Collège de France, 20 March 2009

Les interfaces, l'énergie superficielle et les transformations martensitiques.

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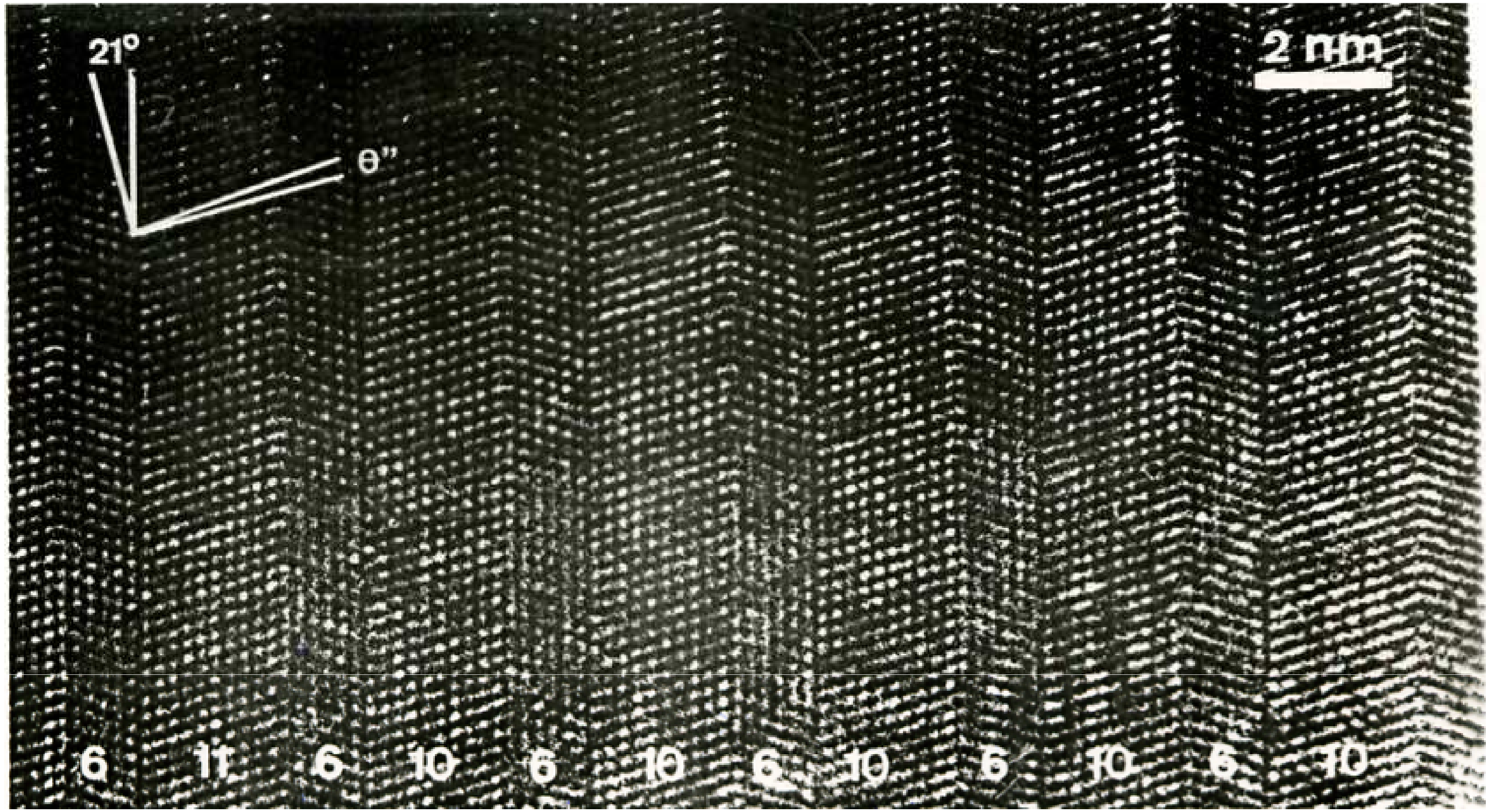
Plan of talk

1. Introduction – sharp and diffuse interfaces in solids.
2. Second gradient model for diffuse interfaces
3. A model allowing for both sharp and diffuse interfaces
4. Nonclassical austenite-martensite interfaces

