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Interfaces and hysteresis in solid phase transformations

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Notes at http://people.maths.ox.ac.uk/ball/teaching.shtml

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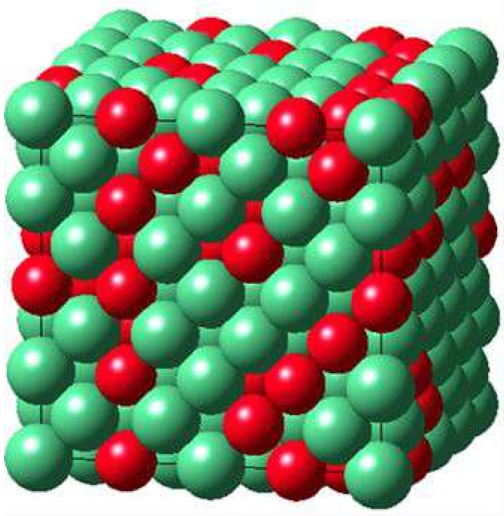
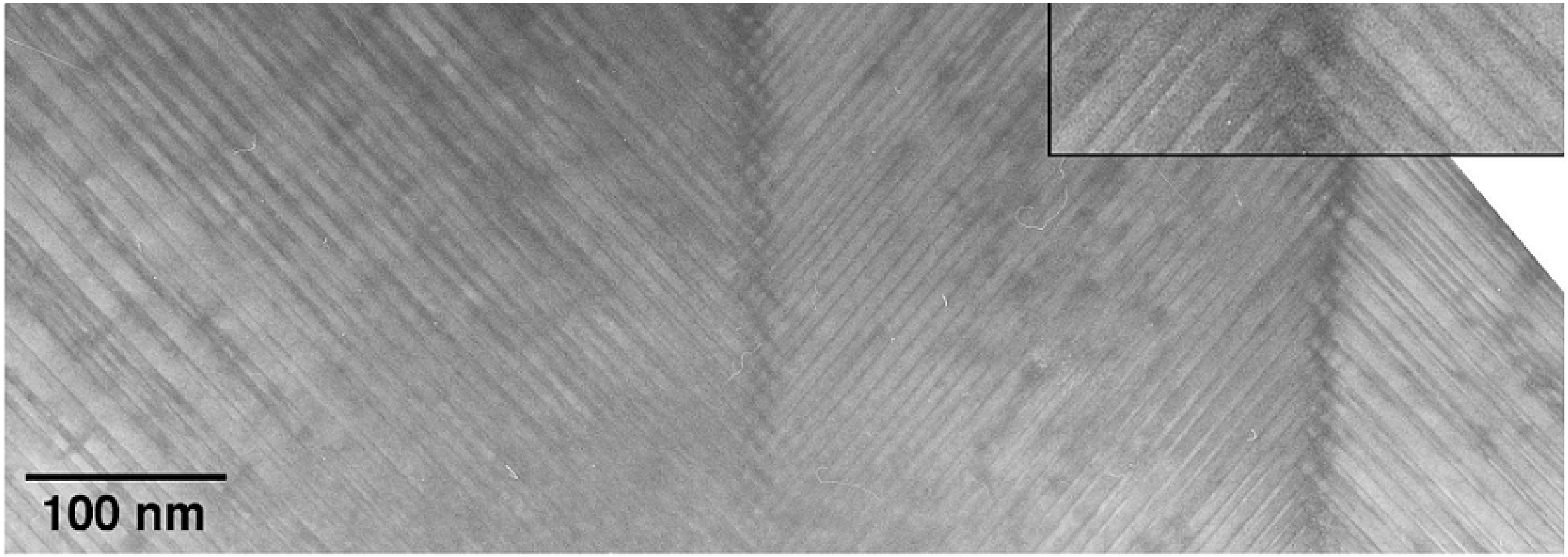
Metallic alloys comprise a mixture of different elements forming a crystal lattice.

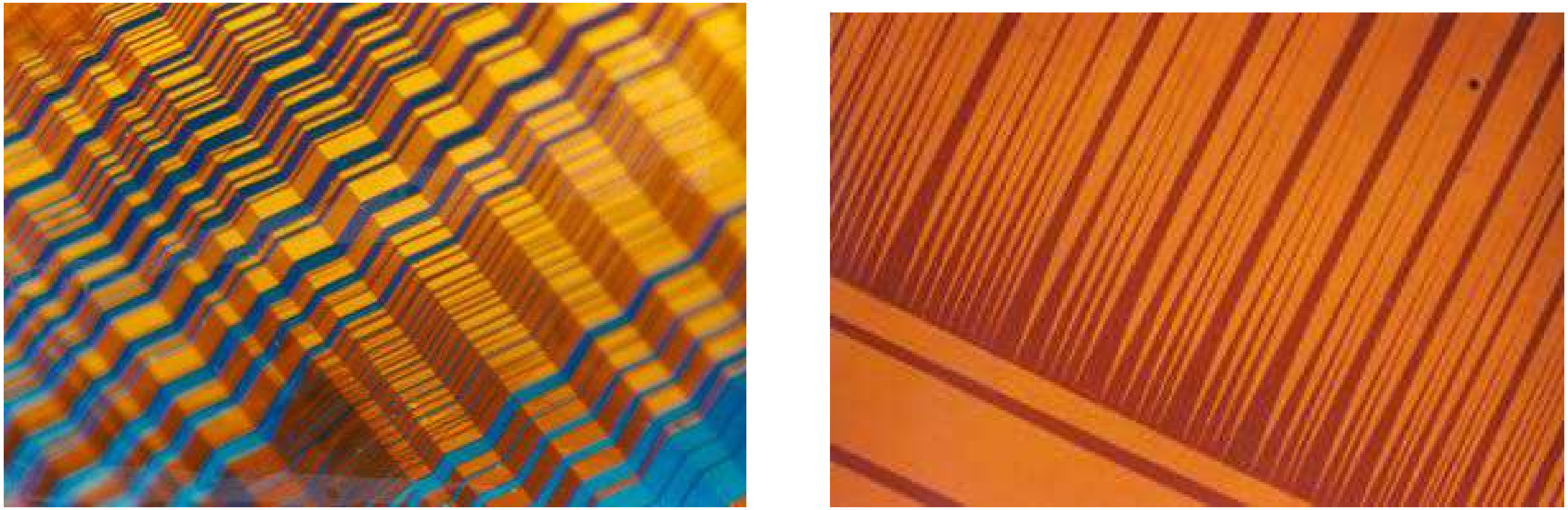


This course is about martensitic phase transformations. These are solid-solid phase transformations in which the underlying crystal lattice of an alloy changes shape as the temperature is reduced through a critical temperature.

