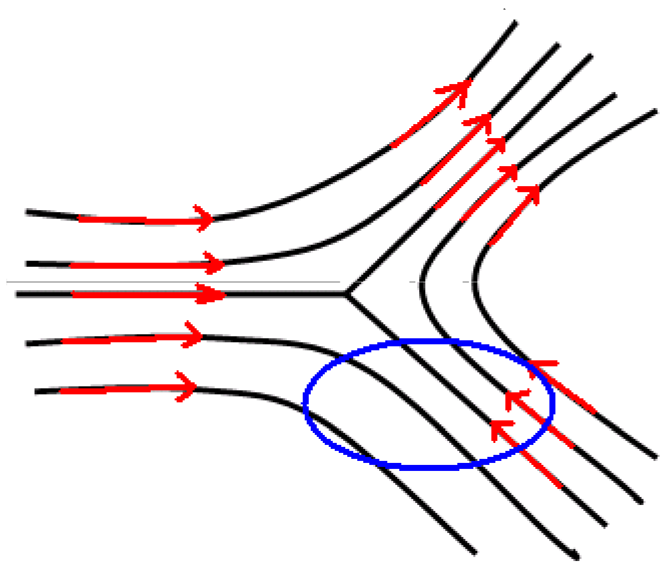
$$\tau(x)n(x) \cdot n(x) = \tau(x)$$

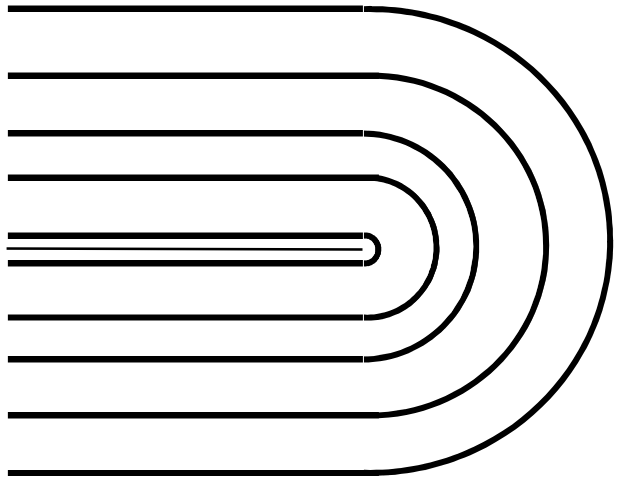
is continuous in x_1. Hence $\tau_{,1}$ exists and is zero. Similarly $\tau_{,2}, \tau_{,3}$ exist and are zero. Thus $\tau \in W^{1,\infty}$ and $\nabla\tau = 0$ a.e. in Ω. Hence $\tau = 1$ a.e. or $\tau = -1$ a.e..

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



The index one half singularities are non-orientable



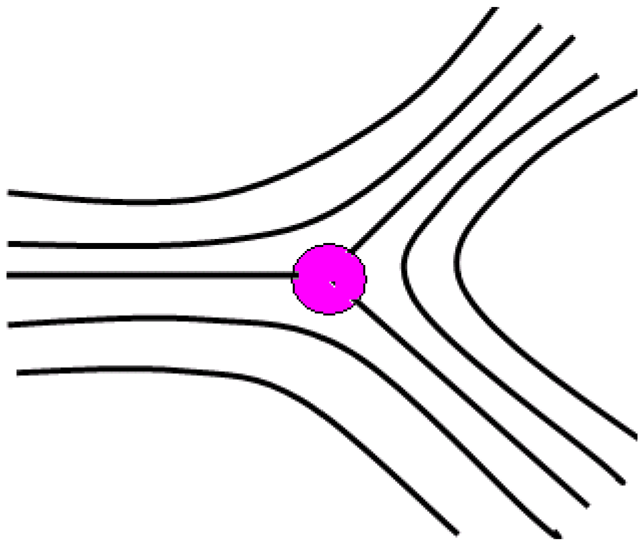


Theorem 2

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:Ω→N.)