1

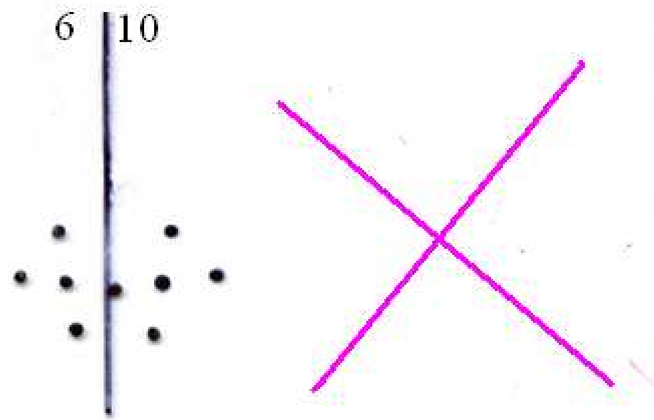
Introduction

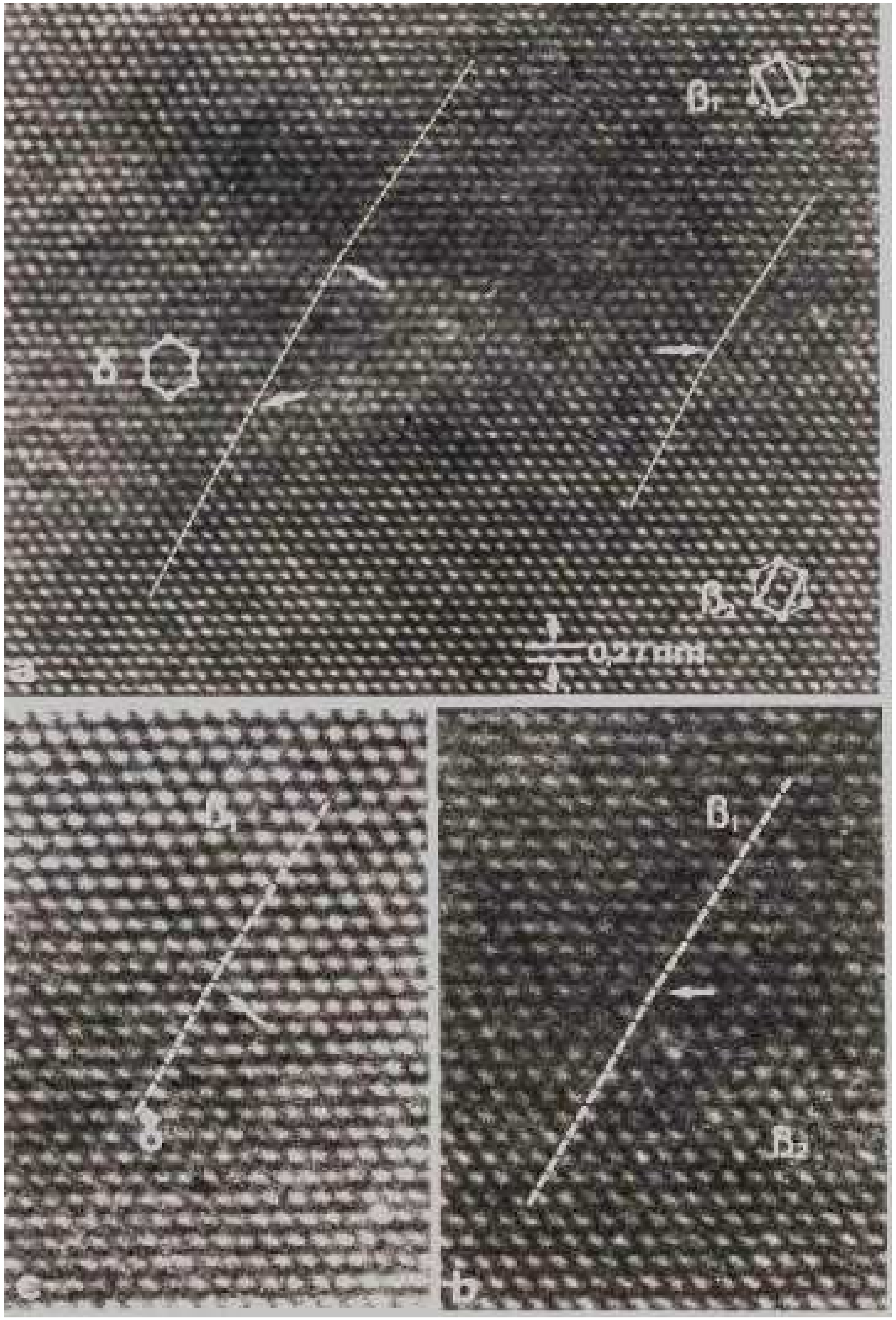
Sharp and diffuse interfaces in solids



Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

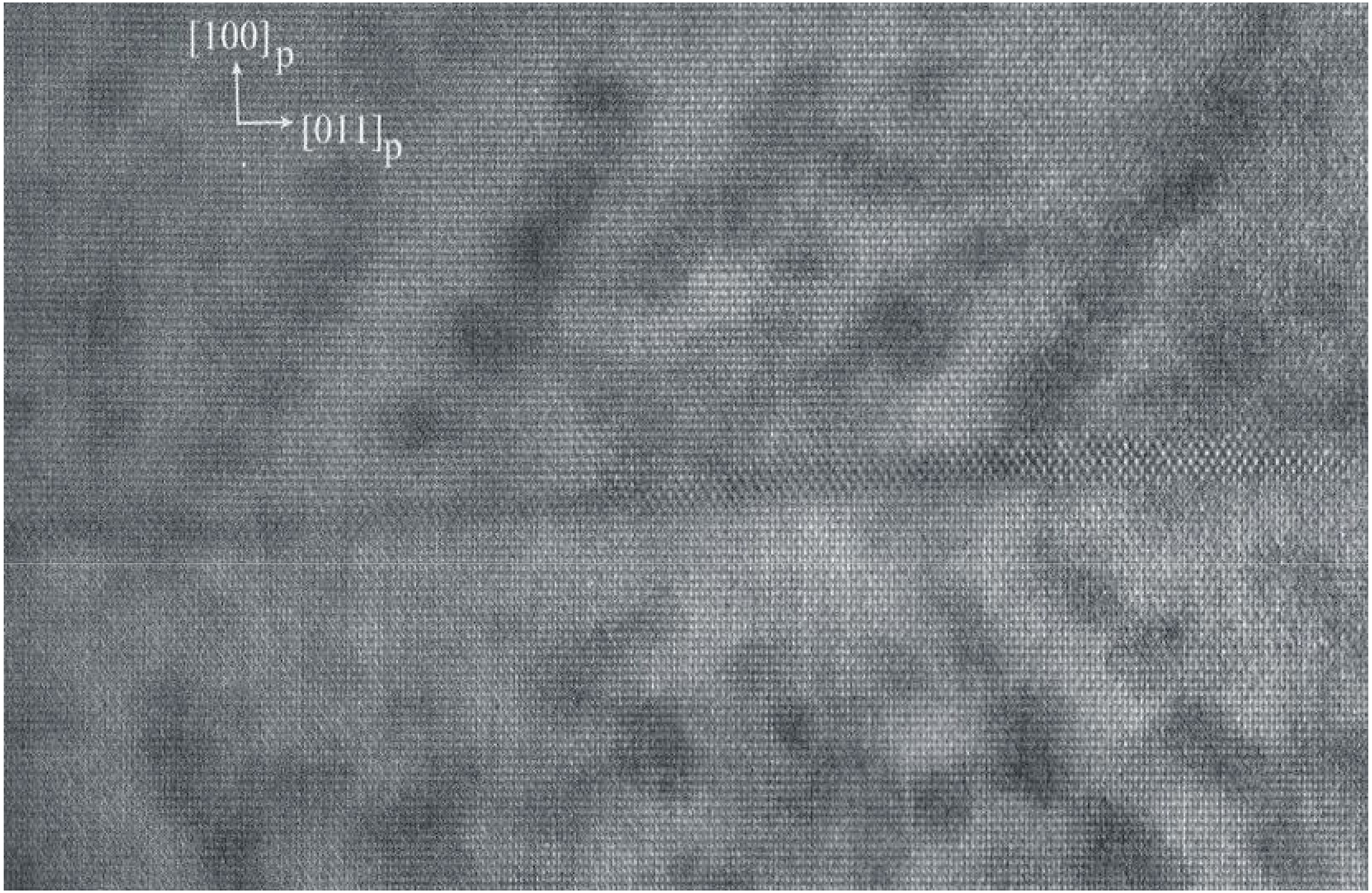
Baele, van Tenderloo, Amelinckx





Diffuse (smooth) interfaces in $Pb_3V_2O_8$

Manolikas, van Tendeloo, Amelinckx



Diffuse interface in perovskite (courtesy Ekhard Salje)

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

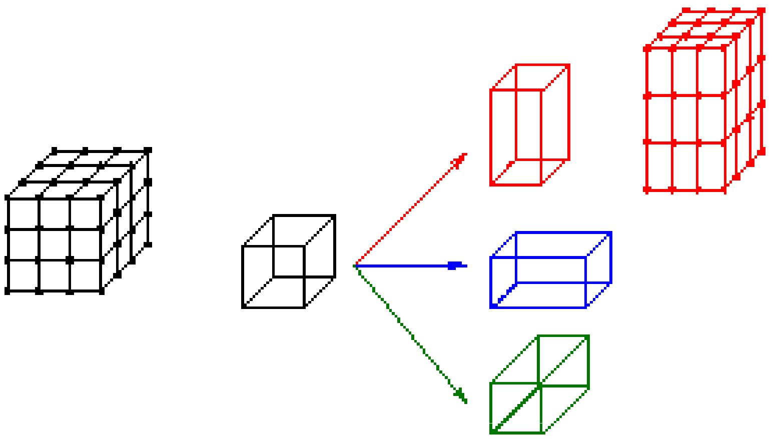
$$K(\theta) = \begin{cases} \alpha(\theta)\mathrm{SO}(3) & \theta > \theta_c \\ \mathrm{SO}(3) \cup \bigcup_{i=1}^{N} \mathrm{SO}(3)U_i(\theta_c) & \theta = \theta_c \\ \bigcup_{i=1}^{N} \mathrm{SO}(3)U_i(\theta) & \theta < \theta_c, \end{cases}$$

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

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. $Ni_{65}Al_{35}$)



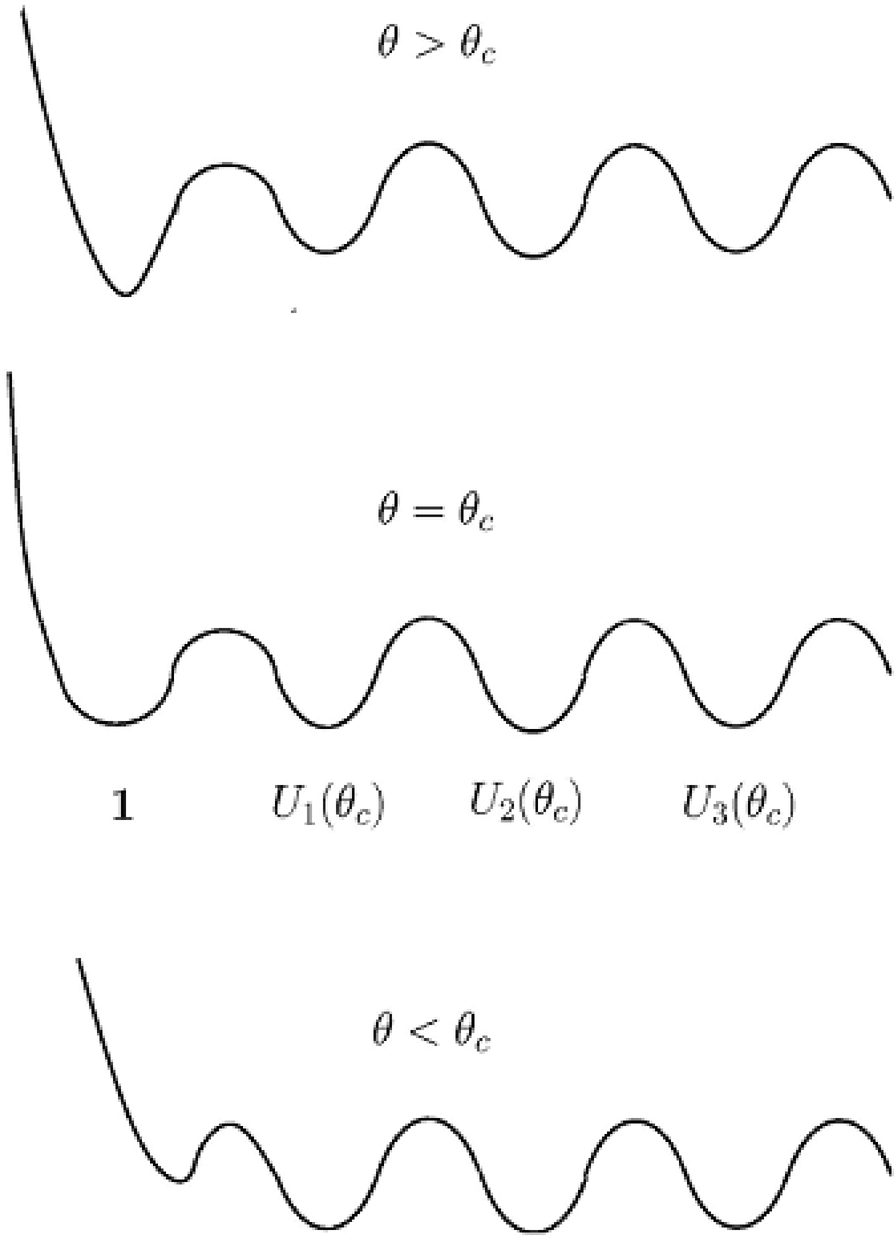
$N = 3$

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

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

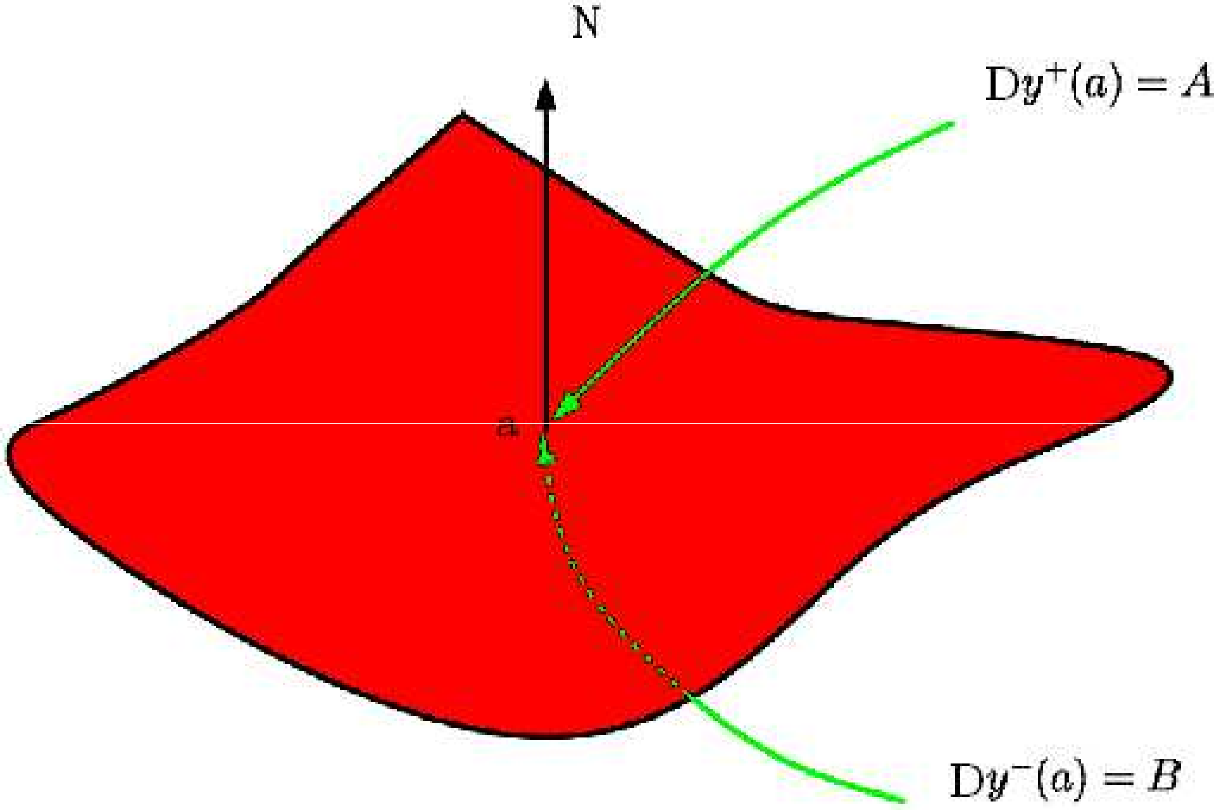
$$U_3 = \operatorname{diag}(\eta_1, \eta_1, \eta_2)$$

