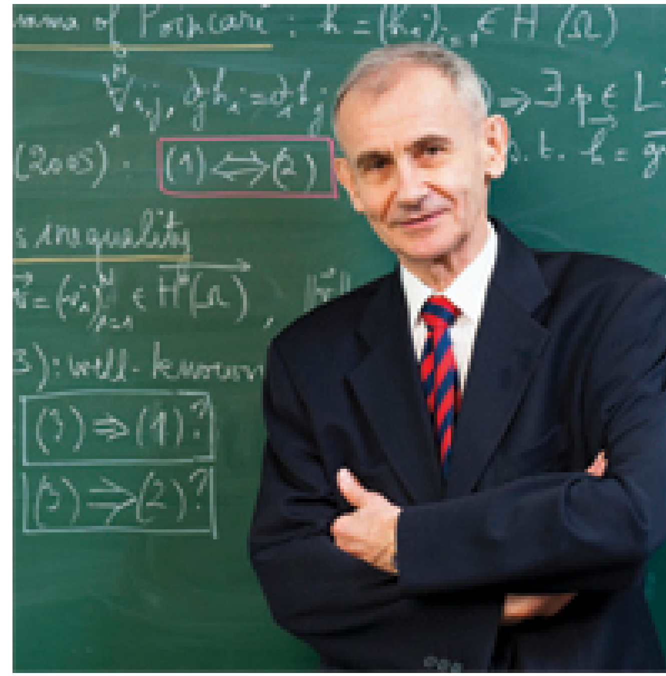
IAS Conference in Honour of Professor Philippe G. Ciarlet's 80th Birthday
City University, Hong Kong, 12 November 2018

Generalized Hadamard jump conditions and martensitic microstructures



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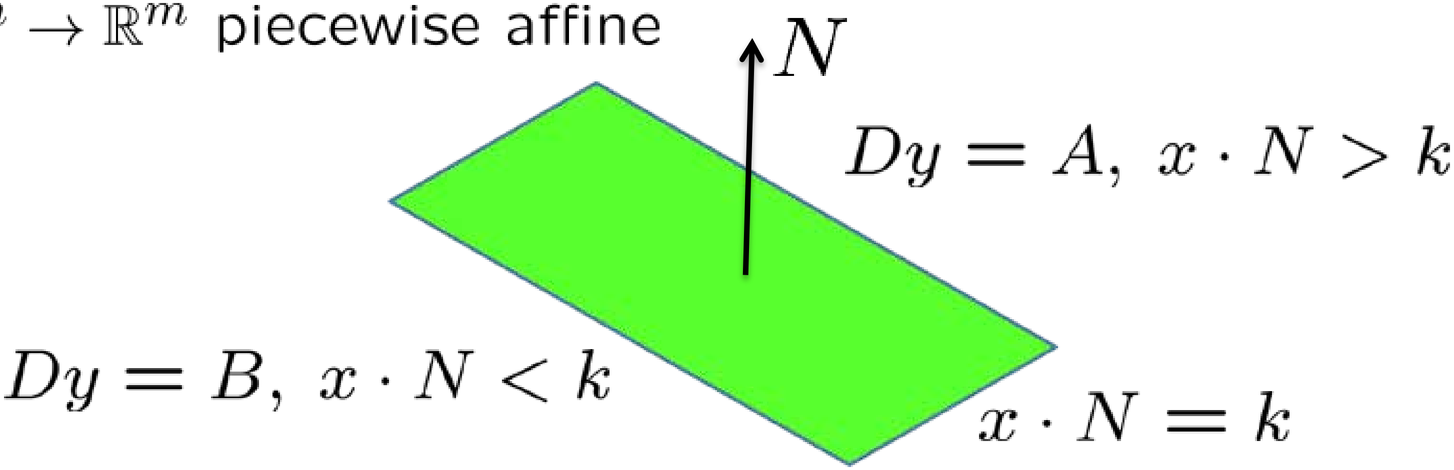
Rank-one matrices and the Hadamard jump condition

$y : \mathbb{R}^n \to \mathbb{R}^m$ piecewise affine



$A, B \in \mathbb{R}^{m\times n} = \{\text{real } m \times n \text{ matrices}\}$

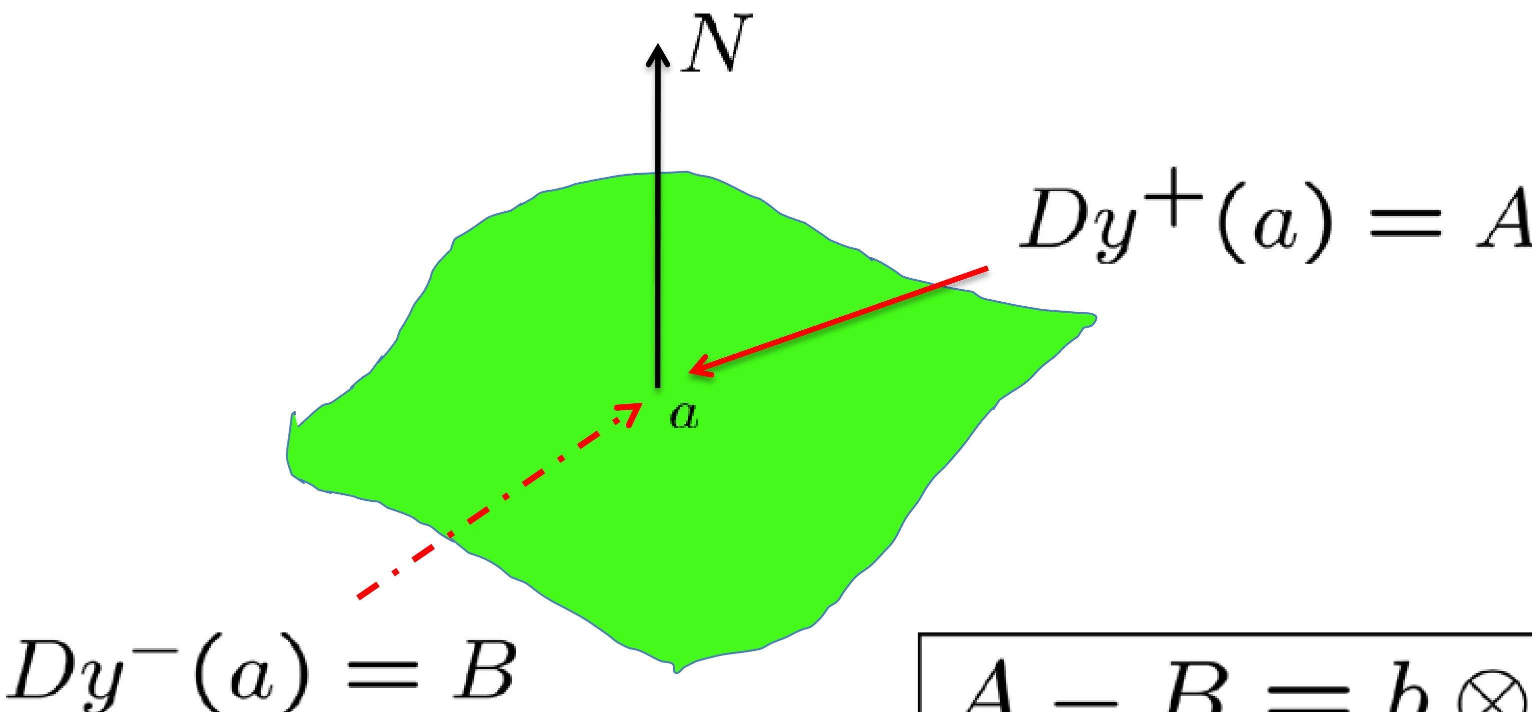
Let $C = A - B$. Then $Cx = 0$ if $x \cdot N = 0$.
Thus $C(z - (z \cdot N)N) = 0$ for all z, and so
$Cz = (CN \otimes N)z$, where $(a \otimes N)_{ij} = a_i N_j$.