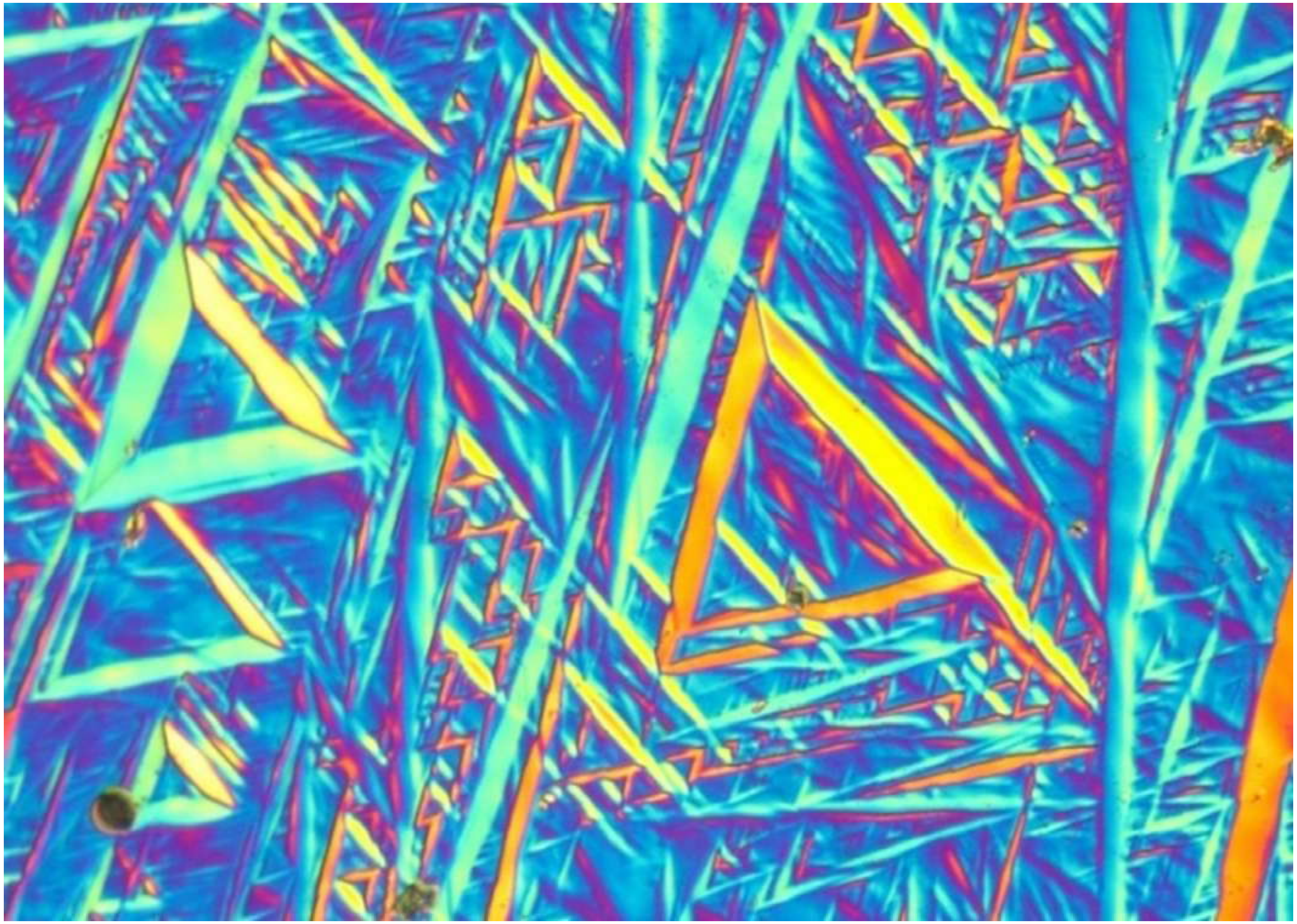
It turns out that there are different possible symmetry related variants of the low temperature phase, and the crystal has to deform in such a way that these different variants are geometrically compatible. This leads to remarkable patterns of microstructure that determine how the alloy behaves macroscopically.



