Mallard's law

Let $\mathbf{U} = \mathbf{U}^T > 0$, $\mathbf{V} = \mathbf{V}^T > 0$ be such that

$$\mathbf{V} = (-\mathbf{1} + 2\mathbf{e} \otimes \mathbf{e})\mathbf{U}(-\mathbf{1} + 2\mathbf{e} \otimes \mathbf{e}), \qquad (\dagger)$$

where $|\mathbf{e}| = 1$. Then $SO(3)\mathbf{U}$ and $SO(3)\mathbf{V}$ are rank-one connected with rank-one connections given by

$$\mathbf{QV} = \mathbf{U} + \mathbf{a} \otimes \mathbf{n},$$

$$\mathbf{a} \otimes \mathbf{n} = \begin{cases} 2\left(\frac{\mathbf{U}^{-1}\mathbf{e}}{|\mathbf{U}^{-1}\mathbf{e}|^2} - \mathbf{Ue}\right) \otimes \mathbf{e} & \text{(Type I)}, \\ 2\mathbf{Ue} \otimes \left(\mathbf{e} - \frac{\mathbf{U}^2\mathbf{e}}{|\mathbf{Ue}|^2}\right) & \text{(Type II)}. \end{cases}$$

(In fact Chen et al (2013) show that if $\mathbf{V} = \mathbf{RUR}^T$ for some $\mathbf{R} \in SO(3)$ then $SO(3)\mathbf{U}$ and $SO(3)\mathbf{V}$ are rank-one connected iff $(\dagger)$ holds for some $\mathbf{e}$.)

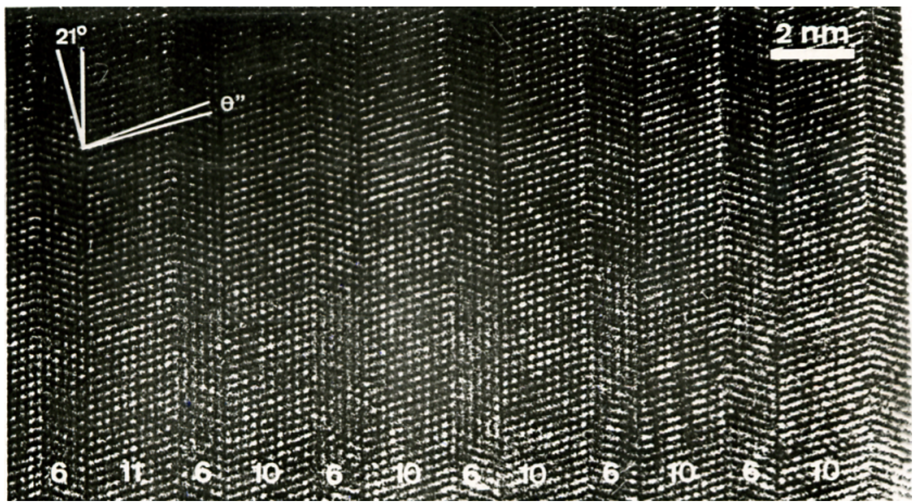
For example, for cubic-to-tetragonal we can take

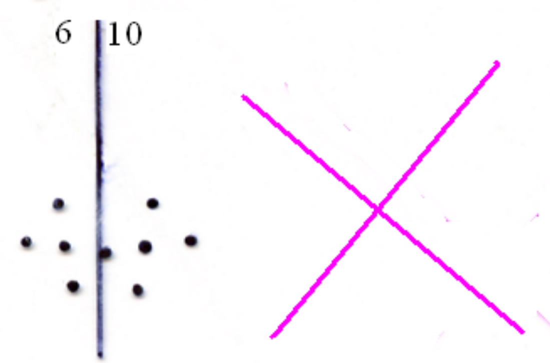
$$\mathbf{U}_1 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_1), \ \ \mathbf{U}_2 = \mathrm{diag}\,(\eta_1, \eta_2, \eta_1),$$

and then

$$\mathbf{U}_1^2 - \mathbf{U}_2^2 = \frac{1}{2}(\eta_2^2 - \eta_1^2)\Big((\mathbf{e}_2 - \mathbf{e}_1)\otimes(\mathbf{e}_2 + \mathbf{e}_1) + (\mathbf{e}_2 + \mathbf{e}_1)\otimes(\mathbf{e}_2 - \mathbf{e}_1)\Big),$$

so that twinning is on [110] planes.