rank one
if $A \neq B$

Hadamard
jump condition

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

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



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

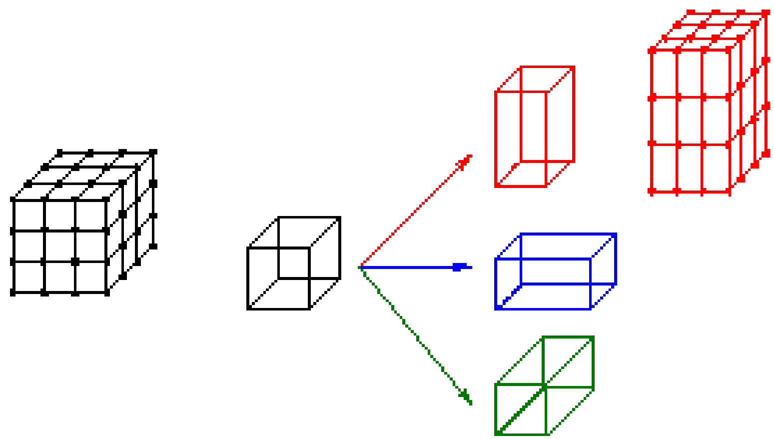
Proof: blow up around x using

$$y_\delta(x) = \delta^{-1}(y(a + \delta x) - y(a)).$$

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

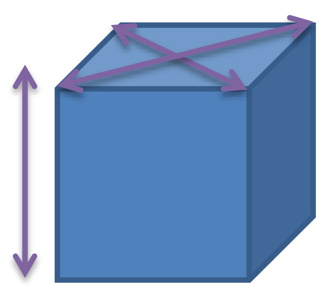
e.g. cubic to tetragonal

$\theta > \theta_c$
cubic
austenite

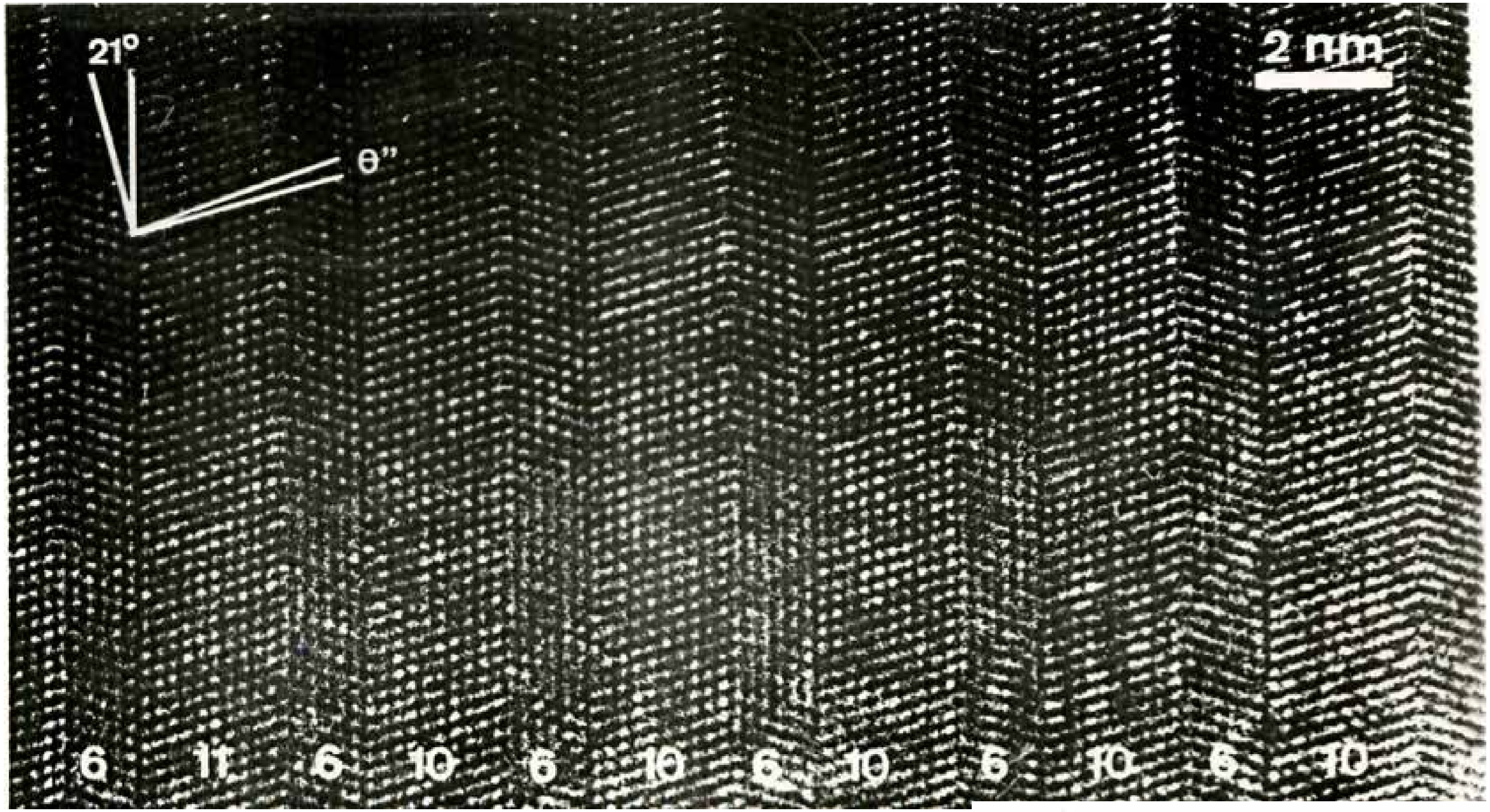


$\theta < \theta_c$
three tetragonal variants of martensite

cubic to orthorhombic (e.g. CuAlNi)

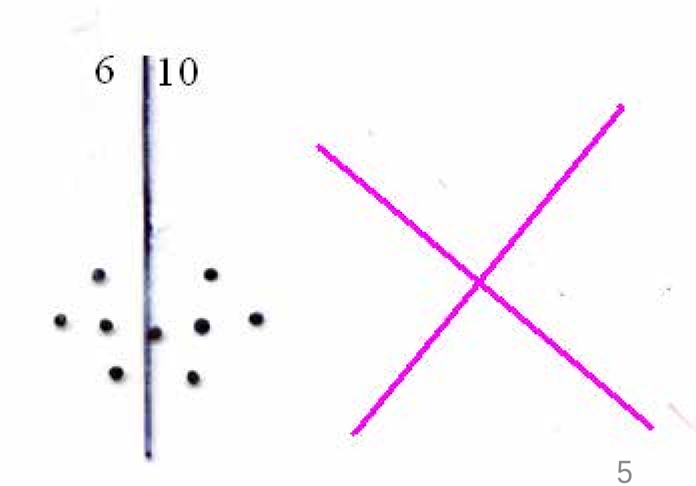


$\theta < \theta_c$
six orthorhombic variants of martensite

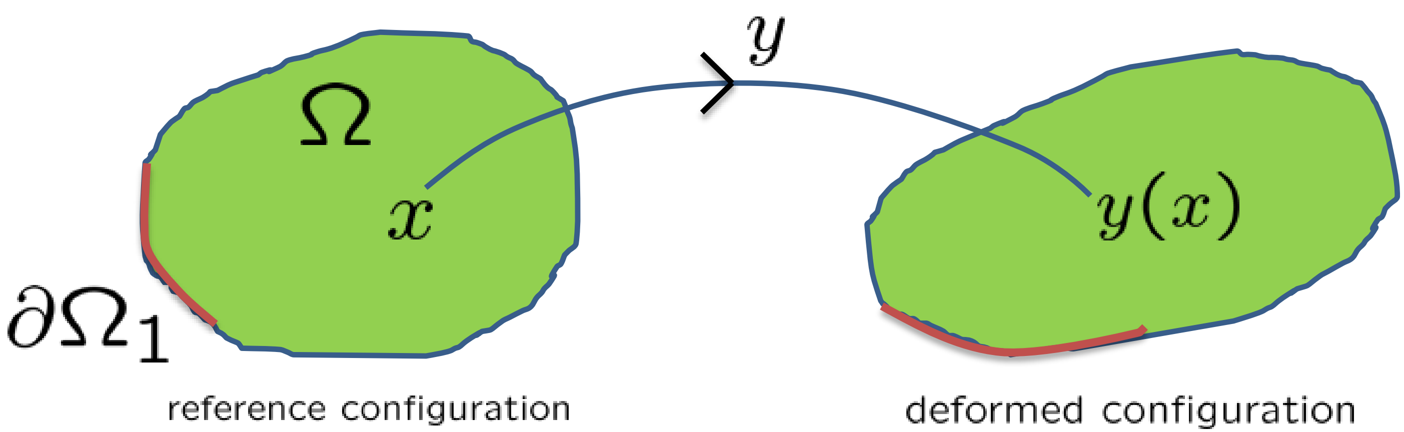


Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

Baele, van Tenderloo, Amelinckx



Energy minimization problem for single crystal



Minimize

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

among (invertible) $y : \Omega \to \mathbb{R}^3$ subject to

$$y|_{\partial\Omega_1} = \bar{y},$$

where $\Omega \subset \mathbb{R}^3$ is a bounded Lipschitz domain, $\partial\Omega_1 \subset \partial\Omega$, and the free-energy density $\psi(A, \theta)$ is defined for $A \in GL^+(3)$, where

$$GL^+(3) = \{\text{real } 3 \times 3 \text{ matrices } A : \det A > 0\}.$$

Energy-well structure

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

Assume

austenite

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

martensite

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

rank-one connections between these wells correspond to twins

e.g. for cubic to tetragonal $M = 3$ and

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

Theorem

Let $U = U^T > 0$, $V = V^T > 0$. Then $\mathrm{SO}(3)\,U$, $\mathrm{SO}(3)\,V$ are rank-one connected iff

$$U^2 - V^2 = c(N \otimes \tilde{N} + \tilde{N} \otimes N) \qquad (*)$$

for unit vectors N, $\tilde{N}$ and some $c \neq 0$.
If $\tilde{N} \neq \pm N$ there are exactly two rank-one connections between V and $\mathrm{SO}(3)\,U$ given by

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

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

(JB/Carstensen version of standard result cf. Ericksen, Gurtin, JB/James ...)

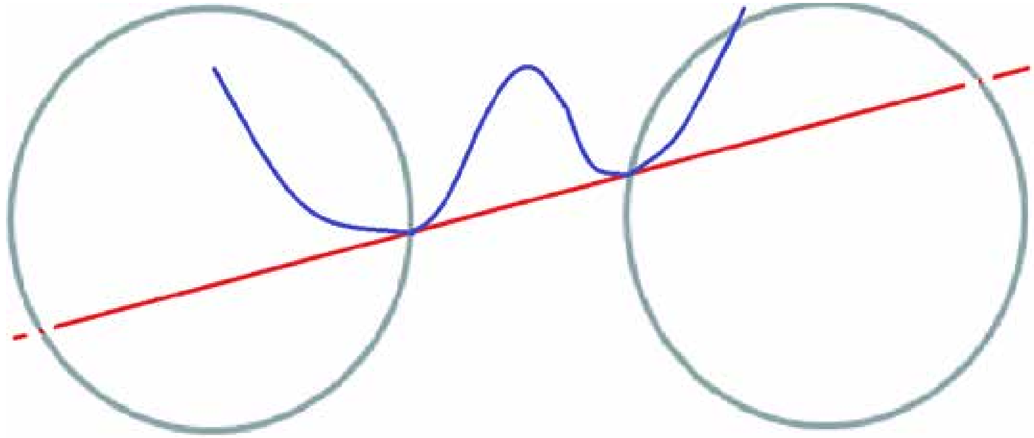
Corollaries.

1. There are no rank-one connections between matrices A, B belonging to the *same* energy well.

Proof. In this case $U = V$, contradicting $c \neq 0$.

2. If $U_i(\theta), U_j(\theta)$ are distinct martensitic variants then $\mathrm{SO}(3)U_i(\theta)$ and $\mathrm{SO}(3)\mathrm{U_j}(\theta)$ are rank-one connected if and only if $\det(U_i(\theta)^2 - U_j(\theta)^2) = 0$, and the possible interface normals are orthogonal. Variants separated by such interfaces are called *twins*.

3. There is a rank-one connection between pairs of matrices $A \in \mathrm{SO}(3)$ and $B \in \mathrm{SO}(3)U_i(\theta_c)$ *if and only if* $U_i(\theta_c)$ *has middle eigenvalue 1.*



The existence of twins implies that the corresponding $\psi(\cdot,\theta)$ is not *rank-one convex* (i.e. convex in the direction of matrices of rank one).

Since quasiconvexity implies rank-one convexity this means that $\psi(\cdot,\theta)$ is not *quasiconvex*.

Definition (Morrey). $f \in C^0(\mathbb{R}^{m\times n})$ is quasiconvex if

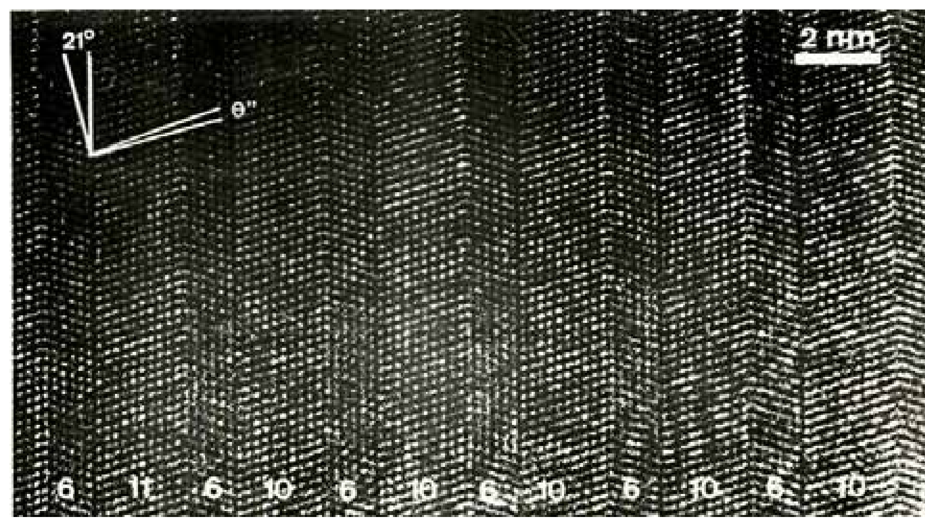
$$\int_\Omega f(Du(x))\,dx \geq \int_\Omega f(A)\,dx = \mathcal{L}^n(\Omega) f(A)$$

for all $A \in \mathbb{R}^{m\times n}$ and smooth $u : \mathbb{R}^n \to \mathbb{R}^m$ with $u(x) = Ax$ for $x \in \partial\Omega$, where $\Omega \subset \mathbb{R}^n$ is bounded open.

Quasiconvexity is the central convexity condition of the multi-dimensional calculus of variations, and is roughly speaking necessary and sufficient of the existence of minimizers.

Therefore we do not expect minimizers of $I_\theta(y)$ to exist in general, the gradients $Dy^{(j)}$ of a minimizing sequence $y^{(j)}$ typically generating an infinitely fine microstructure in the limit $\jmath \to \infty$.