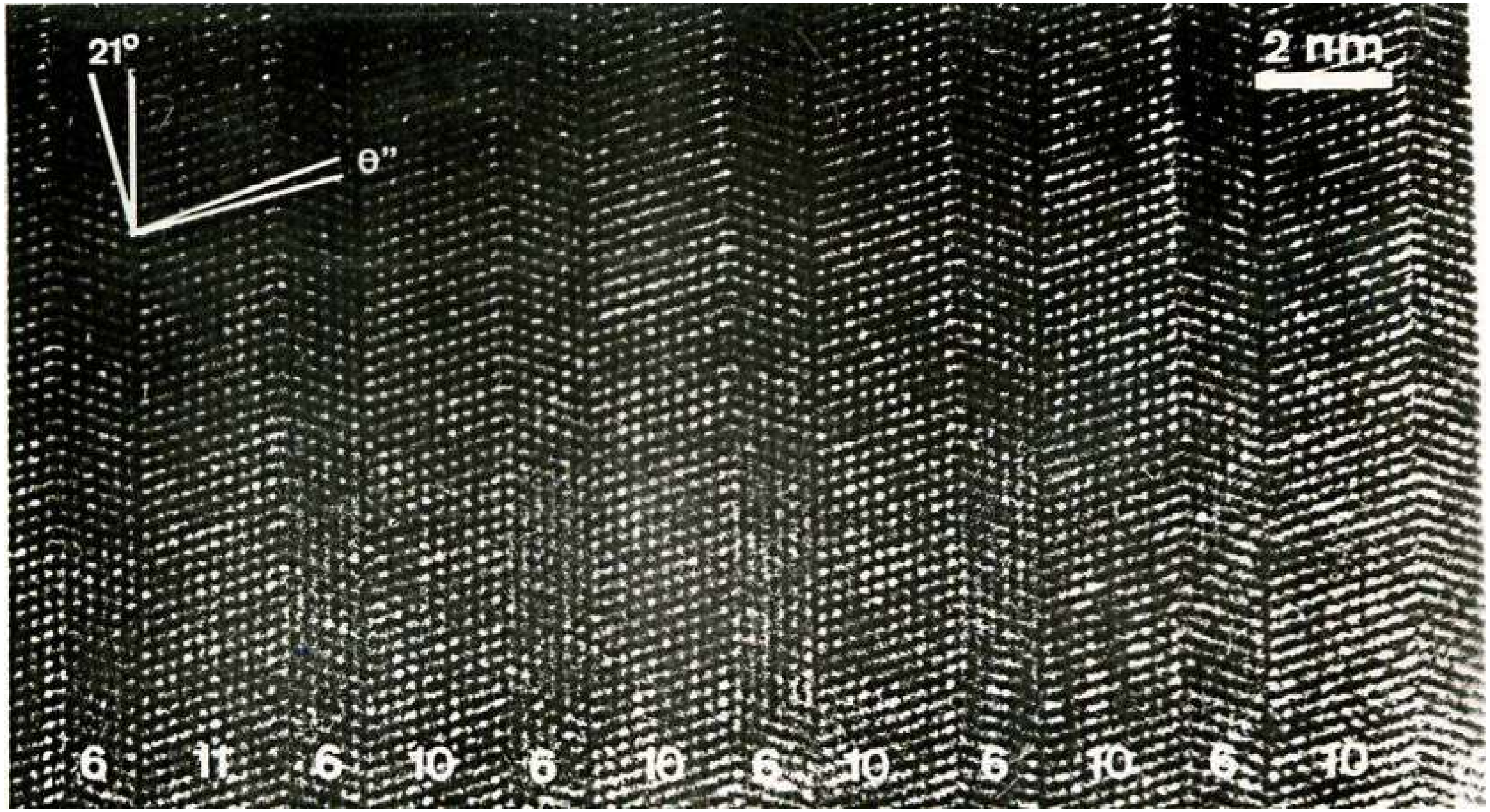
$Ni_{65}Al_{35}$ (Boullay/Schryvers)



CuAlNi (Chu/James)



β-titanium (T. Inamura, M. Ii, N. Kamioka, M. Tahara, H. Hosoda, S. Miyazaki)



NiMn (Baele, van Tendeloo, Amelinckx)

Questions

1. What exactly are we seeing in these micrographs?

2. What is a good mathematical model?

3. Can we predict the microstructure morphology?

4. Why is the microstructure so fine (i.e. the length-scale so small)?

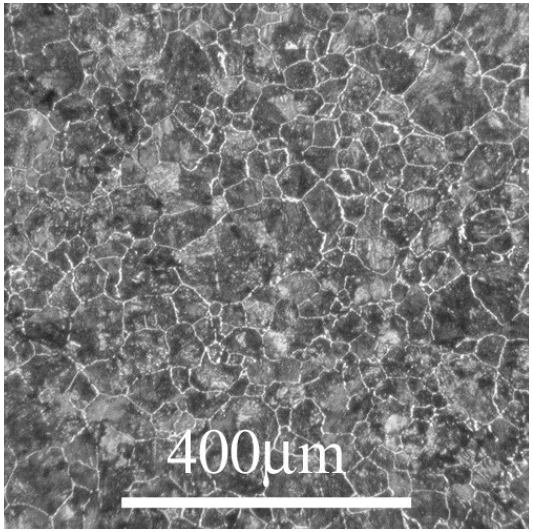
Topics

1. Nonlinear elastostatics.
2. Existence of minimizers and analysis tools.
3. Martensitic phase transformations.
4. Microstructure.
5. Austenite-martensite interfaces.
6. Complex microstructures. Nucleation of austenite.
7. Local minimizers with and without interfacial energy.

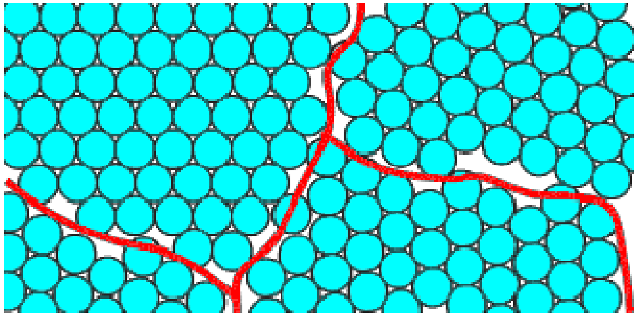
1. Nonlinear elastostatics

The central model of solid mechanics. Rubber, metals (and alloys), rock, wood, bone … can all be modelled as elastic materials, even though their chemical compositions are very different.

For example, metals and alloys are crystalline, with grains consisting of regular arrays of atoms.