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



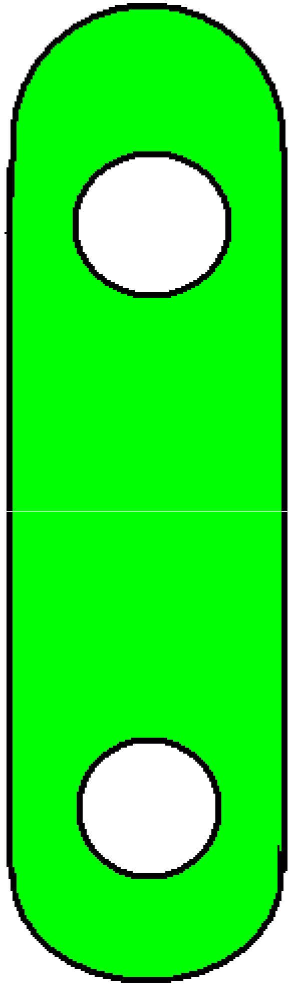
Another consequence is that it is impossible to modify this Q-tensor field in a core around the singular line so that it has finite Landau-de Gennes energy.

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

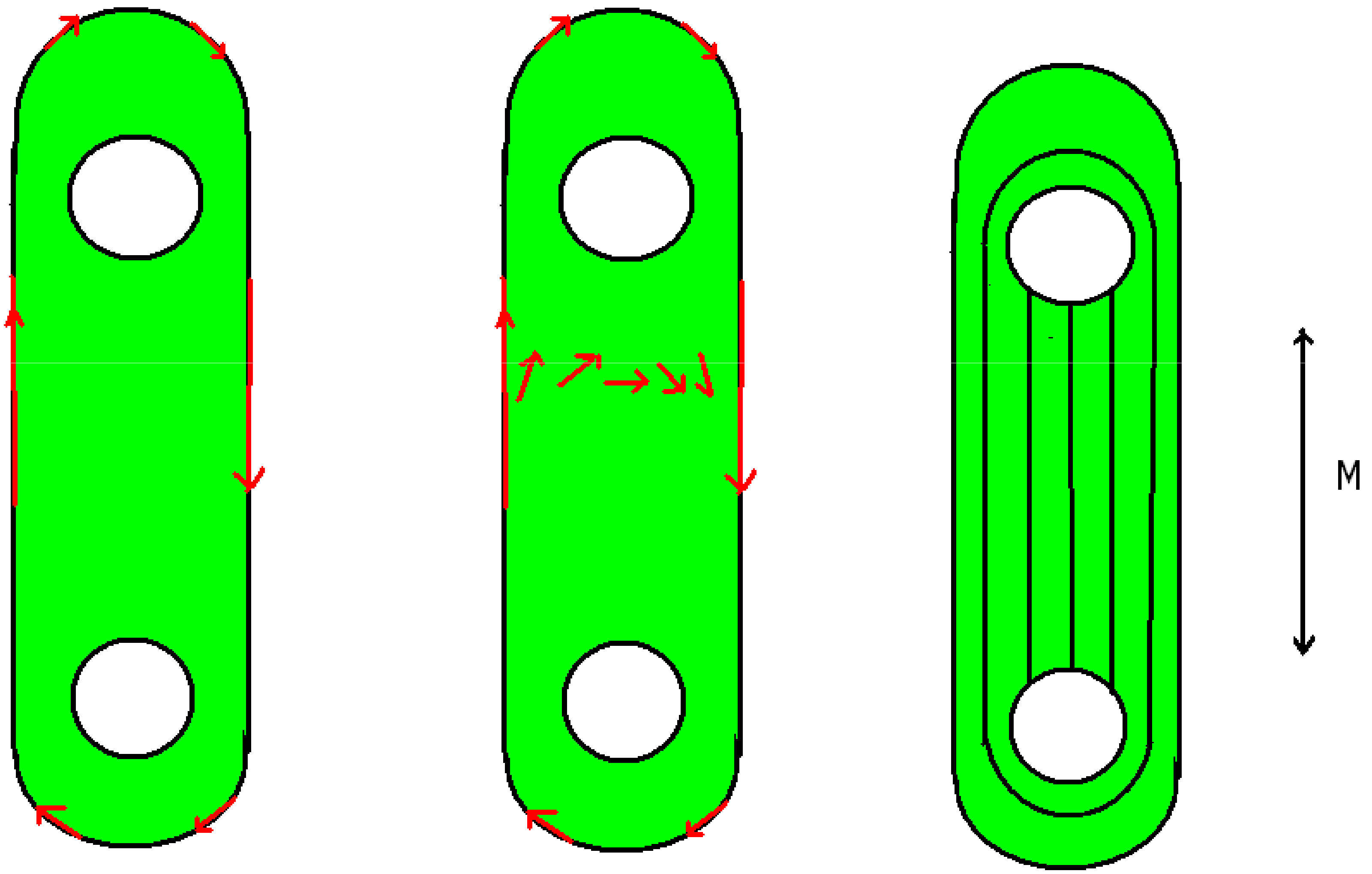
For a 2D domain with smooth boundary and a finite number of holes, $Q \in W^{1,2}$ is orientable if and only if Q is orientable on $\partial\Omega$.