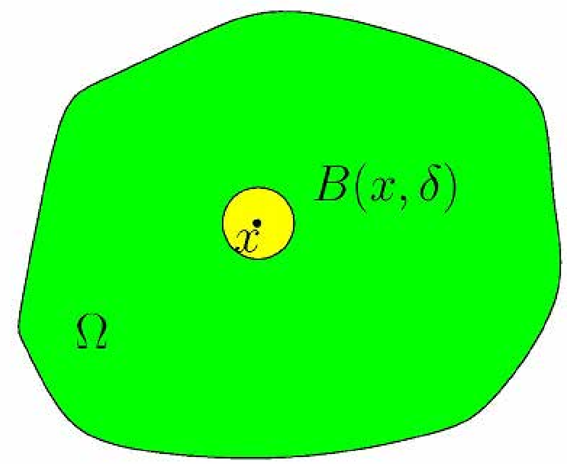
That the fine microstructures observed are not infinitely fine is because interfacial energy contributions are ignored in the elasticity model.



How can we describe infinitely fine microstructures?

Gradient Young measures

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



For $E \subset GL^+(3)$ define

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

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

is the gradient Young measure generated by $Dy^{(j)}$.

$$\bar{\nu}_x := \int_{GL^+(3)} A \, d\nu_x(A) = Dy(x) = \begin{cases} \text{weak limit of } Dy^{(j)} \\ \text{macroscopic} \\ \text{deformation gradient} \end{cases}$$

Semiconvex hulls

$\psi : \mathbb{R}^{m\times n} \to \mathbb{R}$ is polyconvex if $\psi(A) = g(\mathbf{J}(A))$ for a convex function g of the minors $\mathbf{J}(A)$.

Let G be a convex cone of continuous functions $g : \mathbb{R}^{m\times n} \to \mathbb{R}$ containing constants. For $K \subset \mathbb{R}^{m\times n}$ compact define (Šverák)

$$K^G = \{A : \psi(A) \leq \max_K \psi \text{ for all } \psi \in G\}.$$

Theorem (cf Krucik 2000)

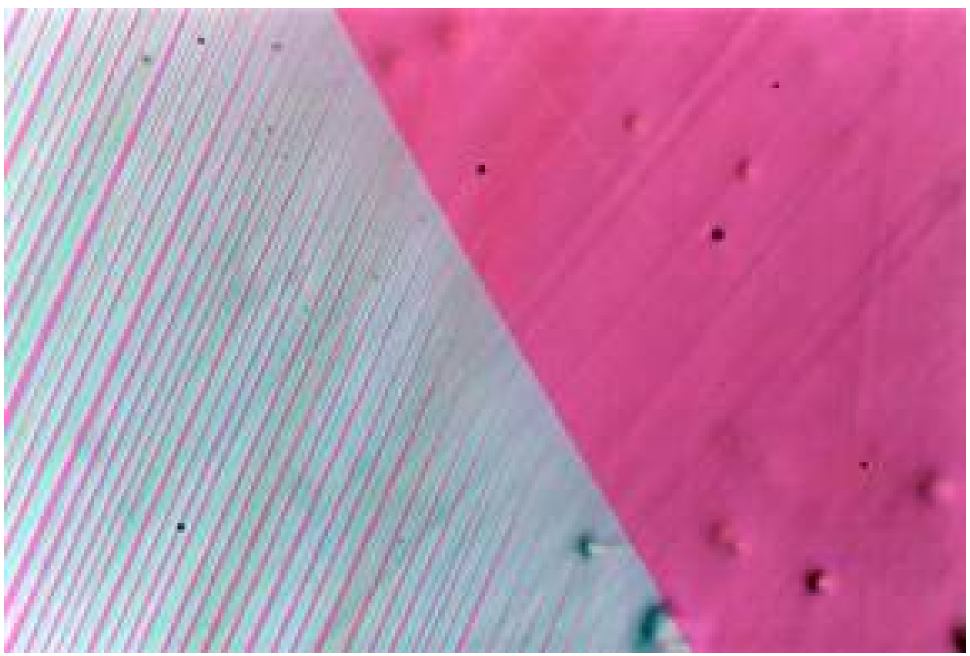
$$K^G = \{A \in \mathbb{R}^{m\times n} : \exists \mu \in \mathcal{P}(K) \text{ with } g(A) \leq \langle \mu, g\rangle \ \forall g \in G\}$$

For $G =$ convex (resp. polyconvex, quasiconvex) functions we write $K^G = K^c$, (resp. K^{pc}, K^{qc}), and then

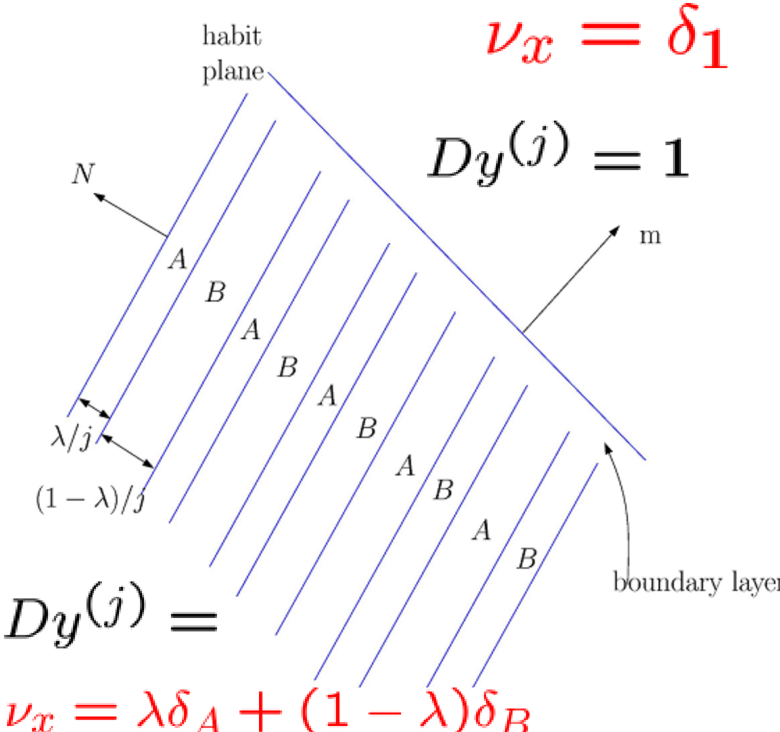
$$K^{qc} \subset K^{pc} \subset K^c.$$

When a new phase is nucleated in a martensitic phase transformation, it has to fit geometrically onto the parent phase. This is is both an important ingredient for determining microstructure morphology, and leads to metastability when the two phases are geometrically incompatible.

e.g. austenite-martensite interfaces



(Classical) austenite-martensite interface in CuAlNi
(courtesy C-H Chu and R.D. James)



$$\nu_x = \delta_1$$

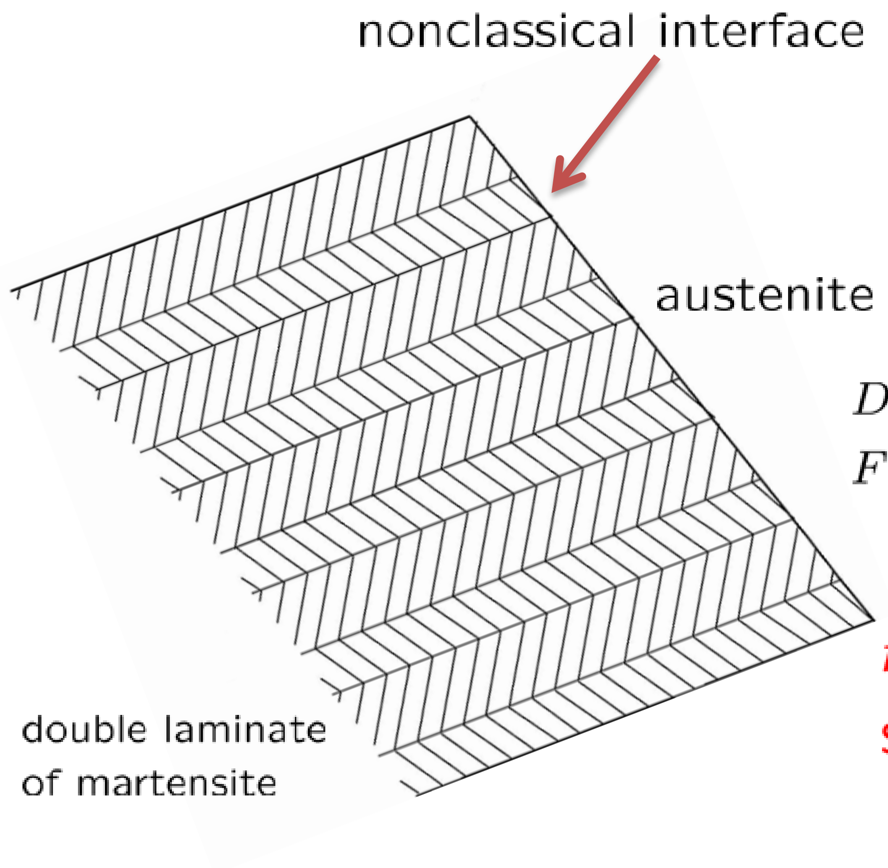
$$Dy^{(j)} = 1$$

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

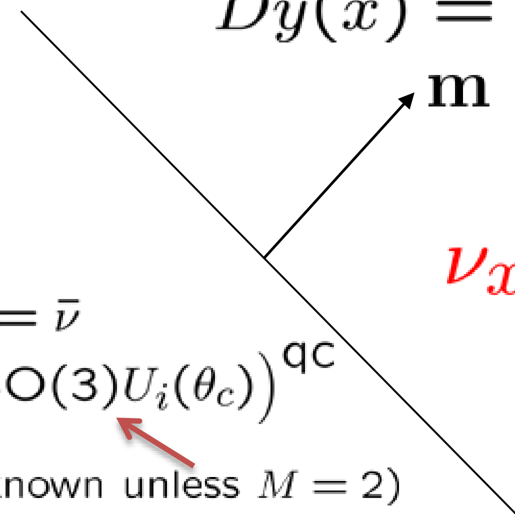
$$\nu_x = \lambda\delta_A + (1-\lambda)\delta_B$$

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

But why (cf JB/Carstensen 1997) should the martensitic microstructure be a simple laminate, rather than something more complicated, such as a double laminate?