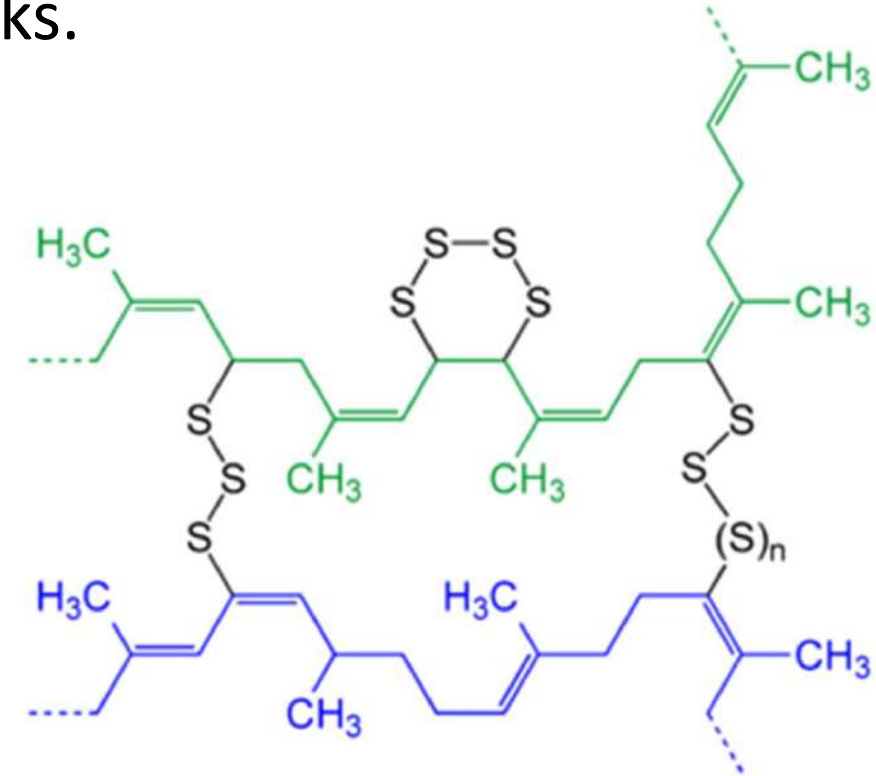


Iron carbon alloy, showing grain structure



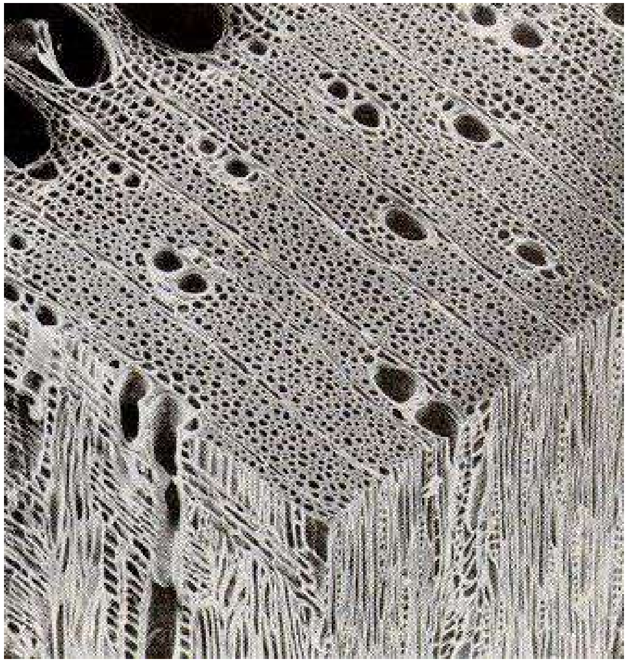
http://www.doitpoms.ac.uk

Polymers (such as rubber) consist of long chain molecules that are wriggling in thermal motion, often joined to each other by chemical bonds called crosslinks.



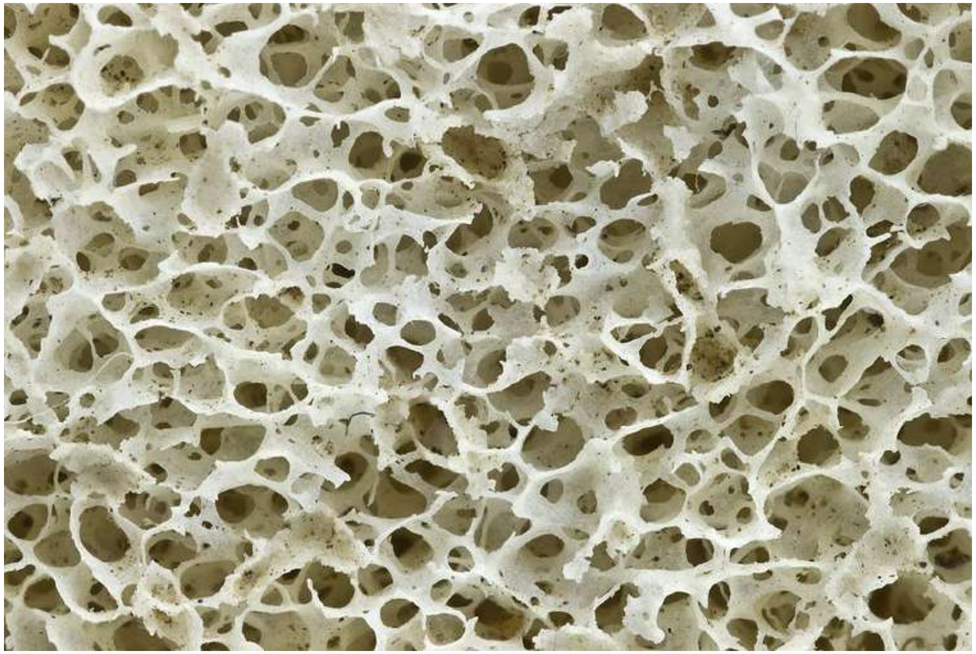
Schematic presentation of two strands (blue and green) of natural rubber after vulcanization with sulphur. (Wikipedia)

Wood and bone have a cellular structure.