Exchange of stability



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

Hadamard jump condition



y piecewise C^1

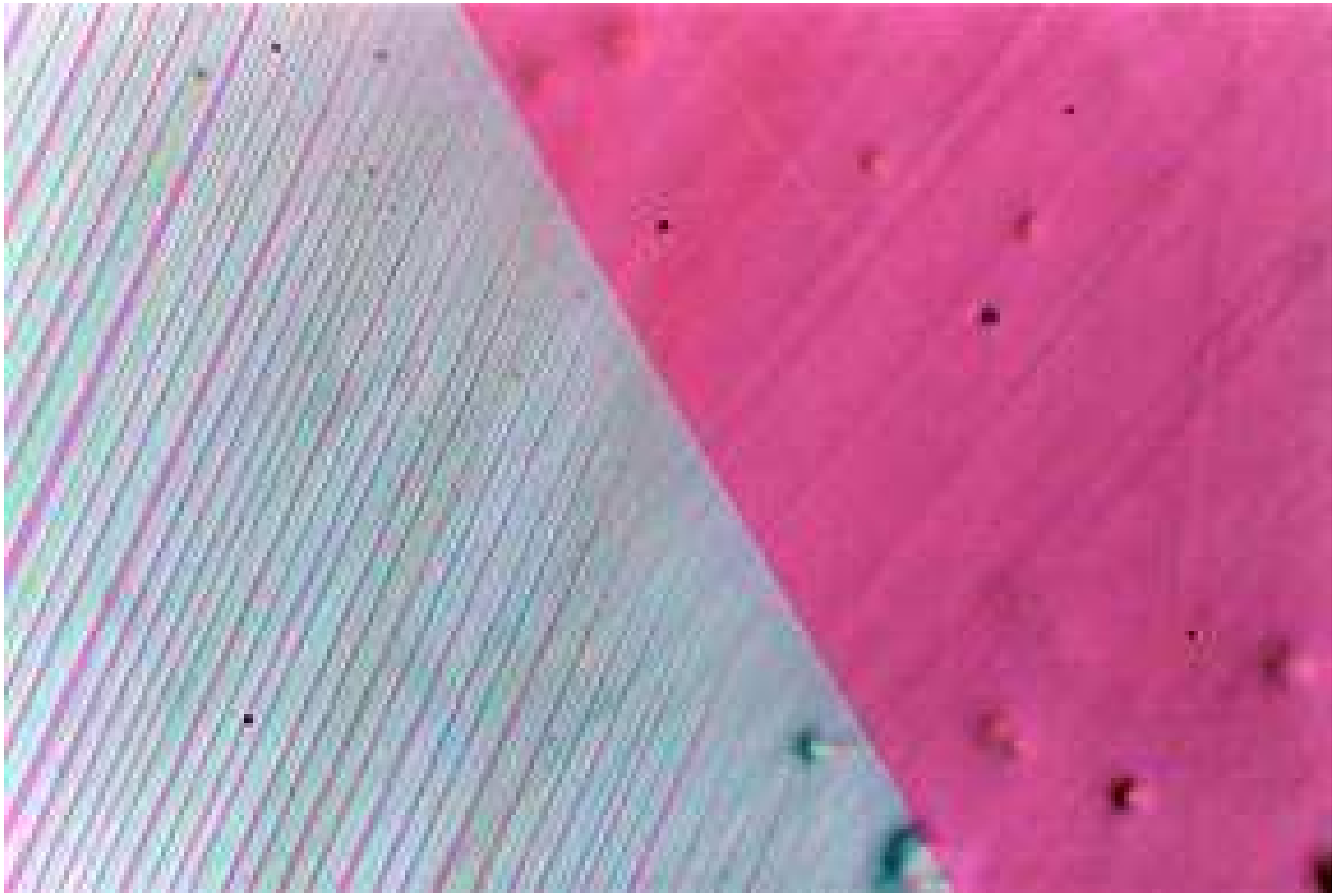
$$A - B = c \otimes N$$

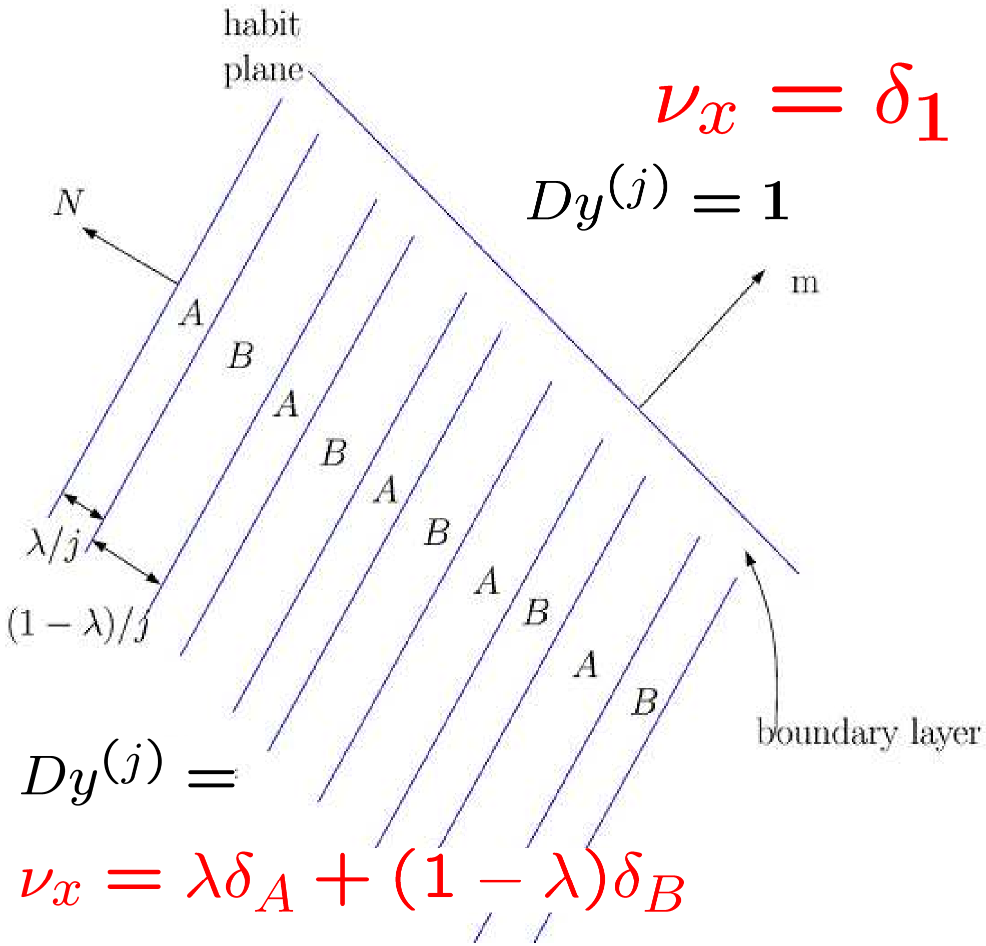
Interfaces correspond to pairs of matrices A, B with $A - B = a \otimes N$, where N is the interface normal. At minimum energy $A, B \in K(\theta)$.

There are no rank-one connections between matrices A, B in the *same* energy well. The rank-one connections between matrices $A \in SO(3)U_i, B \in SO(3)U_j, i \neq j$ correspond to *twins*. In general there is no rank-one connection between $A \in SO(3)$ and $B \in SO(3)U_i$.