$$Dy(x) = 1$$



$$\nu_x = \delta_1$$

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

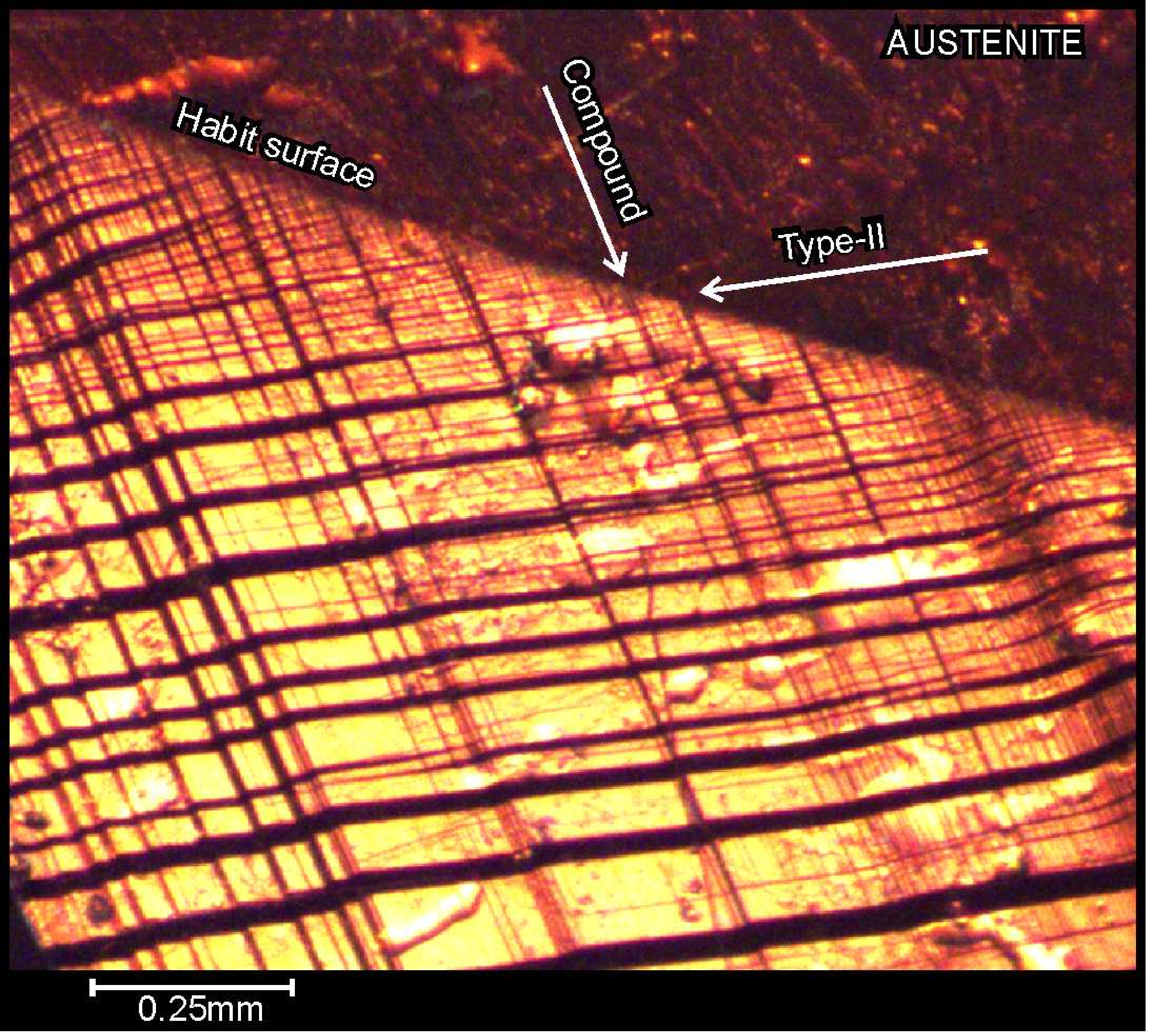
$F \in \left(\bigcup_{i=1}^{M} SO(3) U_i(\theta_c)\right)^{qc}$

(unknown unless $M = 2$)

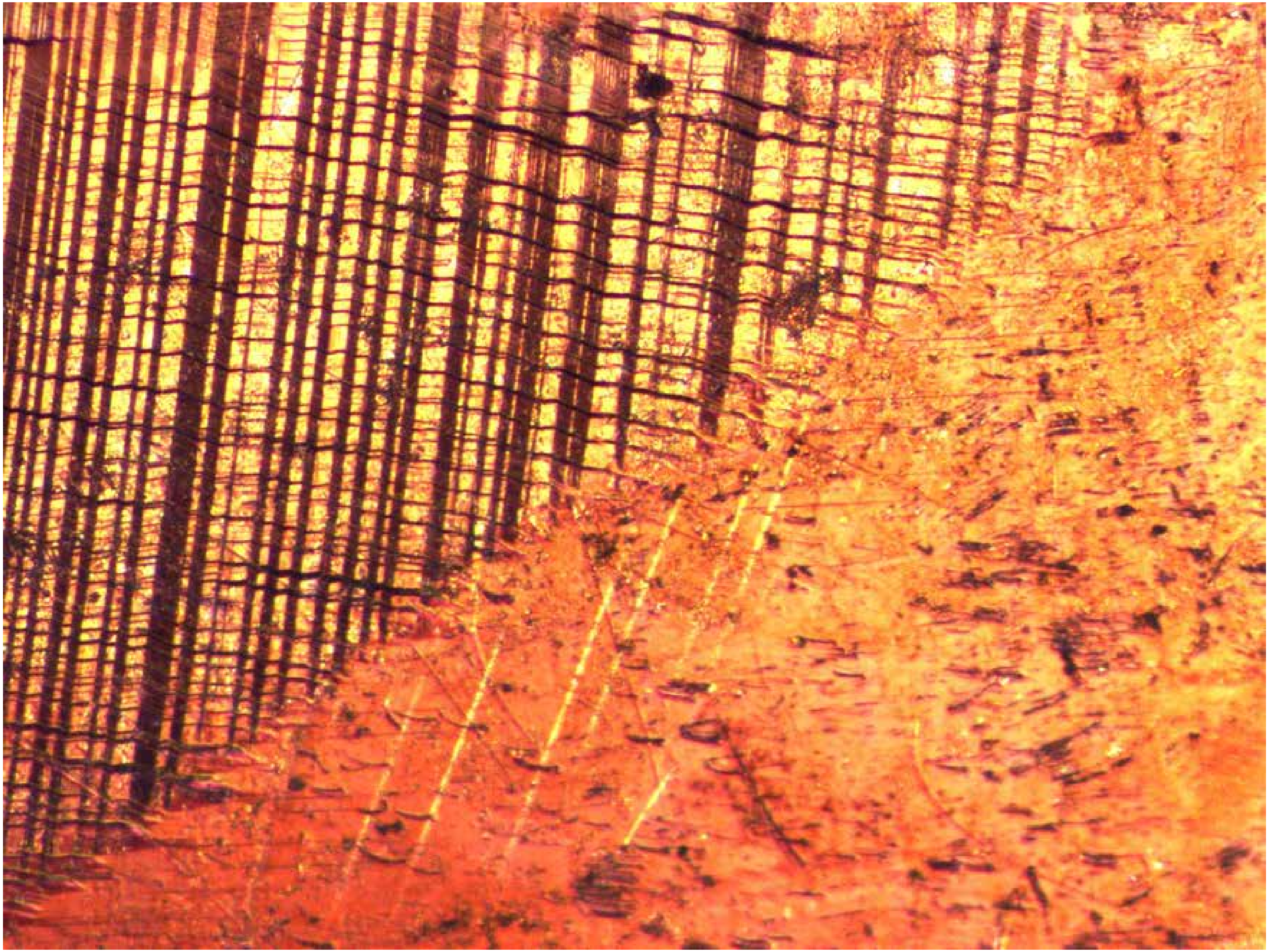
$\nu_x = \nu$

$\mathrm{supp}\,\nu \subset \bigcup_{i=1}^{M} SO(3)\mathbf{U}_i(\theta_c)$

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



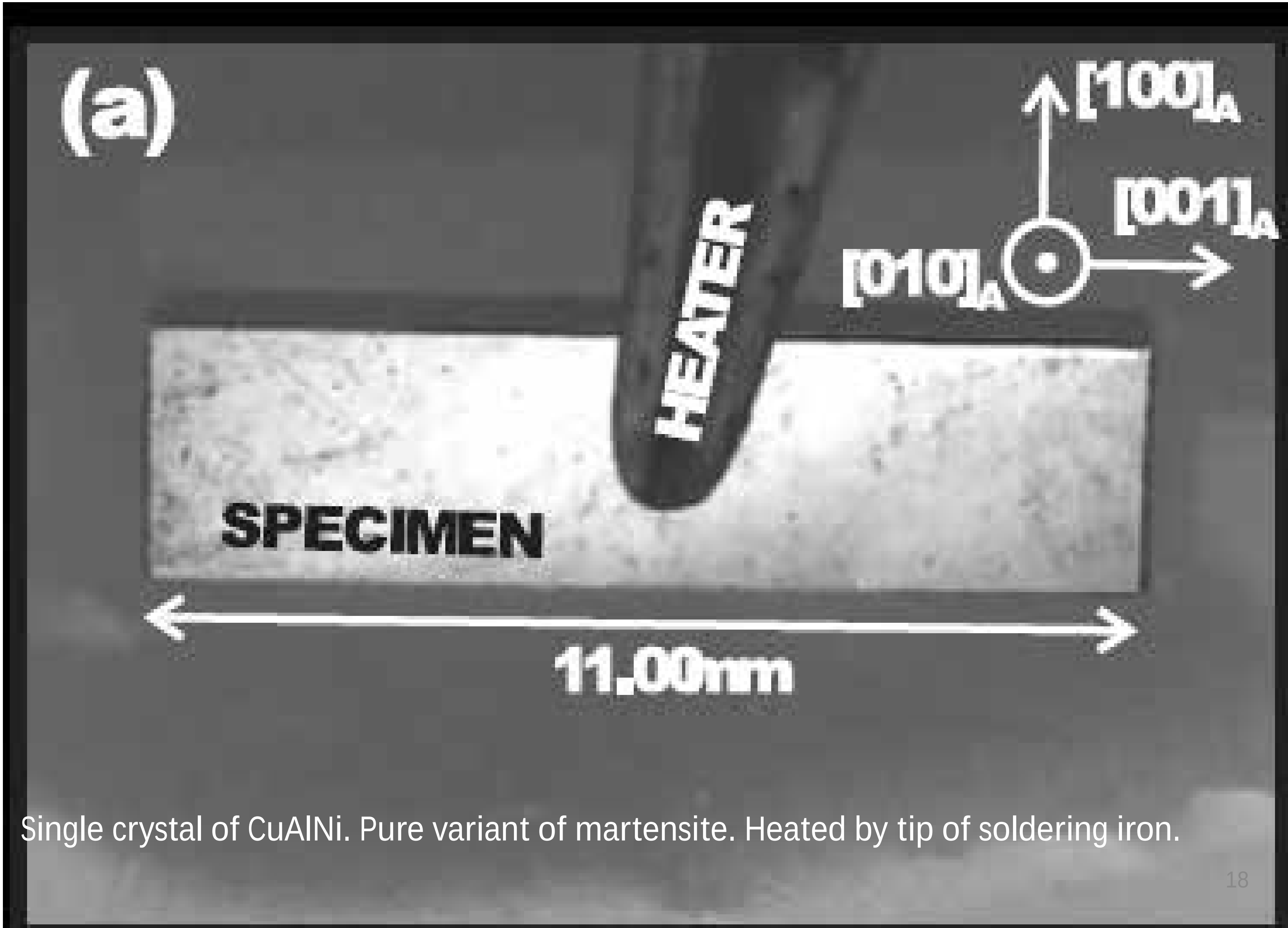
Optical micrograph (H. Seiner) of non-classical interface between austenite and a martensitic microstructure.
The arrows indicate the orientations of twinning planes of Type-II and compound twinning systems