Convexity conditions

Let $\psi : M^{3\times 3} \to \mathbb{R}$ be continuous. We say that

ψ is *rank-one convex* if $t \mapsto \psi(\mathbf{A} + t\mathbf{a} \otimes \mathbf{n})$ is convex for all $\mathbf{A} \in M^{3\times 3}$, and $\mathbf{a}, \mathbf{n} \in \mathbb{R}^3$,

Null Lagrangians

ψ is *polyconvex* if $\psi(\mathbf{A}) = g(\mathbf{A}, \text{cof}\,\mathbf{A}, \det \mathbf{A})$ for all $\mathbf{A} \in M^{3\times 3}$ for some convex g,

ψ is *quasiconvex* if

$$\int_\Omega \psi(D\mathbf{z}(\mathbf{x}))\,d\mathbf{x} \geq \int_\Omega \psi(\mathbf{A})\,d\mathbf{x}$$

whenever $\mathbf{z} \in \mathbf{A}\mathbf{x} + W_0^{1,\infty}(\Omega; \mathbb{R}^3)$.

definition independent of Ω

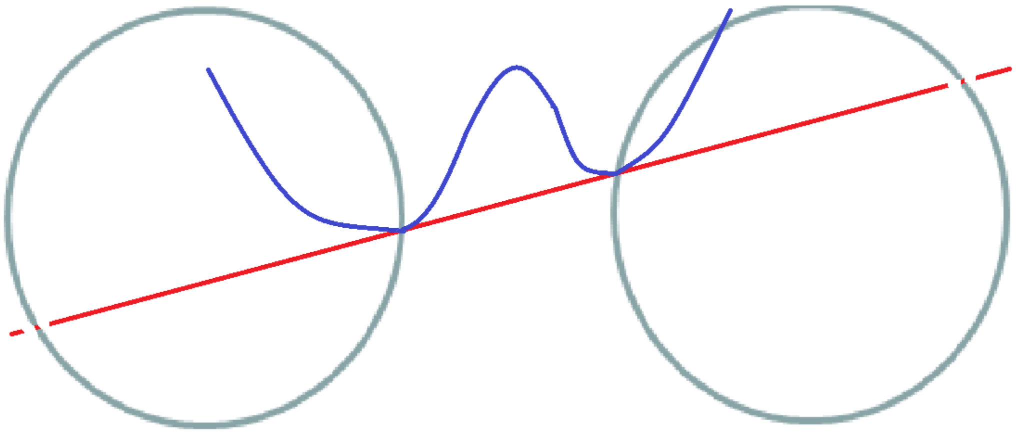
or $C_0^\infty(\Omega; \mathbb{R}^3)$

ψ polyconvex $\Rightarrow$ ψ quasiconvex $\Rightarrow$ ψ rank-one convex

$\not\Leftarrow$ Roughly N&S $\not\Leftarrow$

for existence

of minimizers

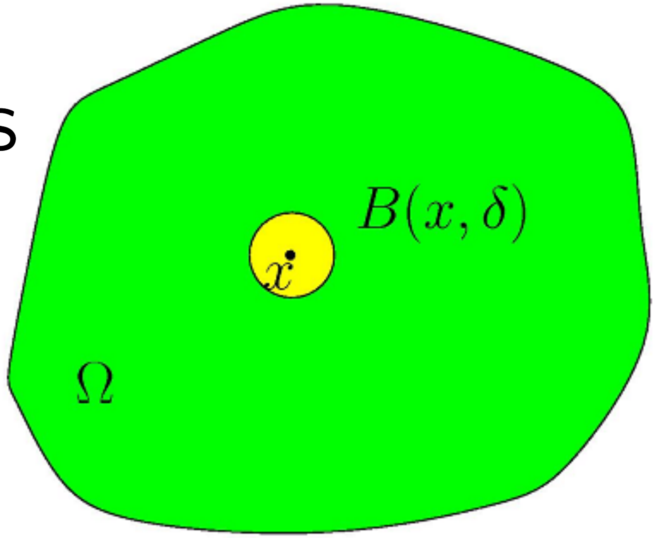


The free-energy function $\psi(\cdot, \theta)$ is not quasiconvex because the existence of rank-one connections between energy wells implies that $\psi(\cdot, \theta)$ is not rank-one convex.

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

Gradient Young measures

Given a sequence of gradients $D\mathbf{y}^{(j)}$, fix $j, \mathbf{x}, \delta$.



Let $E \subset M^{3\times 3}$.