(Classical) austenite-martensite interface in CuAlNi

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





$$\nu_x = \delta_1$$

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

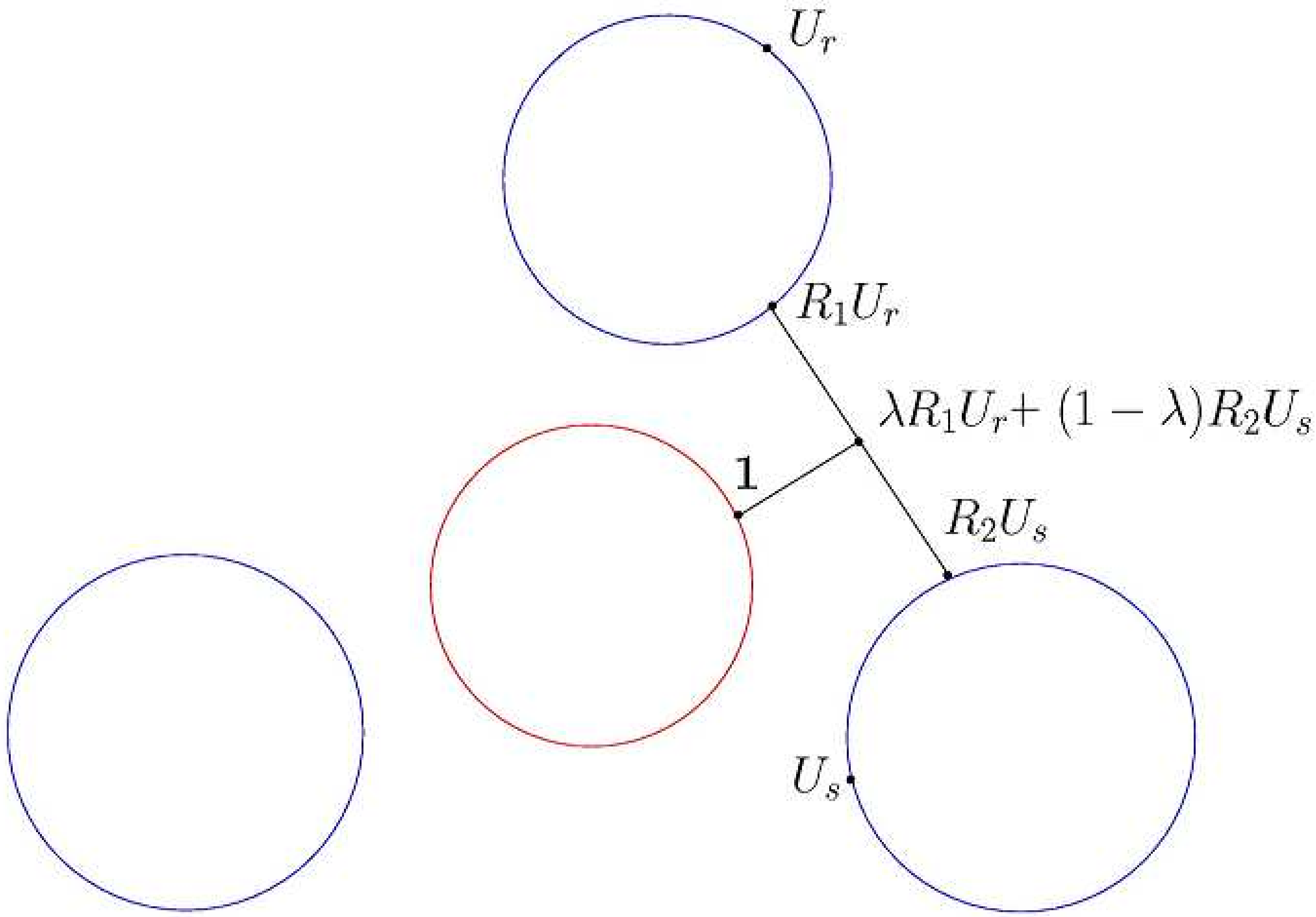
$$Dy^{(j)} =$$

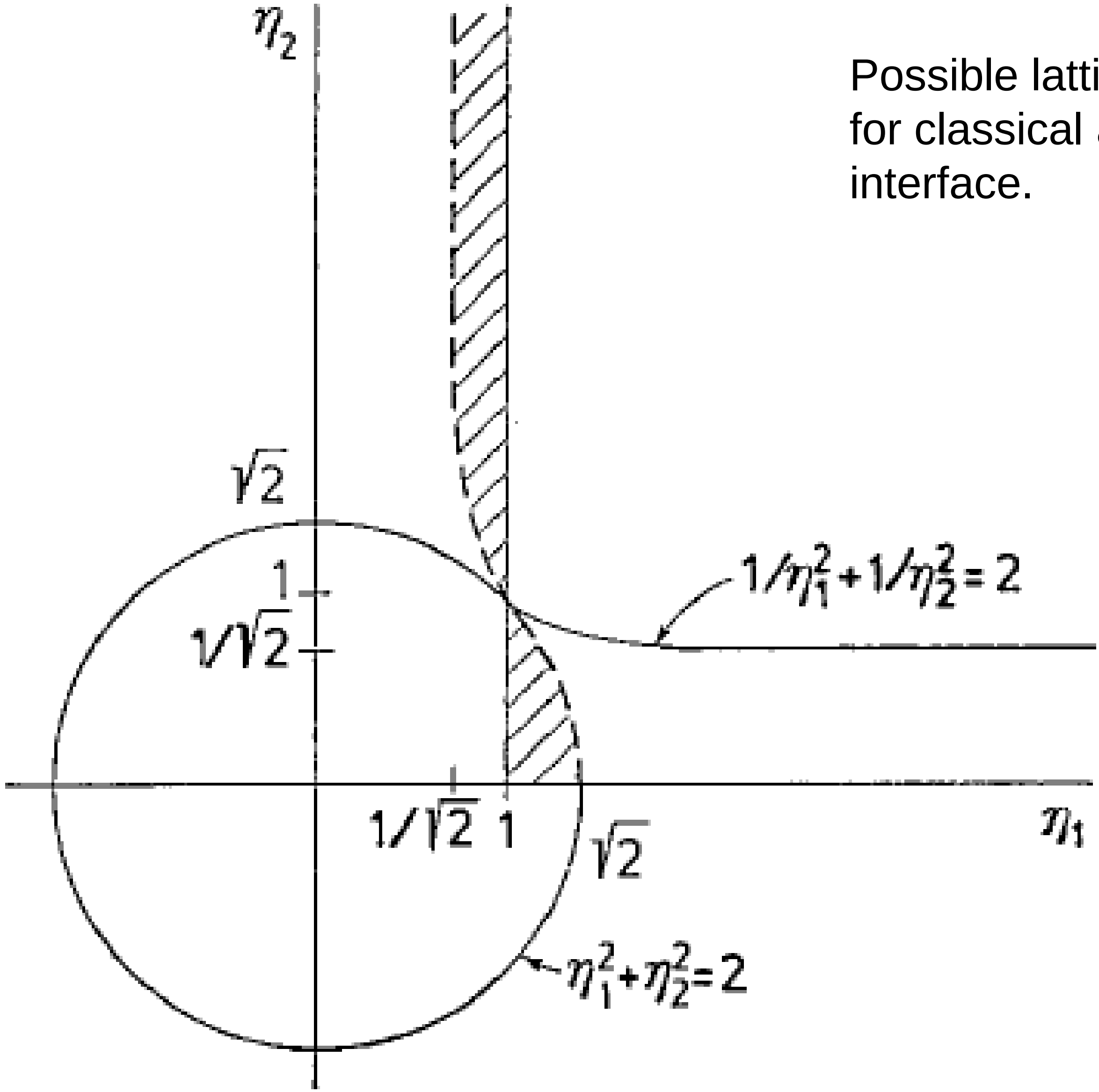
$$\nu_x = \lambda\delta_A + (1-\lambda)\delta_B$$

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.

Commentary on nonlinear elasticity model

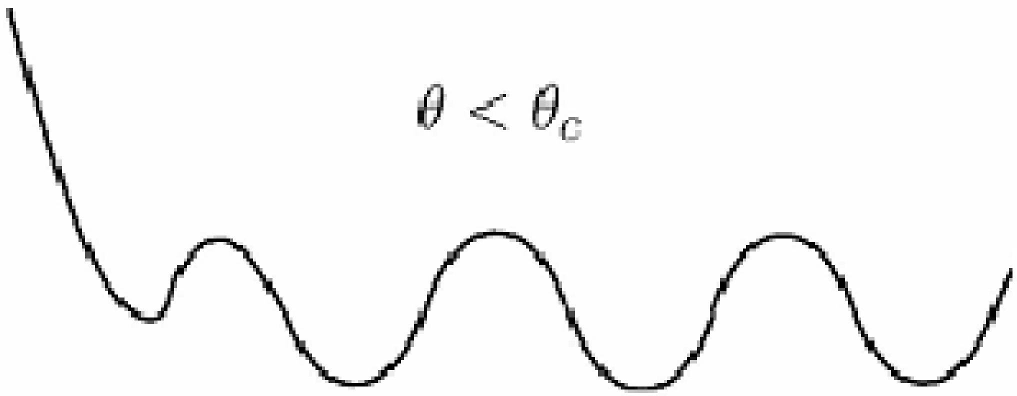
In general the minimum of I_θ is not attained, and the theory thus predicts the existence of infinitely fine microstructures. This is good, because very fine microstructures occur, but bad because they are not infinitely fine. To give a length-scale to the microstructures we need to account for *interfacial energy*.

2

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?



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

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.

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

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

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

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

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

Hypotheses

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

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

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

Theorem. $\bar{y}(x) = \alpha Rx + a$, $R \in \mathrm{SO}(3), a \in \mathbf{R}^3$, *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

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

such that

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

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

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

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

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

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

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

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

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

In particular

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

The ansatz

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

leads to the 1D integral

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

For cubic $\to$ tetragonal or orthorhombic (and probably in general) we have

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

and so by energy minimization (Alikakos & Fusco to appear) we get a smooth solution satisfying $\det Dy(x) > 0$.

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.

A model allowing for both sharp and diffuse interfaces

JB/ Carlos Mora-Corral (Bilbao).

Sharp interface models

A natural idea is to minimize an energy such as

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

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.

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

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

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

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

One-dimensional case

Minimize

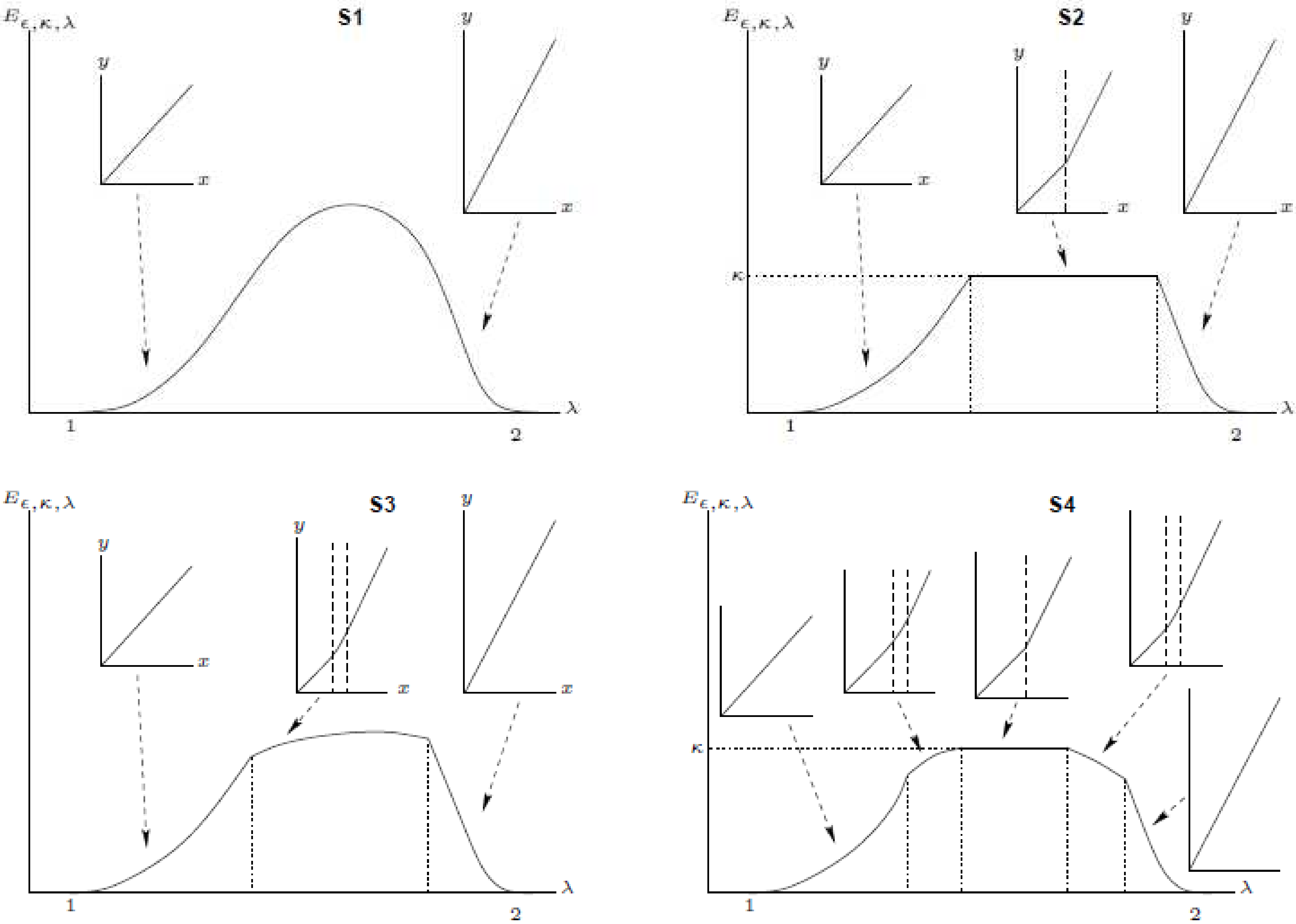
$$I_{\varepsilon,\kappa}(y) = \int_0^1 (\psi(y') + \varepsilon^2 |\nabla^2 y|^2)\, dx + \kappa \mathcal{H}^0(S_{y'})$$

in

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

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

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


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

More realistic 1D model

Minimize

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

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

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

Typically $\gamma(0)=0$ with γ concave on $(0,\infty)$.
For example

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

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

Theorem. Let $\psi : (0,\infty) \to [0,\infty)$ be C^1, $\lim_{t\to 0+}\psi(t) = \infty$, and suppose there exist r_1, r_2 with $0 < r_1 < r_2$ such that

$$-\infty < \sup_{(0,r_i]} \psi' = \inf_{[r_i,\infty)} \psi' < \infty \text{ for } i \in \{1,2\}.$$

Let $\lambda \in (r_1, r_2)$.