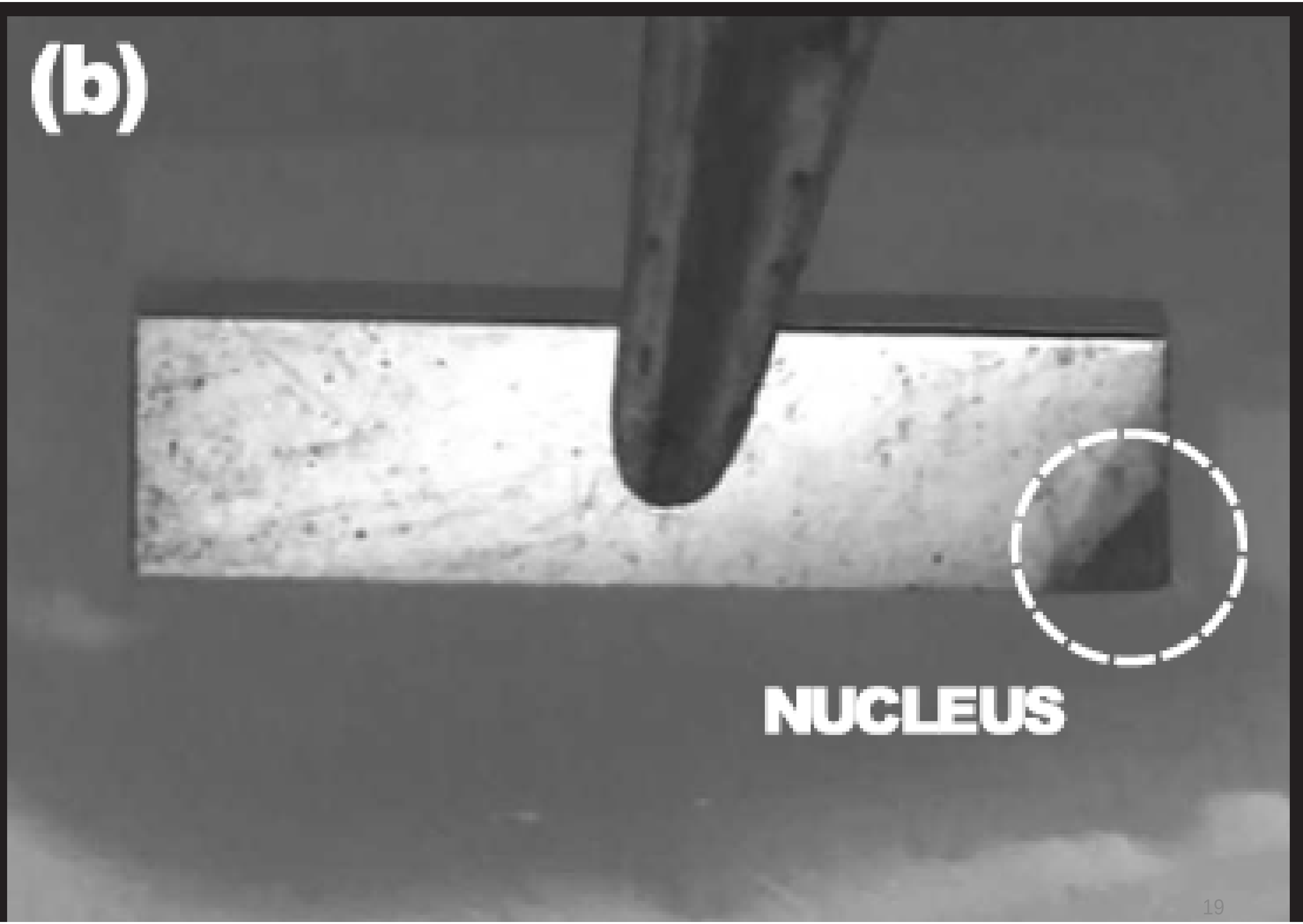
Nonclassical austenite-martensite interface in CuAlNi (H. Seiner)

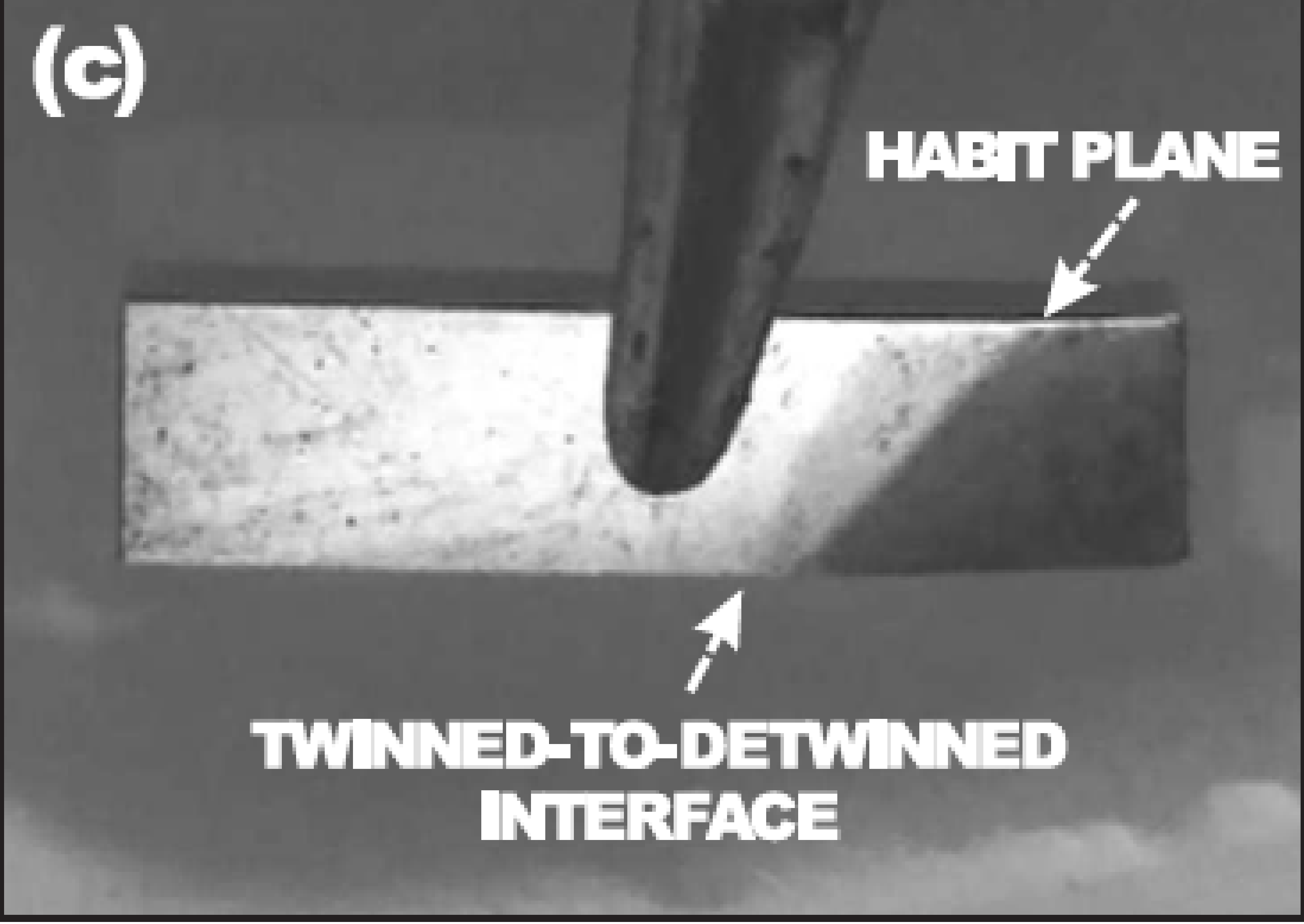
Nucleation of austenite in martensite

(JB/K. Koumatos/H. Seiner 2013,2014)

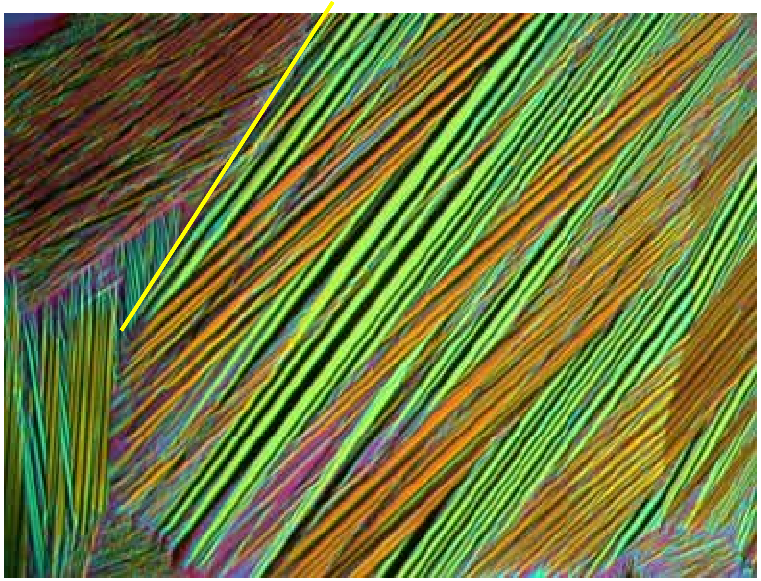


Single crystal of CuAlNi. Pure variant of martensite. Heated by tip of soldering iron.


(b)
NUCLEUS

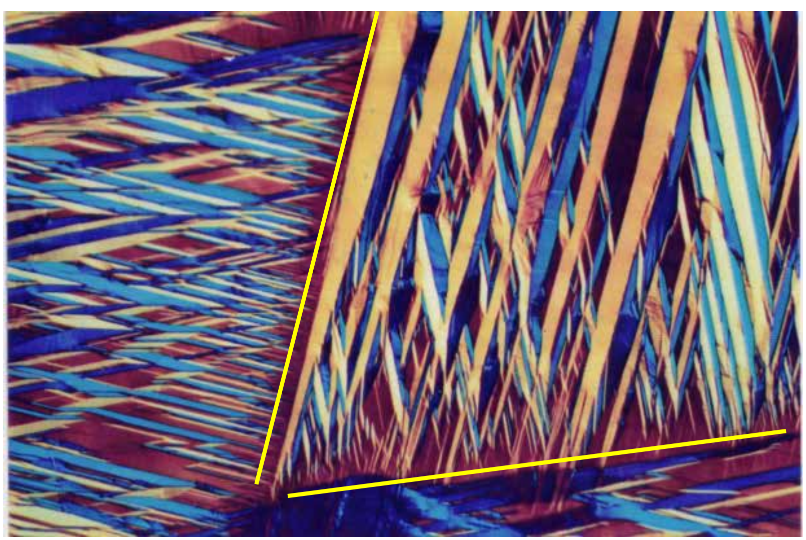

(c)
HABIT PLANE
TWINNED-TO-DETWINNED
INTERFACE

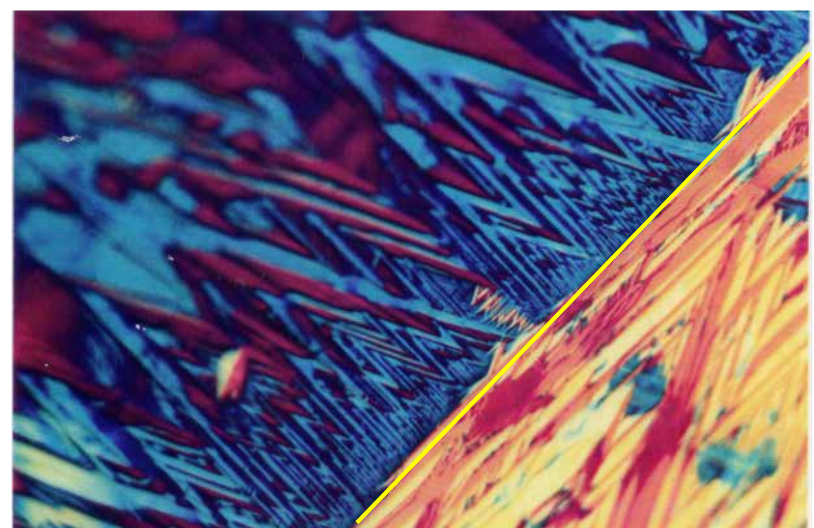
Other complex interfaces



CuZnAl Morin

Cu-14.0wt.%Al-3.9wt.%Ni C. Chu & R. D. James





Question: in general, how are the gradients or gradient Young measures on either side of an interface related?

Knowledge of this could help in understanding microstructure morphology.