White ash

http://classes.mst.edu/civeng120/lessons/wood/cell_structure/index.html



Human hip bone

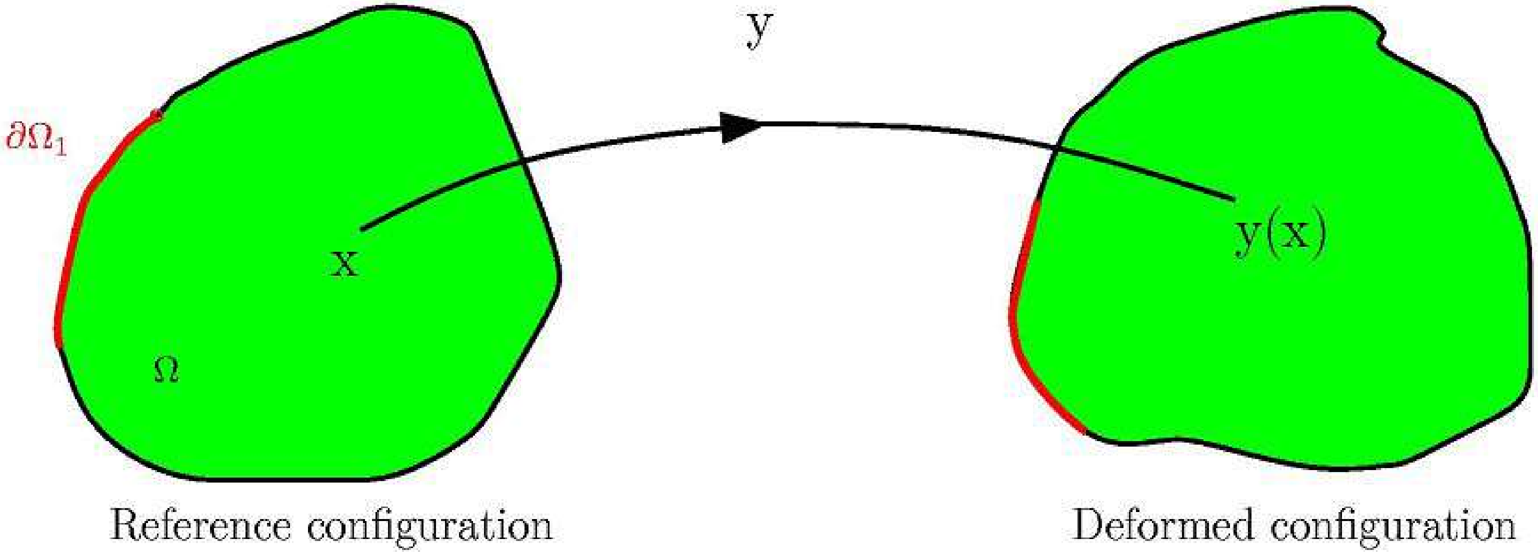
Patrick Siemer, San Francisco, USA

A brief history

1678 Hooke's Law
1705 Jacob Bernoulli
1742 Daniel Bernoulli
1744 L. Euler *elastica* (elastic rod)
1821 Navier, special case of linear elasticity via molecular model
(Dalton’s atomic theory was 1807)
1822 Cauchy, stress, *nonlinear* and linear elasticity

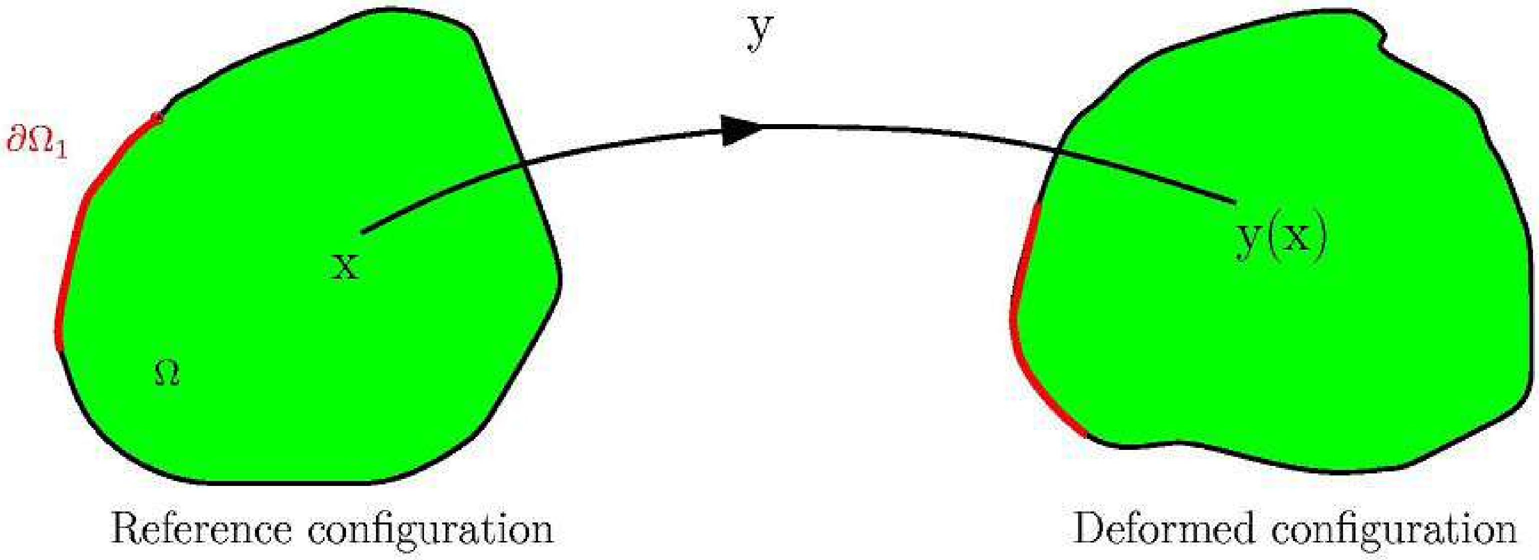
For a long time the nonlinear theory was ignored/forgotten.
1927 A.E.H. Love, Treatise on linear elasticity
1950's R. Rivlin, Exact solutions in *incompressible* nonlinear elasticity (rubber)
1960 - 80 Nonlinear theory clarified by J.L. Ericksen, C. Truesdell …
1980 - Mathematical developments, applications to materials, biology …

Description of deformation



$\Omega \subset \mathbb{R}^3$ bounded domain with closure $\bar{\Omega}$ and (Lipschitz) boundary $\partial\Omega$.

Label the material points of the body by the positions $x \in \Omega$ they occupy in the reference configuration.