Then there exists a minimiser of the functional $I_{\varepsilon,\gamma}$ 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,

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

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

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

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

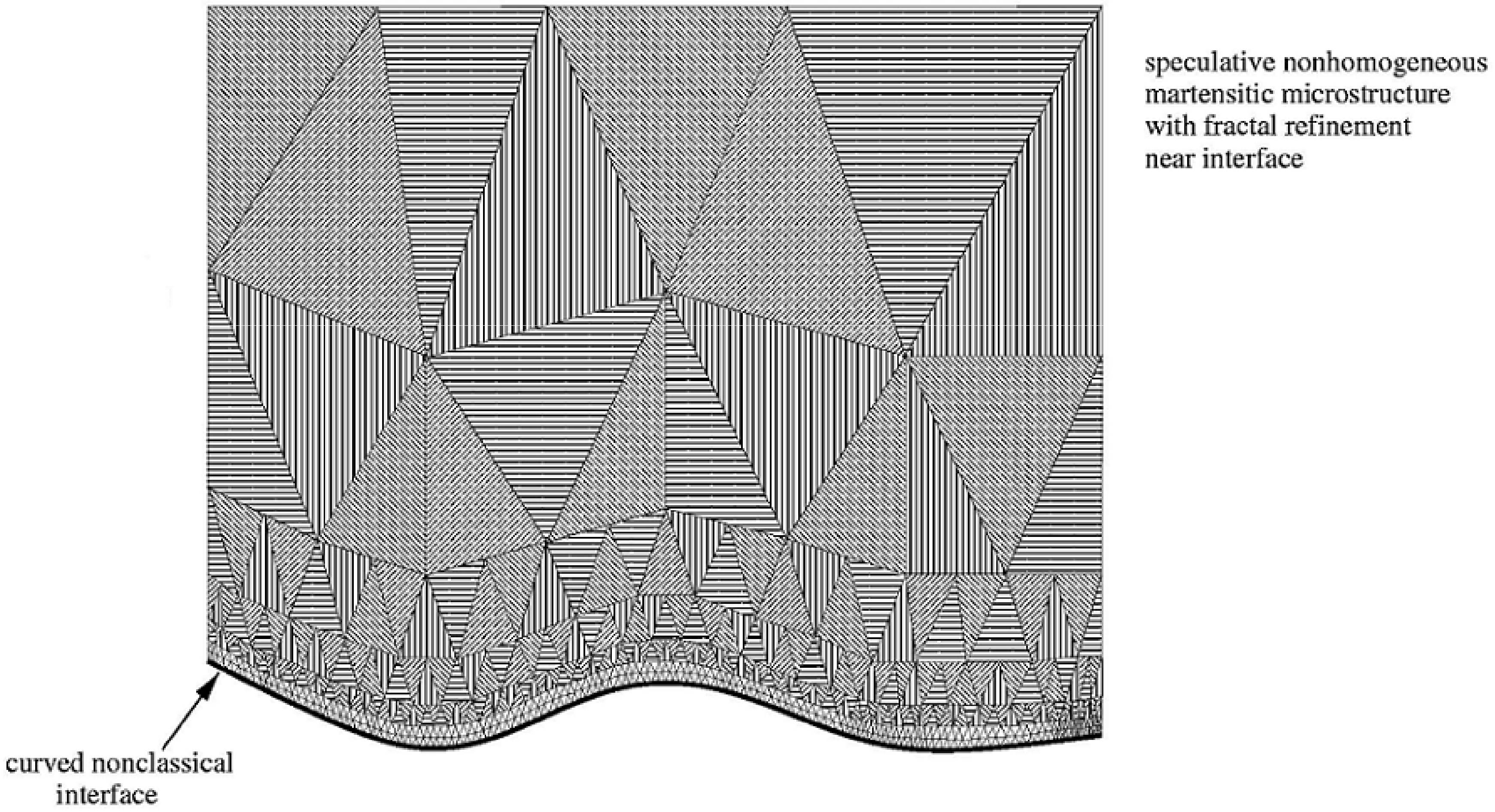
Remarks

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.

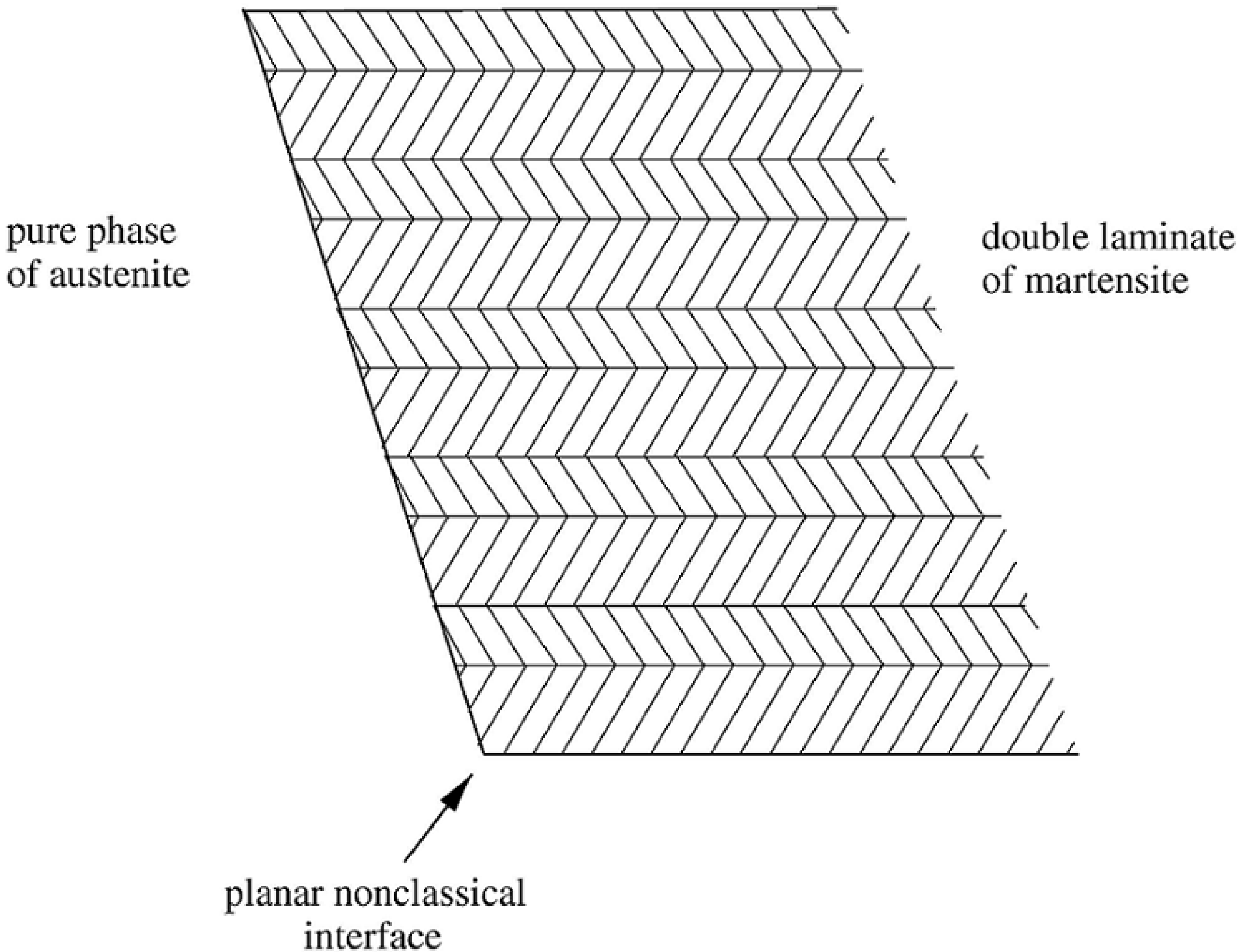
Nonclassical austenite-martensite interfaces

JB/ Konstantinos Koumatos (Oxford)/
Hanus Seiner (Prague).