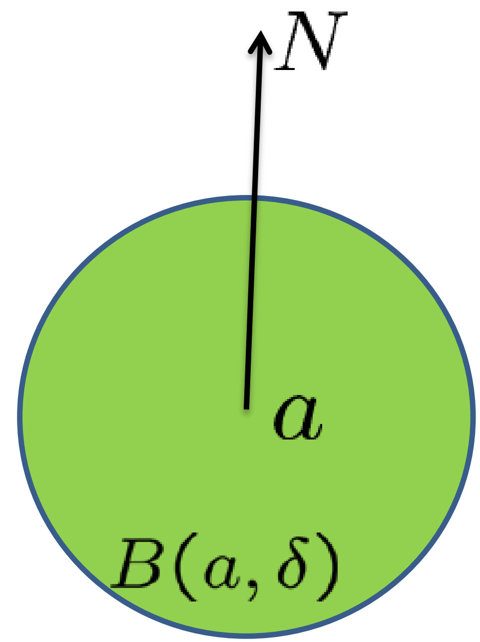
Limiting sets of gradients for Lipschitz maps

$\Omega \subset \mathbb{R}^n$ open,

$y : \Omega \to \mathbb{R}^m$ locally Lipschitz

$a \in \Omega, \ |N| = 1,$

$y \in W^{1,\infty}(B(a,\delta); \mathbb{R}^m)$ for some $\delta > 0$

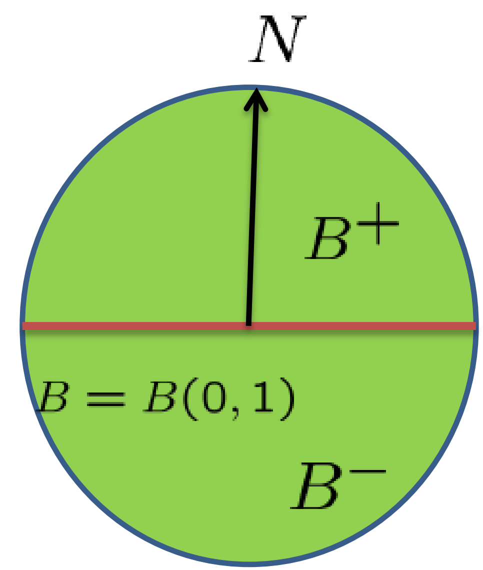


Blow up y around a onto the unit ball $B = B(0,1)$ through

$$z^{(j)}(x) = \delta_j^{-1}(y(a + \delta_j x) - y(a)),$$

where $0 < \delta_j < \delta, \ \delta_j \to 0.$

$$Dz^{(j)}(x) = Dy(a + \delta_j x)$$



Definition

$$D^{\pm N}y(a) \;:=\; \Big\{A\in\mathbb{R}^{m\times n} : \exists\,\delta_j\to 0+ \text{ such that, for all } \varepsilon>0,$$
$$\liminf_{j\to\infty}\mathcal{L}^n(\{x\in B^{\pm} : Dy(a+\delta_j x)\in B(A,\varepsilon)\})>0\Big\}.$$

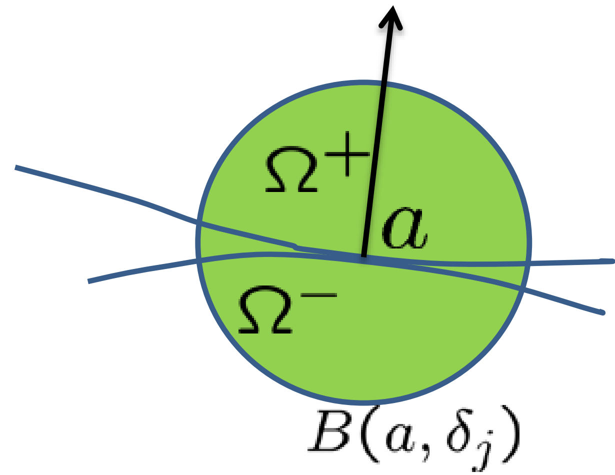
Remark: an equivalent definition can be given in terms of the supports of the Young measures generated by $Dy^{(j)}$.

$D^{\pm N}y(a)$ need not be closed. Indeed there exists a Lipschitz map $y:\mathbb{R}\to\mathbb{R}$ such that $D^{+1}y(0)=\{\frac{1}{k}: k=1,2,\ldots\}$.

Its closure has a slightly simpler characterization

$$\overline{D^{\pm N}y(a)} \;=\; \Big\{A\in\mathbb{R}^{m\times n} : \text{for all } \varepsilon>0$$
$$\liminf_{\delta\to 0+}\mathcal{L}^n(\{x\in B^{\pm} : Dy(a+\delta x)\in B(A,\varepsilon)\})>0\Big\}$$

Remark: The definition can be rephrased in terms of interfaces:



Similar definitions for microstructures.

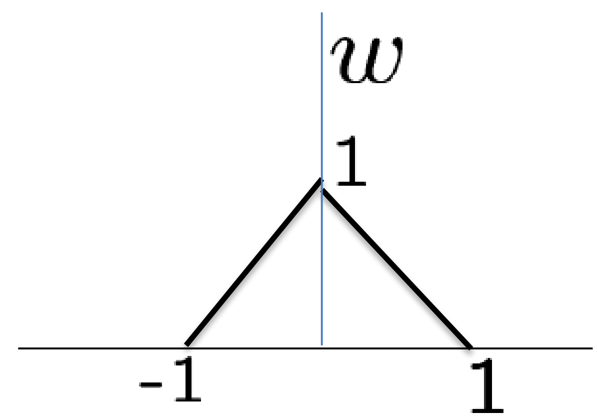
For an open $E \subset \mathbb{R}^n$ define the set of essential gradients

$$Dy(E) = \bigcap\{K \text{ closed}, Dy(x) \in K \text{ a.e. } x \in E\}.$$

Then $D^{\pm N}y(a) \subset \bigcap_{0<\varepsilon<\delta} Dy(a+\varepsilon B^{\pm})$, but in general the inclusion is strict.

For example let $m = n = 1, a = 0$, and

$$y(x) = \sum_{j=1}^{\infty} 2^{-j} w((x - j^{-1})2^j).$$



Then RHS $= \{0, \pm 1\}$, but $D^{+1}y(0) = \{0\}$.

Generalized Hadamard conditions

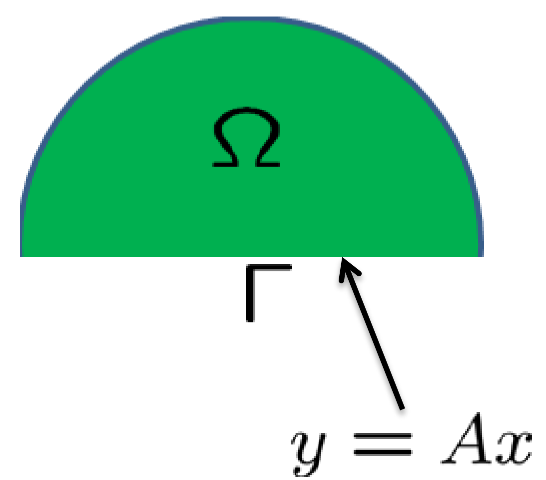
Interface problem on a half ball.

Given a fixed $N \in S^{n-1}$ consider the half-ball

$$\Omega = B^+ = \{x \in B(0,1) : x \cdot N > 0\}$$

and its flat boundary portion

$$\Gamma = \{x \in B(0,1) : x \cdot N = 0\}.$$



Let $y \in W^{1,\infty}(\Omega; \mathbb{R}^m)$ satisfy the affine boundary condition

$$y(x) = Ax \text{ for } x \in \Gamma,$$

where $A \in \mathbb{R}^{m \times n}$ is given.

Question: Does there exist $b \in \mathbb{R}^m$ such that

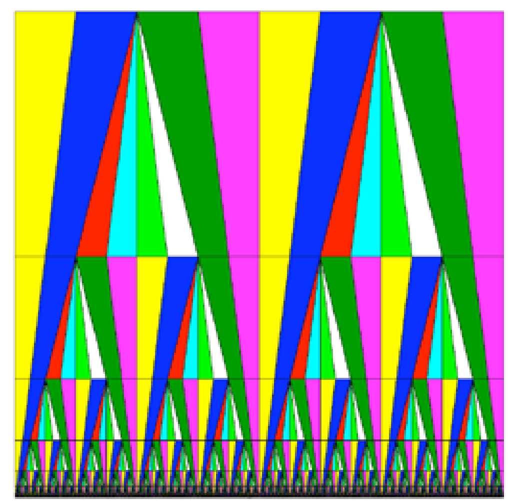
$$A + b \otimes N \in Dy(\Omega)?$$

The answer is no, and counterexamples can be found (JB/James) among maps y such that

$$Dy(x) \in \{A_1, \ldots, A_M\}$$

for $M \geq 3$, where none of the matrices A_i is of the form $A + b \otimes N$.

But see recent work of Della Porta, who describes a situation relevant to low hysteresis materials in which such a result is generically true.



Theorem At every point a in an open set $\Omega \subset \mathbb{R}^n$, for any direction $N \in S^{n-1}$, and for any locally Lipschitz $y : \Omega \to \mathbb{R}^m$, we have

$$0 \in [Dy^{+N}(a)(\mathbf{1}-N\otimes N)]^{\mathrm{qc}}-[Dy^{-N}(a)(\mathbf{1}-N\otimes N)]^{\mathrm{qc}}.$$

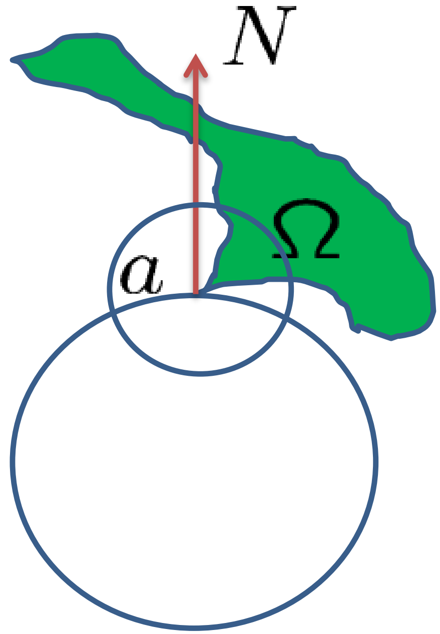
Idea of proof. First consider the case of y defined on a half ball $B^+(0,1)$ with $y(x) = Ax$ on $\Gamma = \{x \in B(0,1) : x \cdot N = 0\}$, and take weak limits of the maps $y^{z_j}(x) = y(x', z_j)$ for a sequence $z_j \to 0+$. Then reduce the general case to this one by doing a second blow-up.

Corollary. There exists $b \in \mathbb{R}^m$ such that

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

Proof. By the theorem

$$\begin{aligned} 0 &\in [Dy^{+N}(a)(\mathbf{1} - N \otimes N)]^c - [Dy^{-N}(a)(\mathbf{1} - N \otimes N)]^c \\ &= [Dy^{+N}(a)^c - Dy^{-N}(a)^c](\mathbf{1} - N \otimes N). \end{aligned}$$



Theorem
Let $\Omega \subset \mathbb{R}^n$ be an arbitrary open set with boundary point a, through which passes a sphere exterior to Ω having exterior normal N. Let $y : \bar{\Omega} \to \mathbb{R}^m$ be Lipschitz with $y(x) = Ax$ for all $x \in \partial\Omega \cap B(a, \delta)$, $\delta > 0$. Then there exists $b \in \mathbb{R}^m$ with $A + b \otimes N \in Dy(\Omega \cap B(a, \delta))^c$.