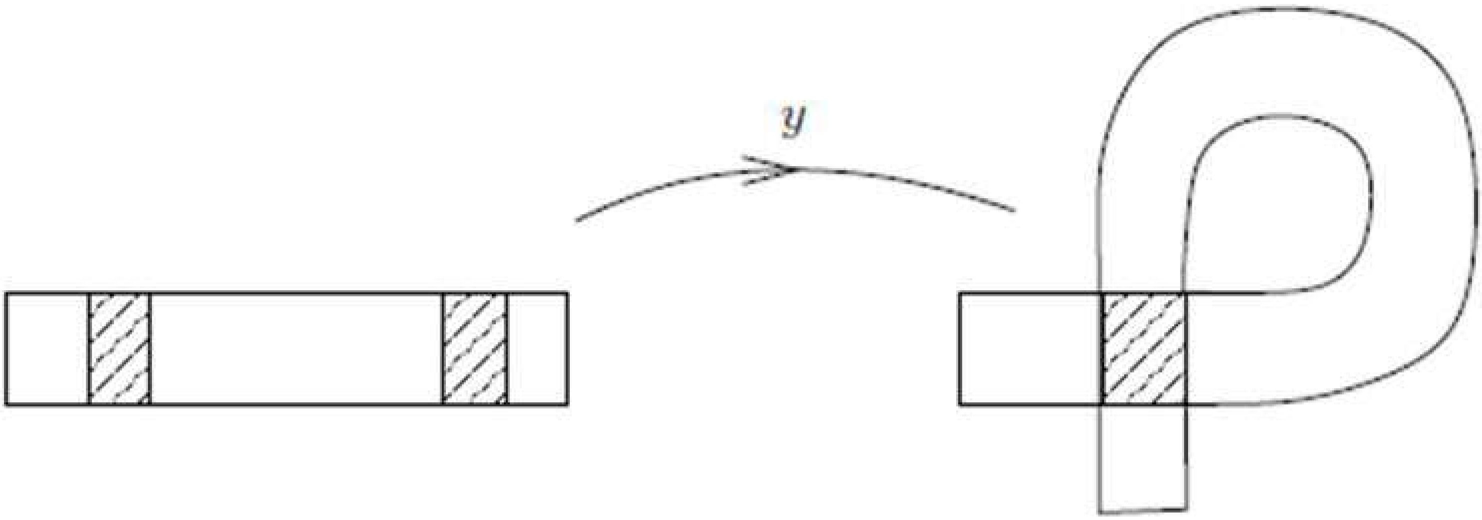
A typical deformation is described by a map $y : \bar{\Omega} \to \mathbb{R}^3$.

For the time being we suppose that y is smooth with deformation gradient

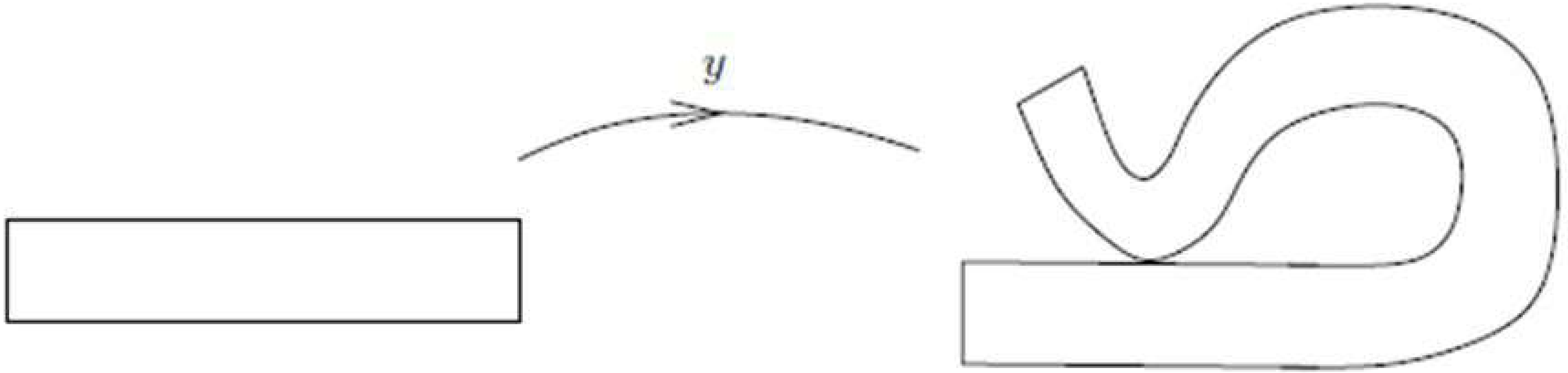
$$F = Dy(x),\ F_{i\alpha} = \frac{\partial y_i}{\partial x_\alpha}.$$

To avoid interpenetration of matter, $y : \Omega \to \mathbb{R}^3$ should be invertible.

Examples.



locally invertible but not globally invertible



invertible on Ω
not on $\overline{\Omega}$

How can we ensure invertibility?

For C^1 maps we can use:

Theorem. Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary $\partial\Omega$ (in particular Ω lies on one side of $\partial\Omega$ locally). Let $y \in C^1(\bar{\Omega}; \mathbb{R}^3)$ with

$$\det Dy(x) > 0 \text{ for all } x \in \bar{\Omega} \qquad (*)$$

and $y|_{\partial\Omega}$ one-to-one. Then y is invertible on $\bar{\Omega}$.

(The proof uses degree theory. See, for example, Meisters & Olech, Duke Math. J. 30 (1963) 63-80.)

When y is not smooth, or is not prescribed on the whole of $\partial\Omega$, things are more complicated. For the rest of this course we ignore issues of invertibility, but we will assume that $(*)$ holds in some sense.

Notation

$$\begin{aligned} M^{3\times 3} &= \{\text{real } 3\times 3 \text{ matrices}\} \\ M^{3\times 3}_{+} &= \{F \in M^{3\times 3} : \det F > 0\} \\ SO(3) &= \{R \in M^{3\times 3}_{+} : R^T R = 1\} \\ &= \{\text{rotations}\}. \end{aligned}$$

If $a \in \mathbb{R}^3$, $b \in \mathbb{R}^3$, the tensor product $a \otimes b$ is the matrix with the components

$$(a \otimes b)_{ij} = a_i b_j.$$

[Thus $(a \otimes b)c = (b \cdot c)a$ if $c \in \mathbb{R}^3$.]

Theorem (Square root theorem) Let C be a positive symmetric 3×3 matrix. Then there is a unique positive definite symmetric 3×3 matrix U such that $C = U^2$. If C has spectral decomposition $C = \sum_{i=1}^{3} \lambda_i \hat{e}_i \otimes \hat{e}_i$, then $U = \sum_{i=1}^{3} \lambda_i^{1/2} \hat{e}_i \otimes \hat{e}_i$. (We write $U = C^{\frac{1}{2}}$.)