Nonclassical austenite-martensite interfaces (B/Carstensen 97)



Nonclassical interface with double laminate



Nonclassical interface calculation

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

m

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

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

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

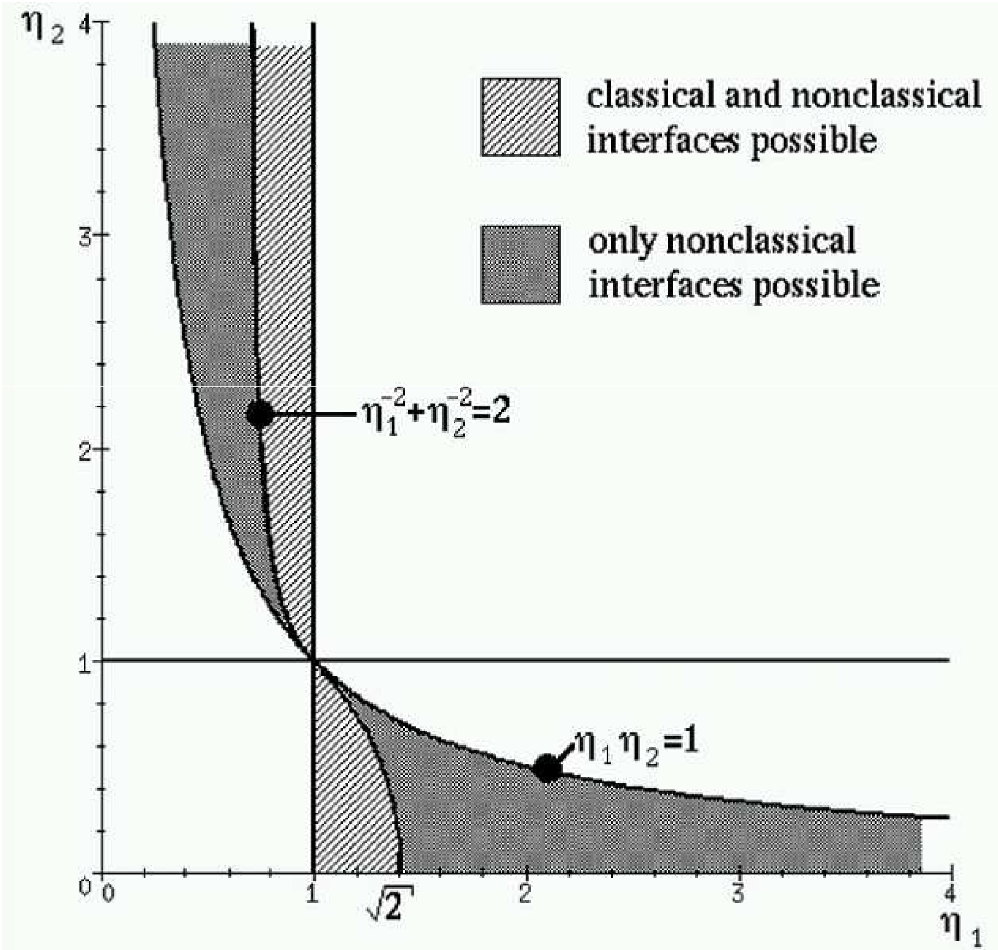
(unknown unless $N = 2$)

$\nu_x = \nu$

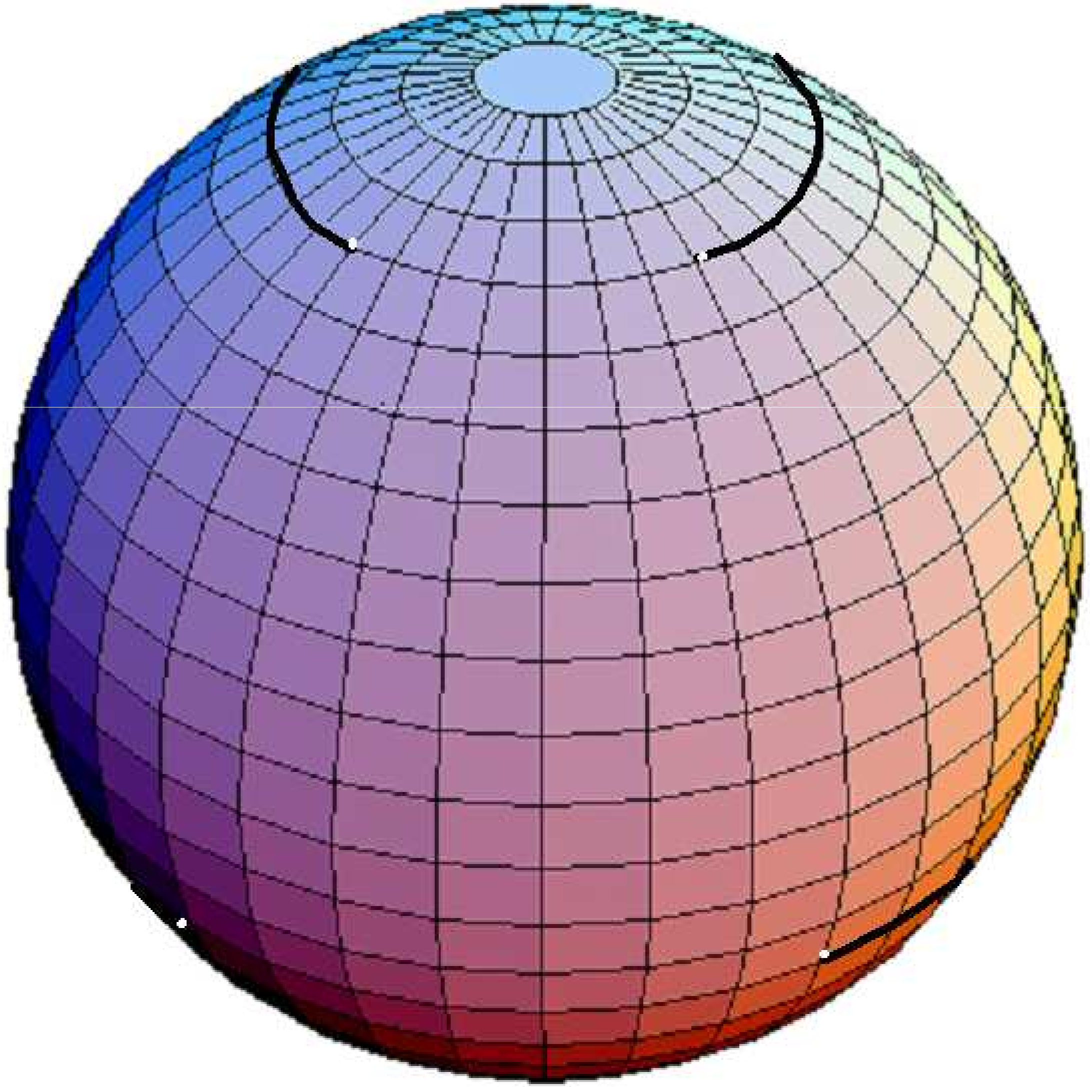
$\operatorname{supp}\nu \subset \bigcup_{i=1}^{N} SO(3)U_i$