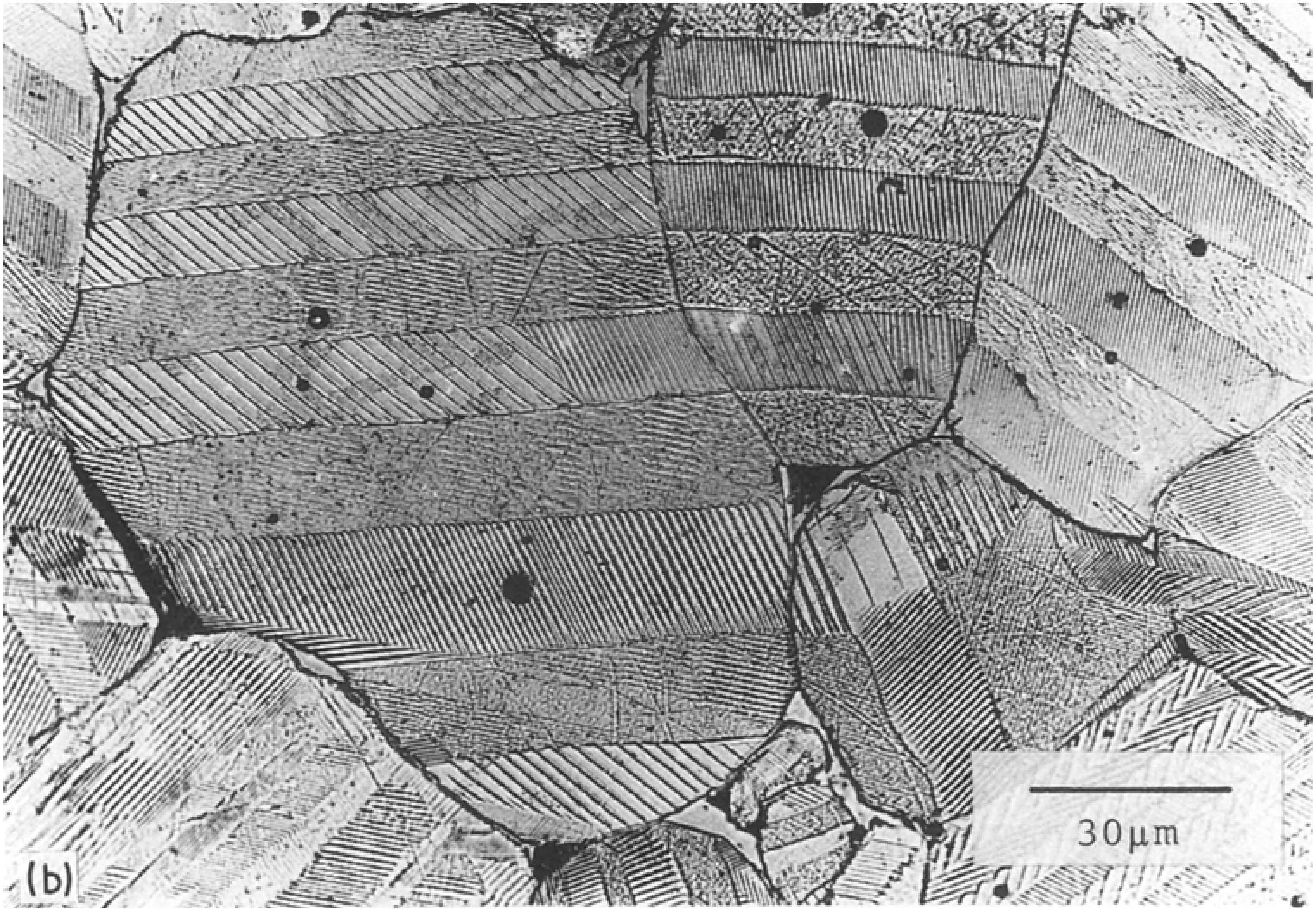
Theorem

Let $m = n = 2$, $\Omega \subset \mathbb{R}^2$ be open, $a \in \mathbb{R}^2$, $N \in S^1$. Then there exists $b \in \mathbb{R}^2$ with

$$b \otimes N \in [D^{-N}y(a)]^{pc} - [D^{+N}y(a)]^{pc}.$$

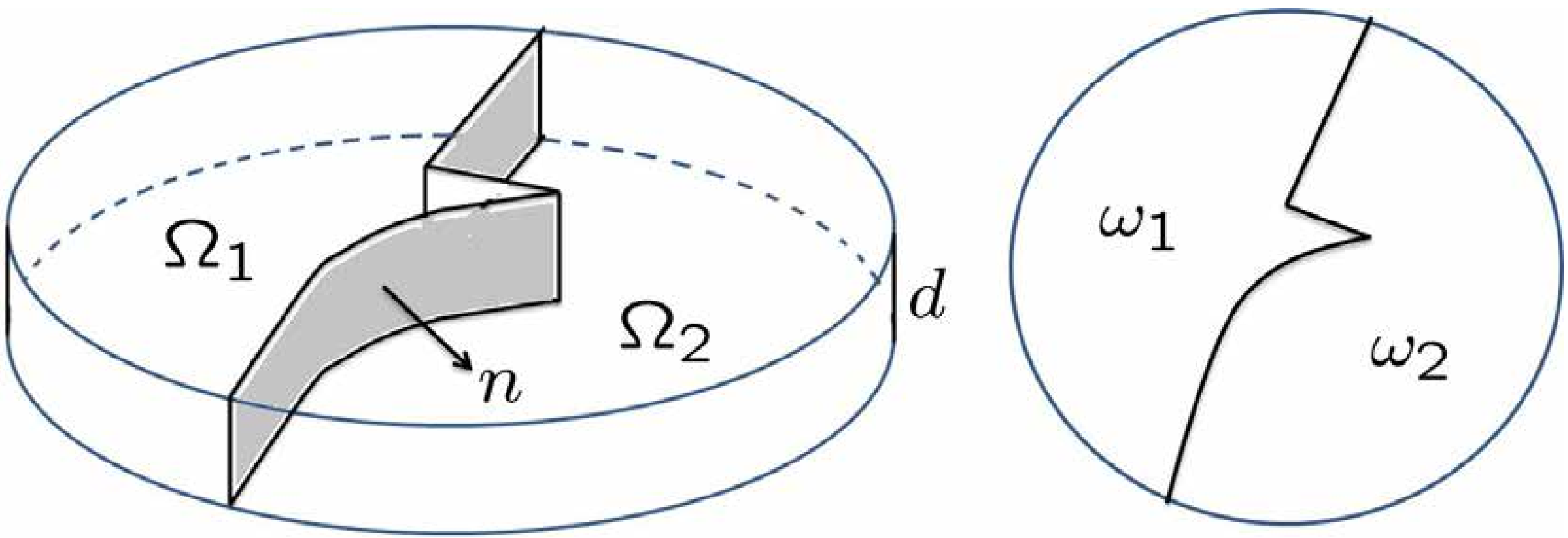
The proof uses results on quasiregular maps. The result was shown to be false for $n = 2$, $m \geq 3$ by Iwaniec, Verchota & Vogel (2002).

Compatibility across grain boundaries



$BaTiO_3$ ceramic: G. Arlt, J. Materials Science, 25 (1990) 2655-2666.

Zero-energy microstructures for a bicrystal



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

$U_1 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_3), U_2 = \mathrm{diag}\,(\eta_1, \eta_2, \eta_3),$
$\eta_2 > \eta_1 > 0, \eta_3 > 0$

Grain 1

$\Omega_1 = \omega_1 \times (0, d)$
$\mathrm{supp}\,\nu_x \subset K$ a.e. $x \in \Omega_1$

Grain 2

$\Omega_2 = \omega_2 \times (0, d)$
$\mathrm{supp}\,\nu_x \subset KR(\alpha)$ a.e. $x \in \Omega_2$
$R(\alpha)e_3 = e_3$

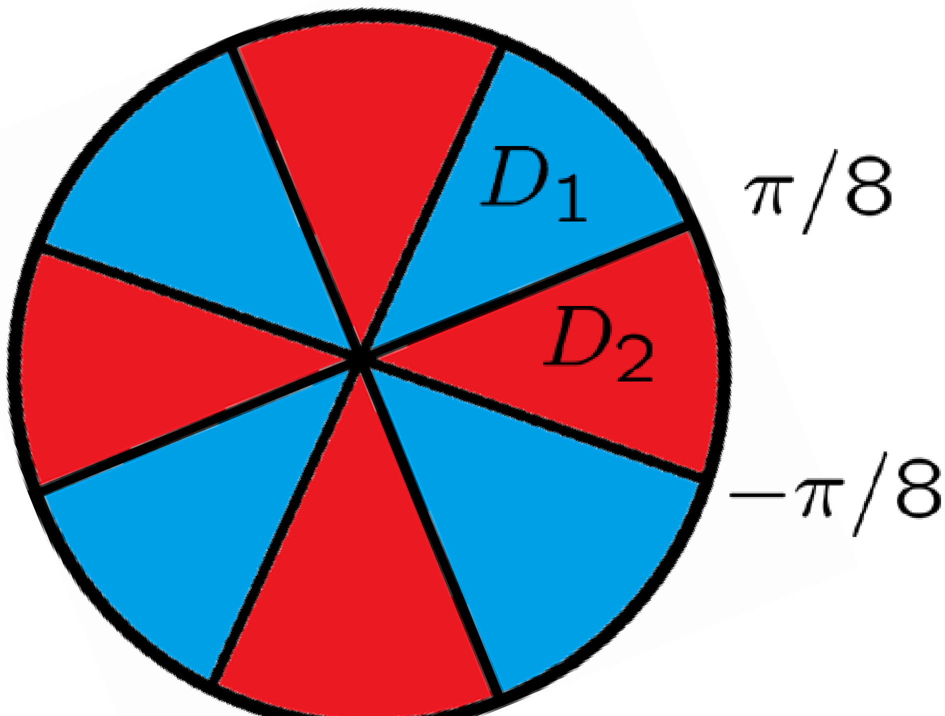
Always possible to have zero-energy microstructure with $Dy = \bar{\nu}_x = (\eta_1\eta_2\eta_3)^{1/3}\mathbf{1}$.

Question: Is it true that every zero-energy microstructure is nontrivial (i.e. not a pure phase $\nu_x = \delta_A$) in each of the grains?

Result 1. If the interface is *planar* then whatever its normal n there always exists a zero-energy microstructure which has a pure phase (i.e. $\nu_x = \delta_A$) in one of the grains.

Therefore the interface needs to be curved in order to show that the microstructure has to be nontrivial. Write the normal to the interface as $n = (\cos\theta, \sin\theta, 0)$.

Result 2. Suppose that $\alpha = \pi/4$. Then it is impossible to have a zero-energy microstructure with a pure phase in one of the grains if the boundary between the grains contains a normal with $\theta \in D_1$ and another normal with $\theta' \in D_2$.