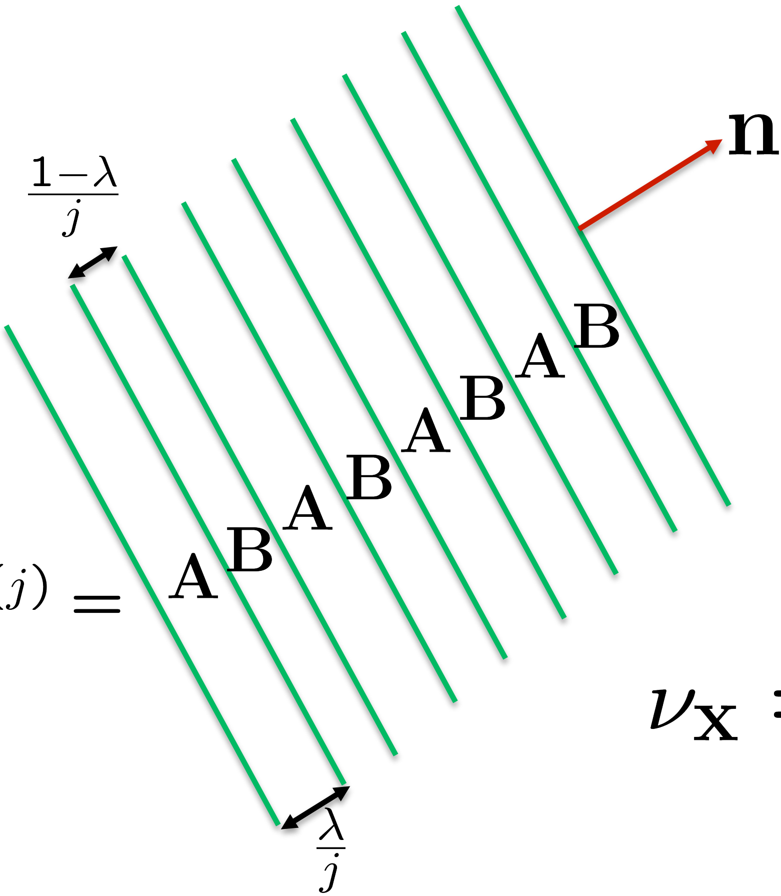
$$\nu_{\mathbf{x},j,\delta}(E) = \frac{\text{vol } \{\mathbf{z} \in B(\mathbf{x},\delta) : D\mathbf{y}^{(j)}(\mathbf{z}) \in E\}}{\text{vol } B(\mathbf{x},\delta)}$$

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

Gradient Young measure

Gradient Young measure of a simple laminate

$D\mathbf{y}^{(j)} =$



$$\mathbf{A} - \mathbf{B} = \mathbf{a} \otimes \mathbf{n}$$

$$0 < \lambda < 1$$

$$\nu_{\mathbf{x}} = \lambda \delta_{\mathbf{A}} + (1-\lambda)\delta_{\mathbf{B}}$$

$$D\mathbf{y}^{(j)} \rightharpoonup \lambda \mathbf{A} + (1-\lambda)\mathbf{B} = \bar{\nu}_{\mathbf{x}} = \int_{M^{3\times 3}} \mathbf{C}\, d\nu_x(\mathbf{C})$$

Theorem (Kinderlehrer/Pedregal)

A family of probability measures $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ *is the Young measure of a sequence of gradients* $D\mathbf{y}^{(j)}$ *bounded in* L^{∞} *if and only if*

(i) $\bar{\nu}_{\mathbf{x}}$ *is a gradient (*$D\mathbf{y}$*, the weak limit of* $D\mathbf{y}^{(j)}$*)*

(ii) $\langle \nu_{\mathbf{x}}, f\rangle := \int_{M^{3\times 3}} f(\mathbf{C})\, d\nu_{\mathbf{x}}(\mathbf{C}) \geq f(\bar{\nu}_{\mathbf{x}})$

for all quasiconvex f*.*

Convexifications with respect to a cone

Let G be a convex cone of continuous functions $f : M^{3\times 3} \to \mathbb{R}$. Examples are the cones of convex, poly-convex, quasiconvex and rank-one convex functions.

For a continuous $\psi : M^{3\times 3} \to \mathbb{R}$ define the $G-$convexification ψ^G of ψ by

$$\psi^G = \text{sup}\{f \in G : f \leq \psi\}.$$

Then $\psi^c \leq \psi^{pc} \leq \psi^{qc} \leq \psi^{rc}$.

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

Similarly, for $K \subset M^{3\times 3}$ compact define (Šverák)

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

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

Theorem (JB/Carstensen (to appear) following Krucik 2000)

$$K^G = \{\mathbf{A} \in M^{3\times 3} : \exists \mu \in \mathcal{P}(K) \text{ with } f(\mathbf{A}) \leq \langle \mu, f \rangle \; \forall f \in G\}$$

In particular

$$K^{qc} = \{\bar{\nu} : \nu \text{ homogeneous gradient YM}, \operatorname{supp} \nu \subset K\}.$$

$K(\theta)^{\text{qc}}$ is the set of macroscopic deformation gradients corresponding to zero-energy microstructures.

Phase nucleation

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 $\mathbf{U}_i(\theta)$ to be one, which in general is not the case (but see later).

So what does it do?