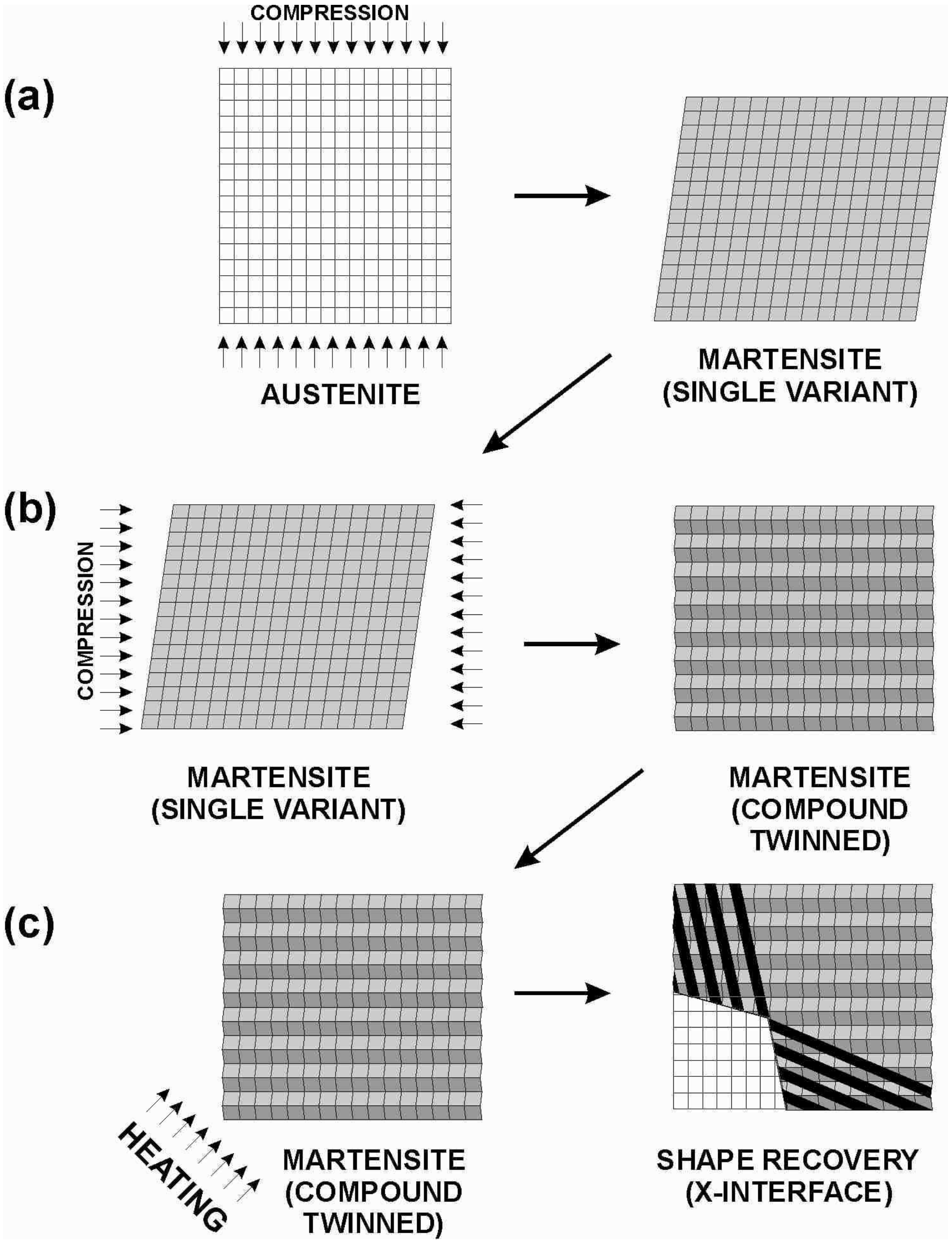
$$F = \mathbf{1} + b \otimes m$$

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



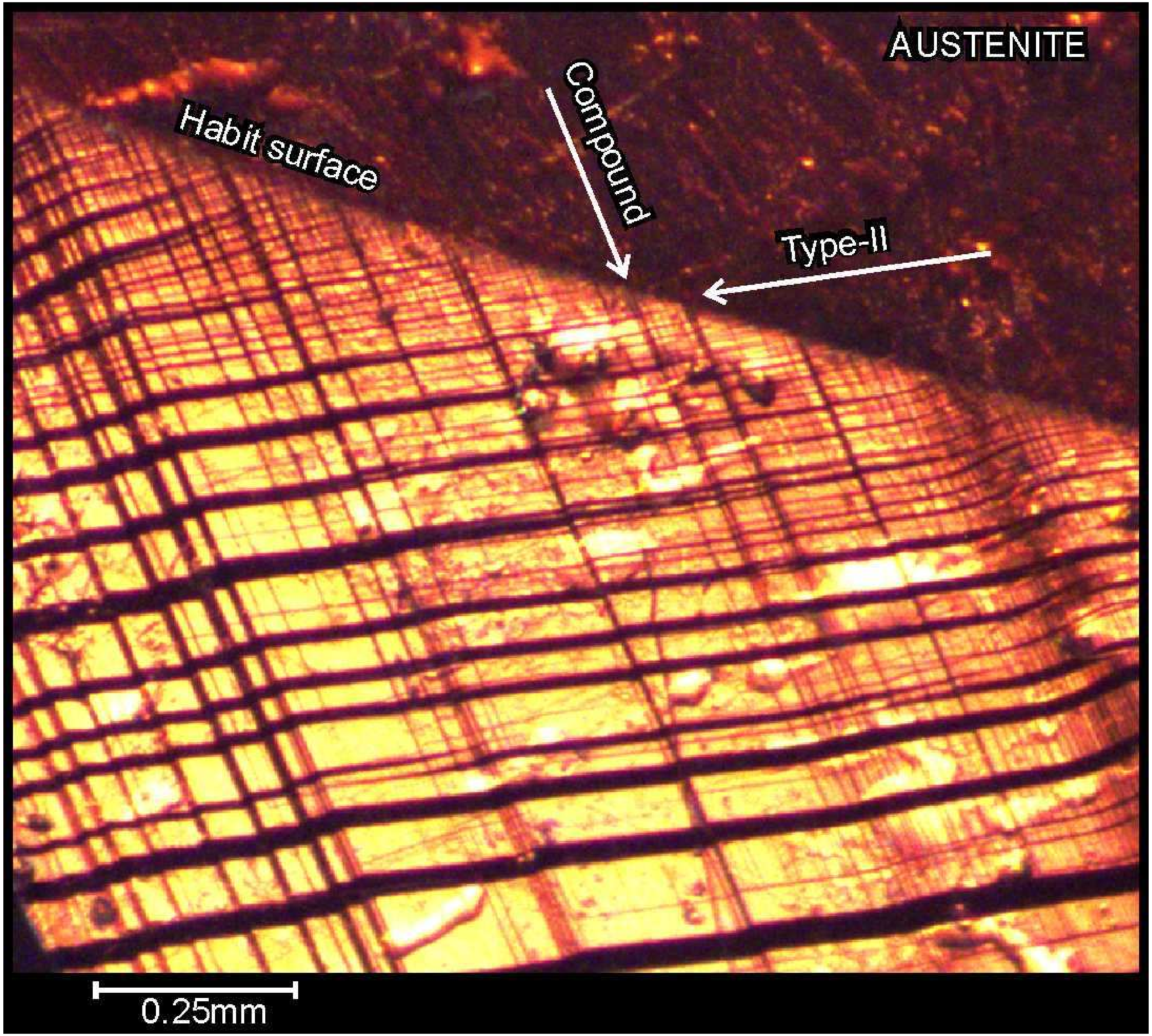
Interface normals



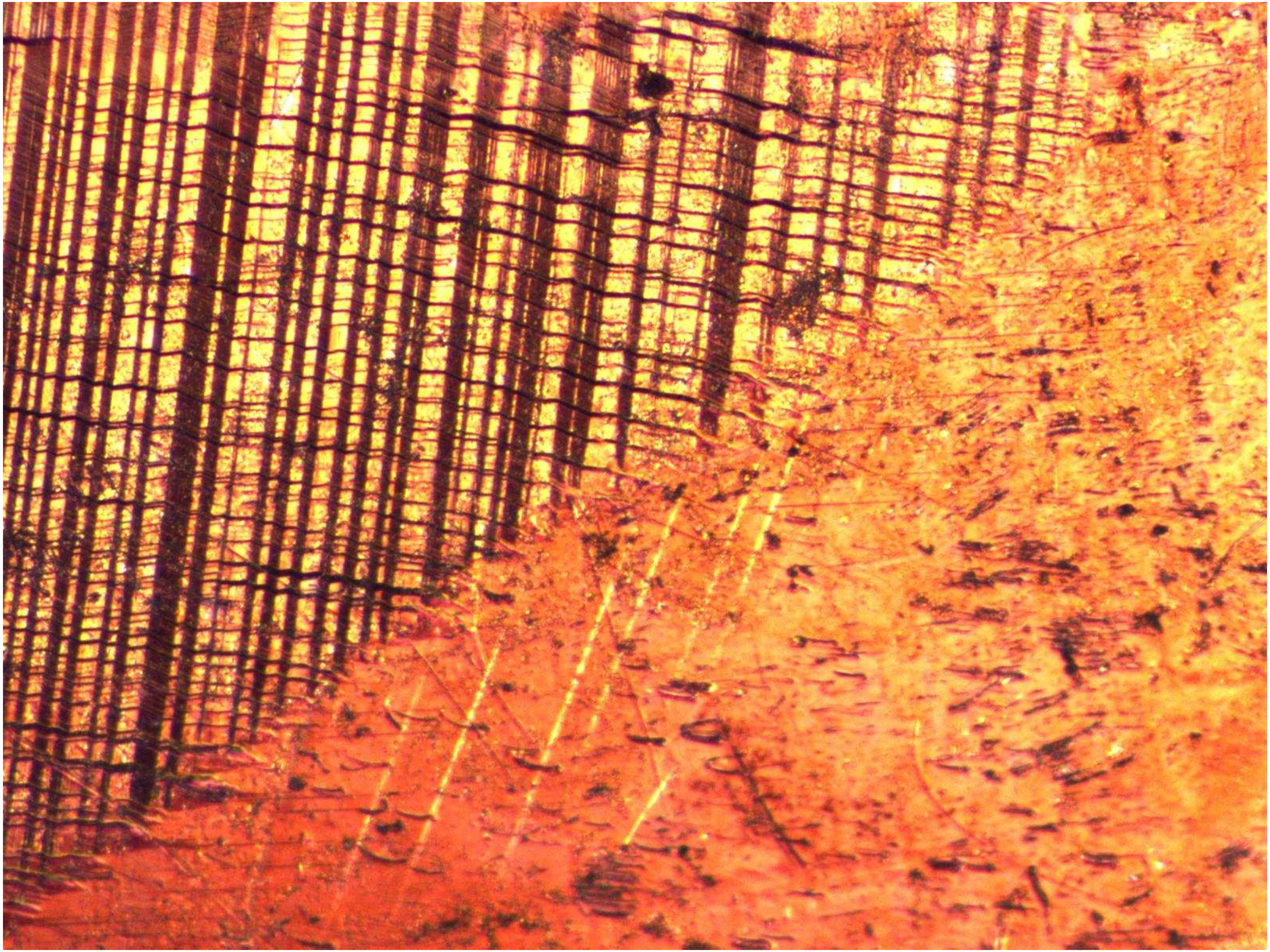


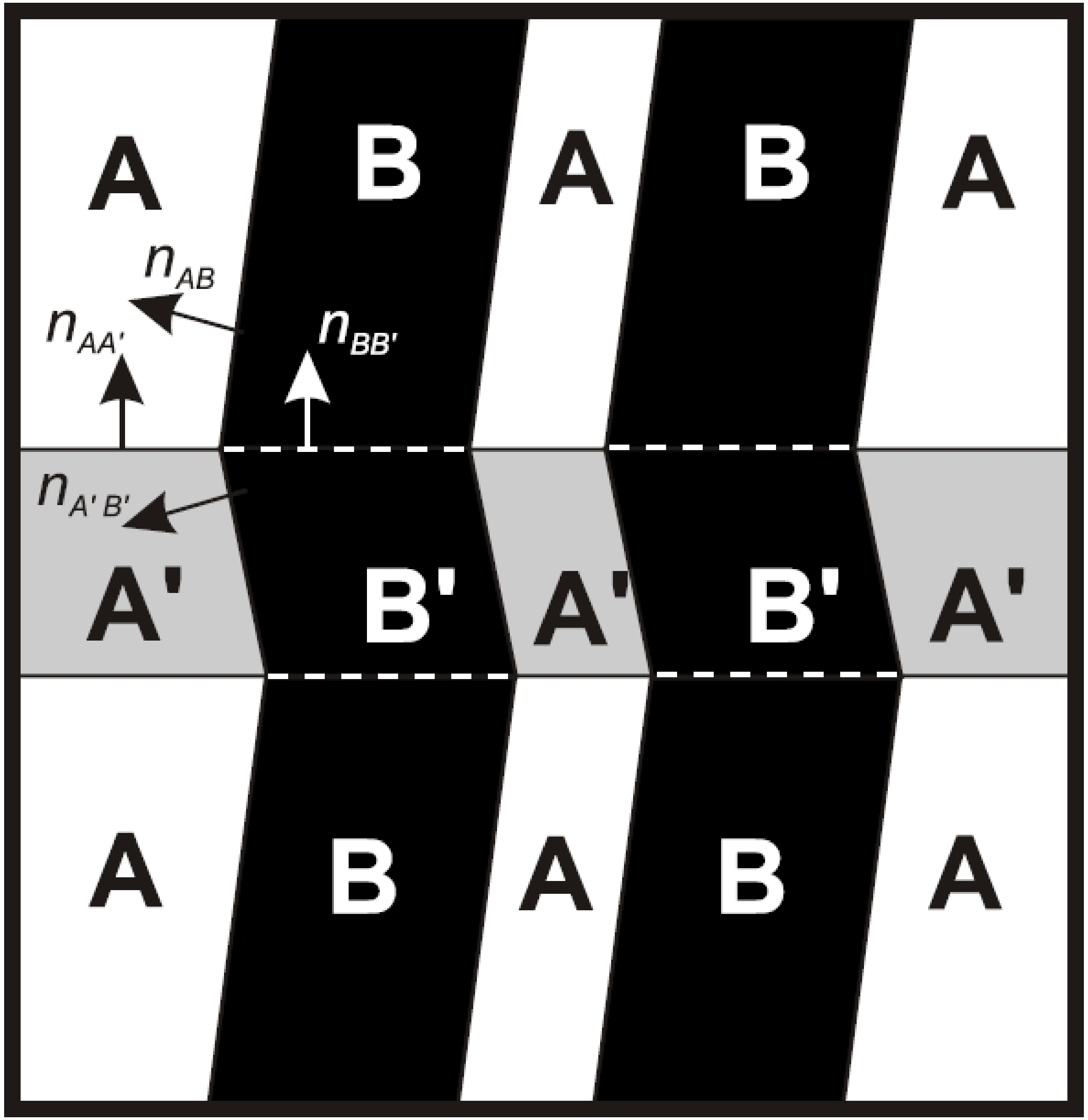
Experimental procedure

$3.9 \times 3.8 \times 4.2$mm 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-orthorhombic energy wells