Proofs use:

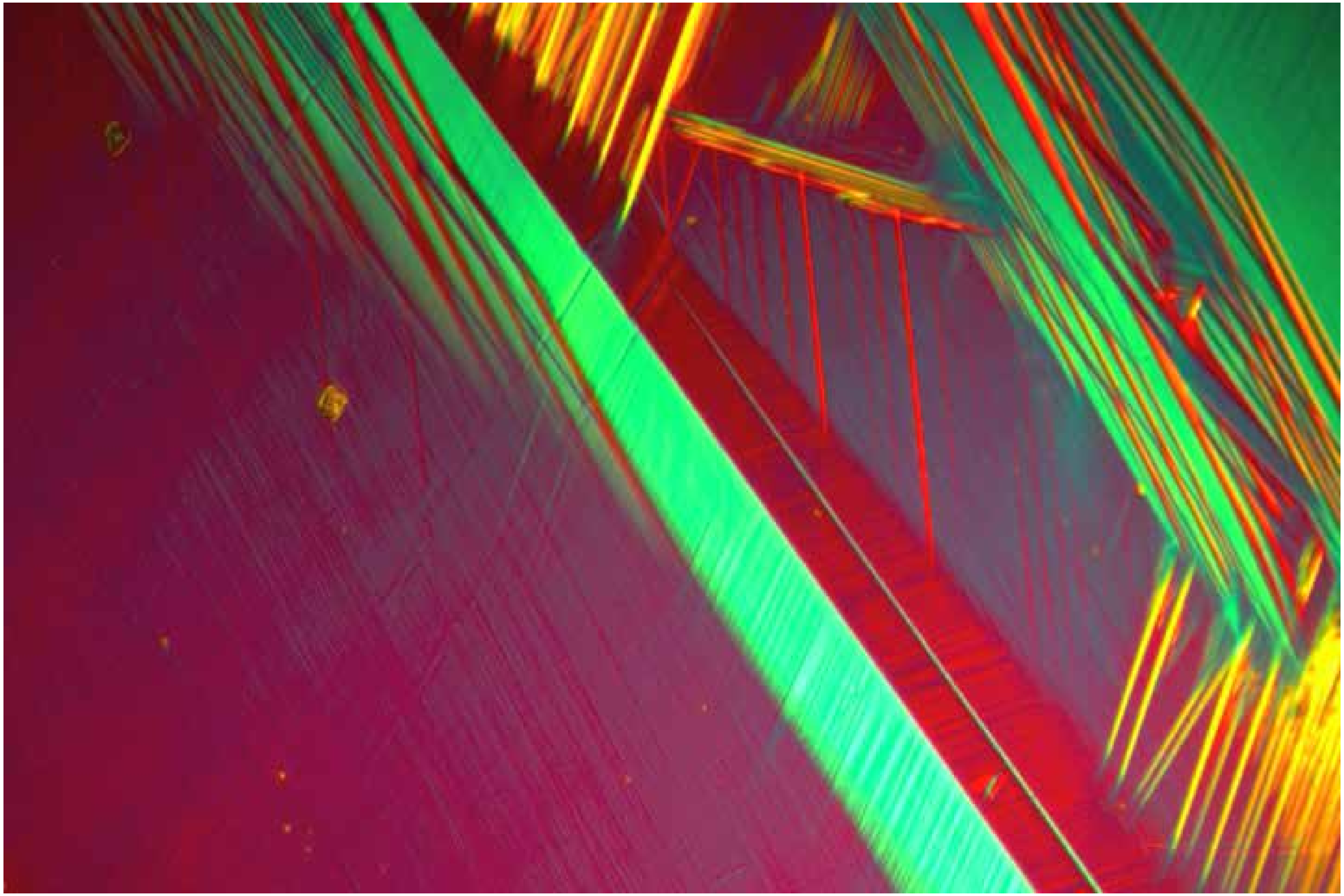
1. A reduction to 2D using the plane strain result for the two-well problem (JB/James).

2. The characterization of the quasiconvex hull of two wells (JB/James), which equals their polyconvex hull.

3. Use of the generalized Hadamard jump condition in 2D to show that there has to be a rank-one connection $b \otimes N$ between the polyconvex hulls for each grain.

4. Long and detailed calculations.

For the details see, JB & C. Carstensen, *Interaction of martensitic microstructures in adjacent grains*, ICOMAT 2017 Proceedings.



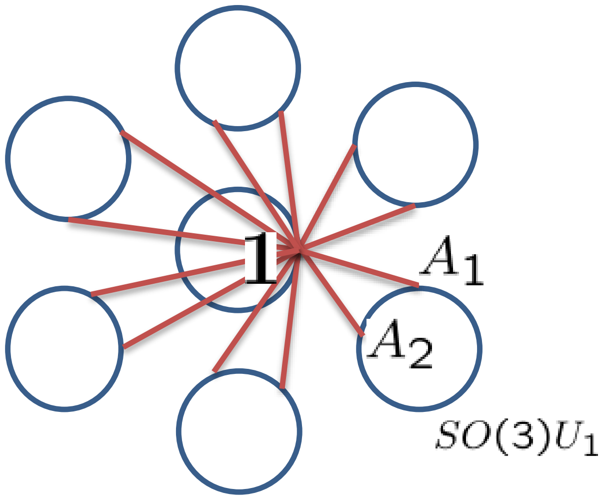
$Zn_{45}Au_{30}Cu_2$ ultra-low hysteresis alloy satisfying cofactor conditions Song, Chen, Dabade, Shield, James, 2013

'Moving mask' approximation analyzed by Della Porta (2018), who has also identified further conditions on the $\mathbf{U}_i$ allowing new microstructures, closely satisfied in this alloy.

$Ti_{76}Nb_{22}Al_2$ (T. Inamura)

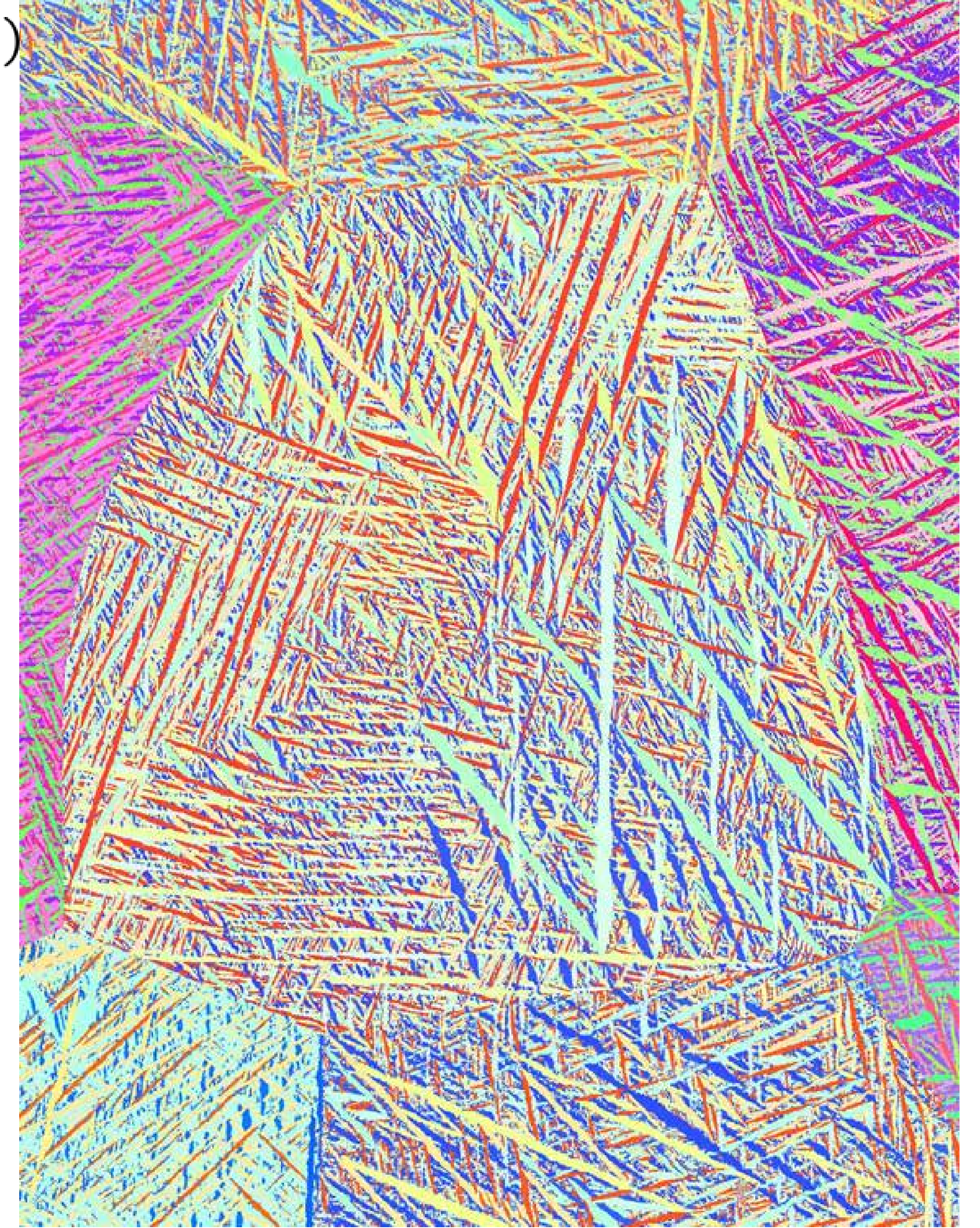
Cubic to orthorhombic

$\lambda_2 = 1$



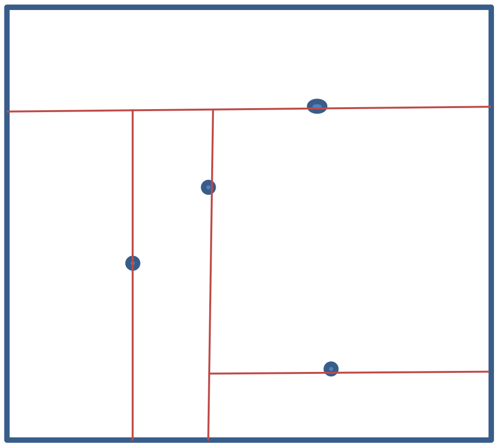
$$\mathrm{rank}\,(\mathbf{A_i} - \mathbf{1}) = 1,$$
$$i = 1, \ldots, 12$$

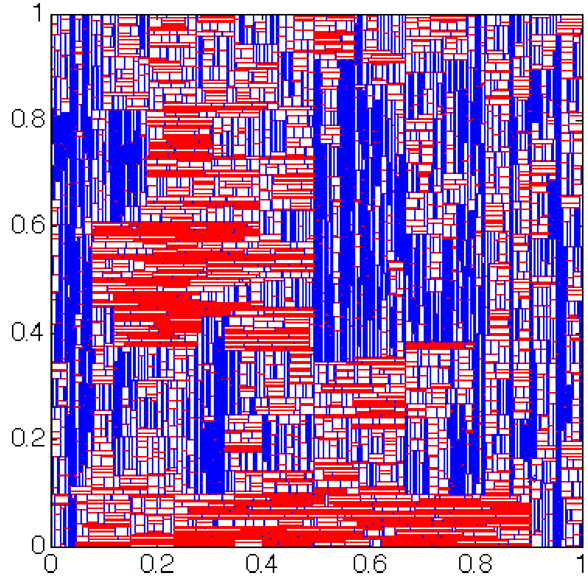
$$\mathrm{rank}\,(\mathbf{A_i} - \mathbf{A_j}) > 1,$$
$$i \neq j$$



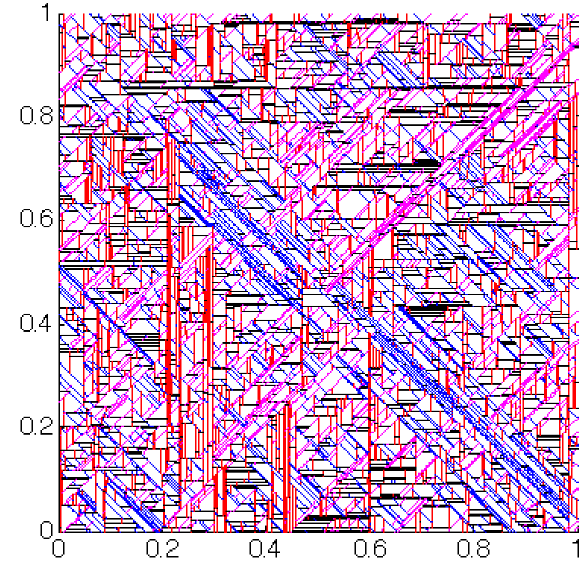
A probabilistic model for martensitic avalanches.

JB/P. Cesana/B. Hambly 2015





2 directions



4 directions

General branching random walk analysis (Cesana/Hambly) predicts approximate power laws for plate lengths, as observed for acoustic emissions.