Theorem (Polar decomposition)
Let $F \in M_+^{3\times 3}$. Then there exist positive definite symmetric U, V and $R \in SO(3)$ such that

$$F = RU = VR,$$

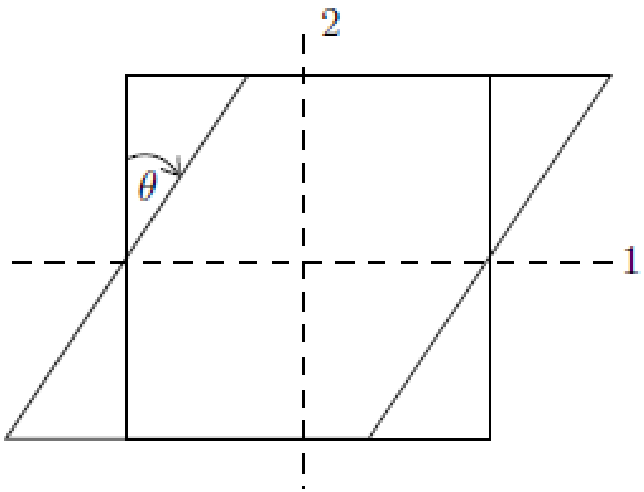
and $U = (F^T F)^{\frac{1}{2}}, V = (FF^T)^{\frac{1}{2}}$.
These representations are unique.

Because $V = RUR^T$ the strictly positive eigenvalues v_1, v_2, v_3 of U and V are the same. They are called the *singular values* of F, or the *principal stretches*.

Exercise: simple shear

$$y(x) = (x_1 + \gamma x_2, x_2, x_3).$$

$$\gamma = \tan\theta$$
$$\theta = \text{angle of shear}$$

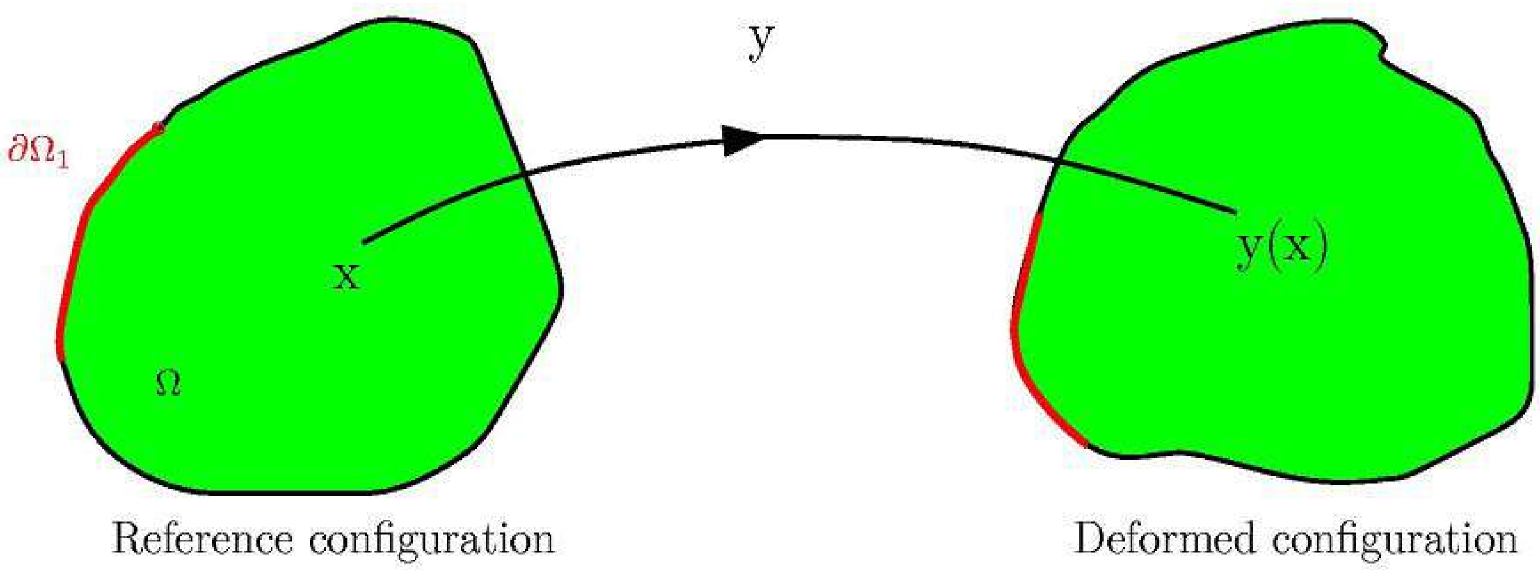


Show that

$$F = \begin{pmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\psi & \sin\psi & 0 \\ \sin\psi & \frac{1+\sin^2\psi}{\cos\psi} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$\tan\psi = \frac{\gamma}{2}$. As $\gamma \to 0+$ the eigenvectors of U and V tend to $\frac{1}{\sqrt{2}}(e_1 + e_2), \frac{1}{\sqrt{2}}(e_1 - e_2), e_3$.

Variational formulation of nonlinear elasticity



Find a deformation $y = y(x)$ minimizing the total free energy given by

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

subject to suitable boundary conditions, for example $y|_{\partial\Omega_1} = \bar{y}$, where $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$ is given.

Properties of the free-energy density ψ.

Assume

(H1) $\psi(\cdot) : M_{+}^{3\times 3} \to [0,\infty)$ is C^1.

(H2) $\psi(F) \to \infty$ as $\det F \to 0+$.

(H3) (Frame indifference) $\psi(QF) = \psi(F)$ for all $Q \in SO(3),\ F \in M_{+}^{3\times 3}$.

Hence $\psi(F) = \psi(RU) = \psi(U)$.