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

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

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

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

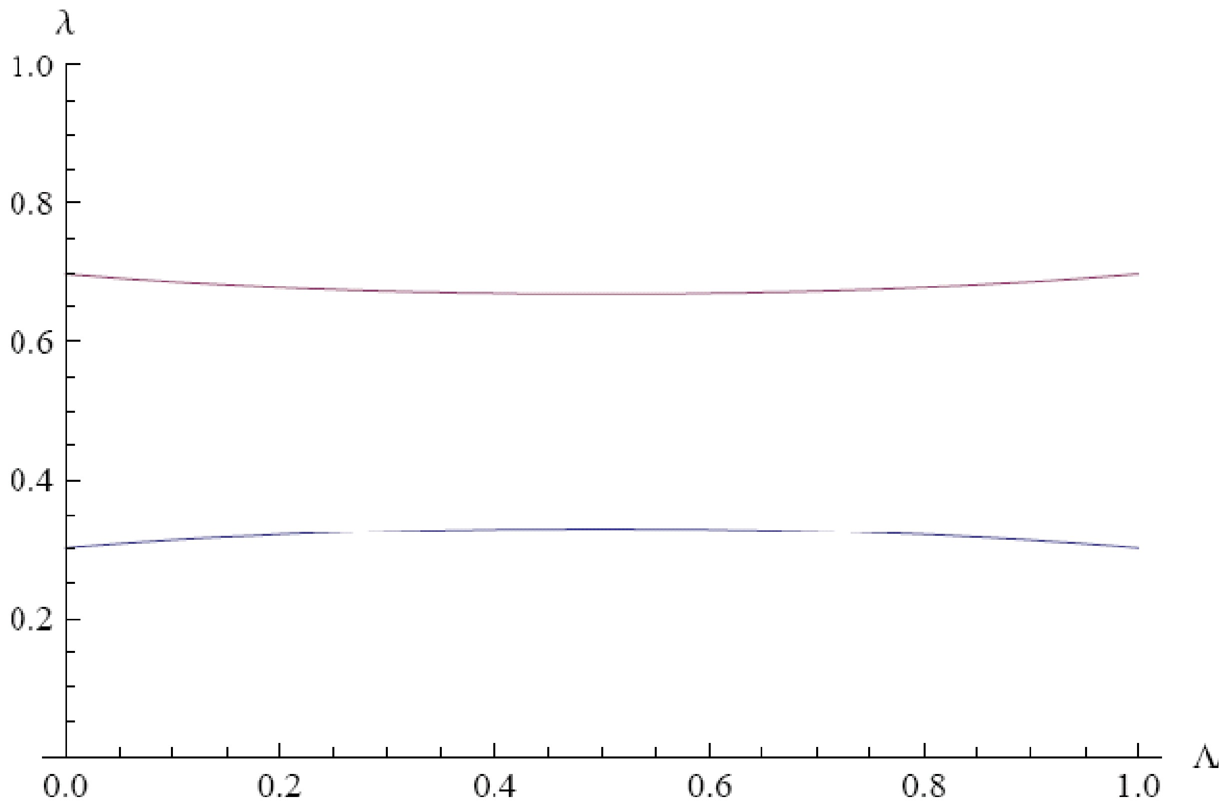
$$M = (1-\Lambda) M_{AB} + \Lambda R_{AA'} M_{A'B'}.$$

For compatibility with the austenite we need

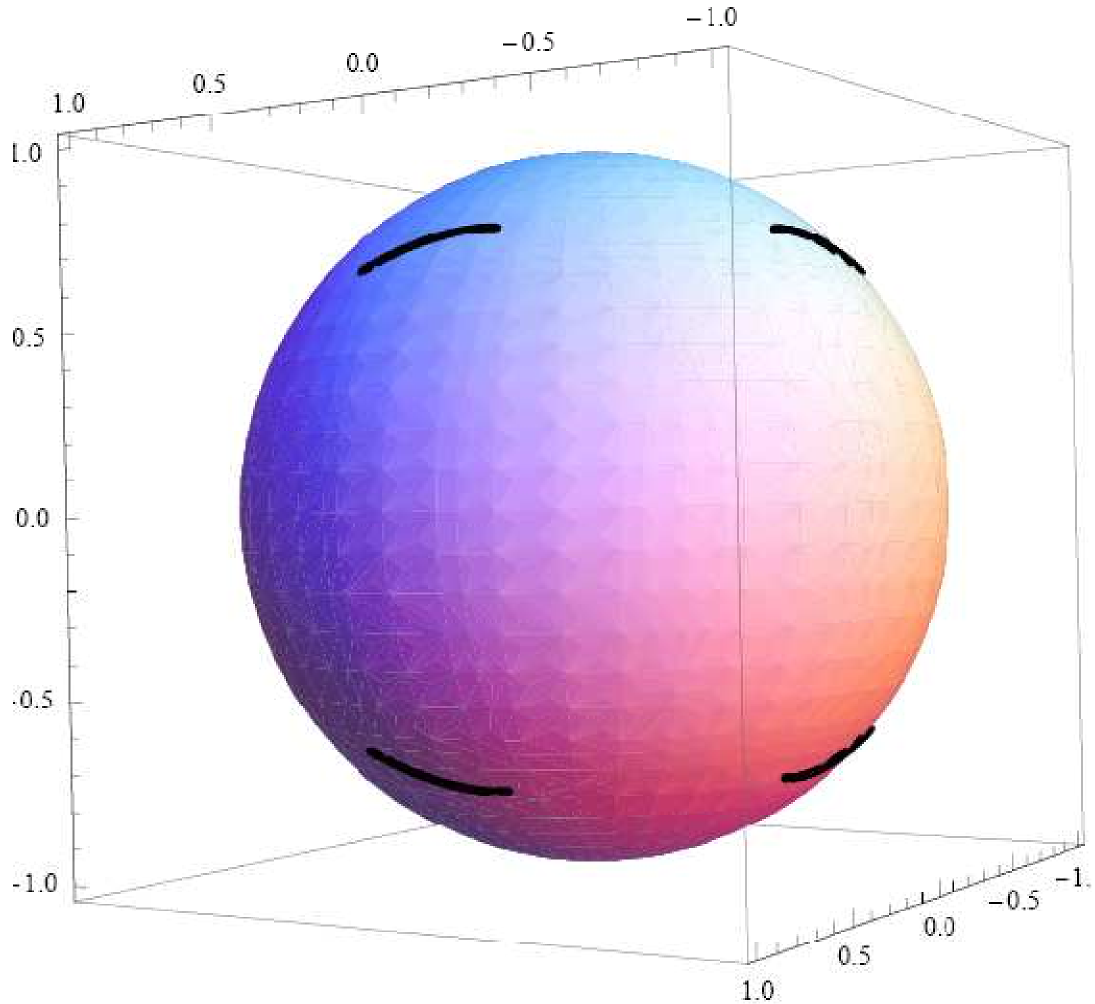
$$\lambda_{\text{mid}}(M^T M) = 1$$

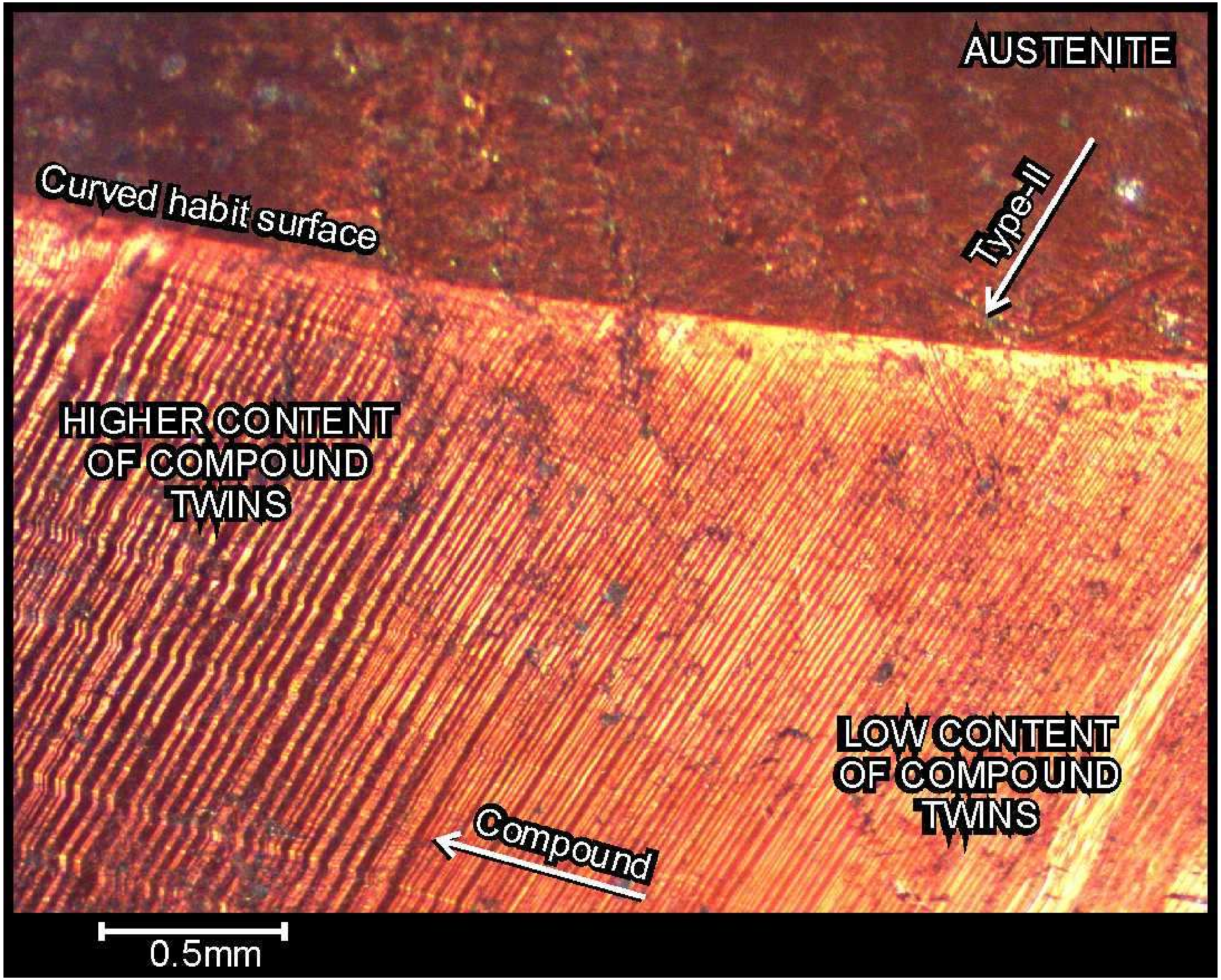
Possible volume fractions

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



Possible nonclassical interface normals





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