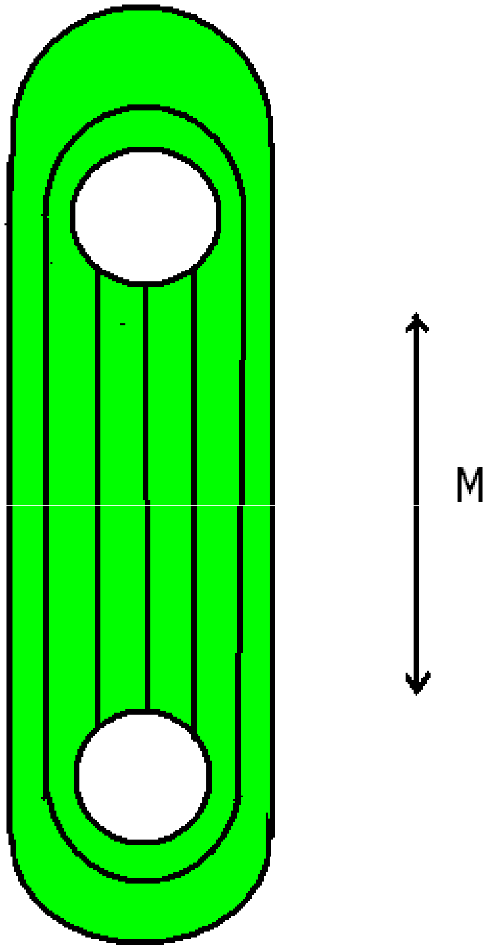


Tangent boundary conditions on outer boundary. No (free) boundary conditions on inner circles.

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

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


M



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

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

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, $\mathcal{E}=\{Q\in M^{3\times3}:Q=Q^T,\mathrm{tr}\,Q=0\}$, (e.g. of the quartic form considered previously) and

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

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

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

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

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 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, 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

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

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

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

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 super-linearly 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

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

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

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

where

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

The μ_i 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 $\mathcal{H}^2(E) > 0$. There exists $z \in L^\infty(S^2)$ such that

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

(this is possible since $1 = \sum_{i,j=1}^{3} (D_{ij}(p_i p_j - \frac{1}{3}\delta_{ij})$ is impossible for constants D_{ij}). Define for $\varepsilon > 0$ sufficiently small

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

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

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

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.

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

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 $Q = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$,

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

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

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

Consequences

1. Logarithmic divergence of ψ_B as $\min \lambda_i(Q) \to -\frac{1}{3}$.

2. All critical points of ψ_B are uniaxial.

3. Phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

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

5. Using a maximum principle we can show that minimizers of

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

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

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

for some $\varepsilon > 0$.

(Compare nonlinear elasticity, for which the energy is $I(y) = \int_\Omega W(\nabla y(x))\, dx$, with $W(A) \to \infty$ for $\det A \to 0+$.)

Voir http://www.maths.ox.ac.uk/~ball

sous teaching pour les diapositives

The end