The *Piola-Kirchhoff stress tensor* is given by

$$T_R(Dy) = DW(Dy).$$

Material symmetry

Some materials have a mechanical response that depends on how they are oriented in the reference configuration. To make this precise we ask the question as to which initial linear deformations $H \in M_{+}^{3\times3}$ do not change ψ? That is, for which H do we have

$$\psi(F) = \psi(FH) \qquad \text{for all } F \in M_{+}^{3\times3}?$$

These H form a subgroup $\mathcal{S}$ of $M_{+}^{3\times3}$, the *symmetry group* of ψ. For example, if ψ has cubic symmetry we can take

$$\mathcal{S} = P^{24} = \{\text{rotations of a cube}\}.$$

Isotropic materials

These are materials for which all rotations are in the symmetry group, i.e. $SO(3) \subset \mathcal{S}$.

Theorem
ψ is isotropic iff $\psi(F) = \Phi(v_1, v_2, v_3)$ for some Φ that is symmetric with respect to permutations of v_1, v_2, v_3.

Examples of isotropic ψ are given by the Ogden models of rubber:

$$\begin{aligned}\Phi = \sum_{i=1}^{N} \alpha_i(v_1^{p_i} + v_2^{p_i} + v_3^{p_i} - 3) \\ + \sum_{i=1}^{M} \beta_i((v_2v_3)^{q_i} + (v_3v_1)^{q_i} + (v_1v_2)^{q_i} - 3) \\ + h(v_1v_2v_3)\end{aligned}$$

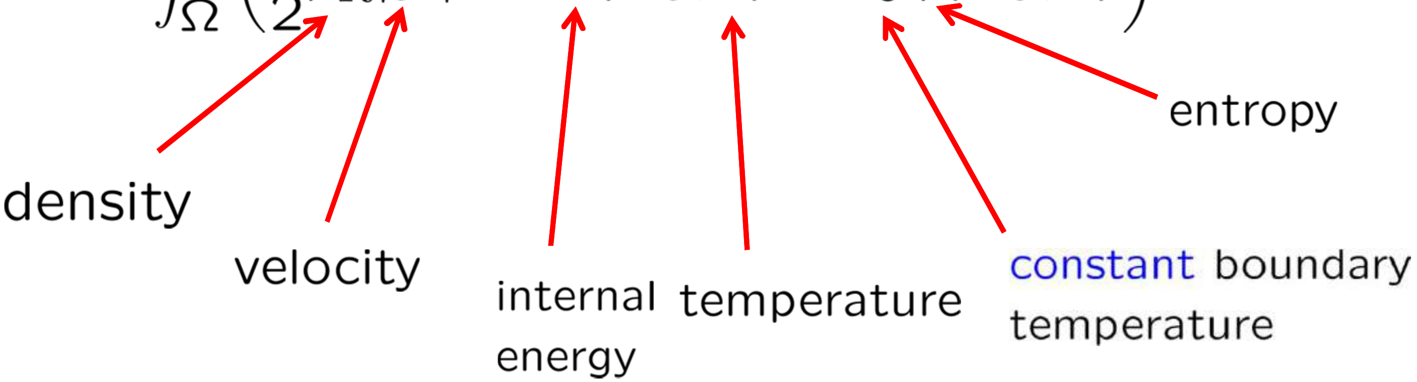
where $\alpha_i, \beta_i, p_i, q_i$ are constants and $h(\delta) \to \infty$ as $\delta \to 0+$.

Why do we minimize energy?

This is a deep question, the rough answer being the Second Law of Thermodynamics.

Under suitable mechanical and thermal boundary conditions the Second Law endows (Duhem, Ericksen) the equations of dynamic (thermo)elasticity with a Lyapunov function

$$\int_\Omega \left(\frac{1}{2}\rho_R|y_t|^2 + \epsilon(Dy,\theta) - \theta_0\eta(Dy,\theta)\right)\,dx$$



entropy

density

velocity

internal energy

temperature

constant boundary temperature

and we expect $y_t \to 0$, $\theta \to \theta_0$ as $t \to \infty$. Thus we expect the dynamics to generically give minimizing sequences for $\int_\Omega \psi(Dy(x))\,dx$, where $\psi(Dy) = \epsilon(Dy,\theta_0) - \theta_0\eta(Dy,\theta_0)$.

2. Existence of minimizers and analysis tools

L^p spaces

All mappings, sets assumed measurable, all integrals Lebesgue integrals.

Let $1 \le p \le \infty$.

$$L^p(\Omega) = \{u : \Omega \to \mathbb{R} : \|u\|_p < \infty\},$$

where

$$\|u\|_p = \begin{cases} \left(\int_\Omega |u(x)|^p \, dx\right)^{\frac{1}{p}} & \text{if } 1 \le p < \infty \\ \operatorname{ess\,sup}_{x \in \Omega} |u(x)| & \text{if } p = \infty \end{cases}$$

$$L^p(\Omega; \mathbb{R}^n) = \{u = (u_1, \ldots, u_n) : u_i \in L^p(\Omega)\}.$$

$$u^{(j)} \to u \text{ in } L^p \text{ if } \|u^{(j)} - u\|_p \to 0.$$

The Sobolev space $W^{1,p}$

$W^{1,p} = \{y : \Omega \to \mathbb{R}^3 : \|y\|_{1,p} < \infty\}$, where

$$\|y\|_{1,p} = \begin{cases} \left(\int_\Omega [|y(x)|^p + |Dy(x)|^p]\,dx\right)^{1/p} & \text{if } 1 \le p < \infty \\ \operatorname{ess\,sup}_{x\in\Omega}\,(|y(x)| + |Dy(x)|) & \text{if } p = \infty \end{cases}$$

i.e. $y \in L^p(\Omega; \mathbb{R}^3), Dy \in L^p(\Omega; M^{3\times 3})$.

Dy is interpreted in the weak (or distributional) sense, so that

$$\int_\Omega \frac{\partial y_i}{\partial x_\alpha}\,\varphi\,dx = -\int_\Omega y_i\,\frac{\partial \varphi}{\partial x_\alpha}\,dx$$

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

Weak convergence

$=$ convergence of averages

$u^{(j)}$ converges *weakly* to u (or weak* if $p = \infty$) in L^p, written $u^{(j)} \rightharpoonup u$ (or $u^{(j)} \overset{*}{\rightharpoonup} u$ if $p = \infty$) if

$$\int_\Omega u^{(j)} \varphi \, dx \to \int_\Omega u\varphi \, dx \text{ for all } \varphi \in L^{p'},$$

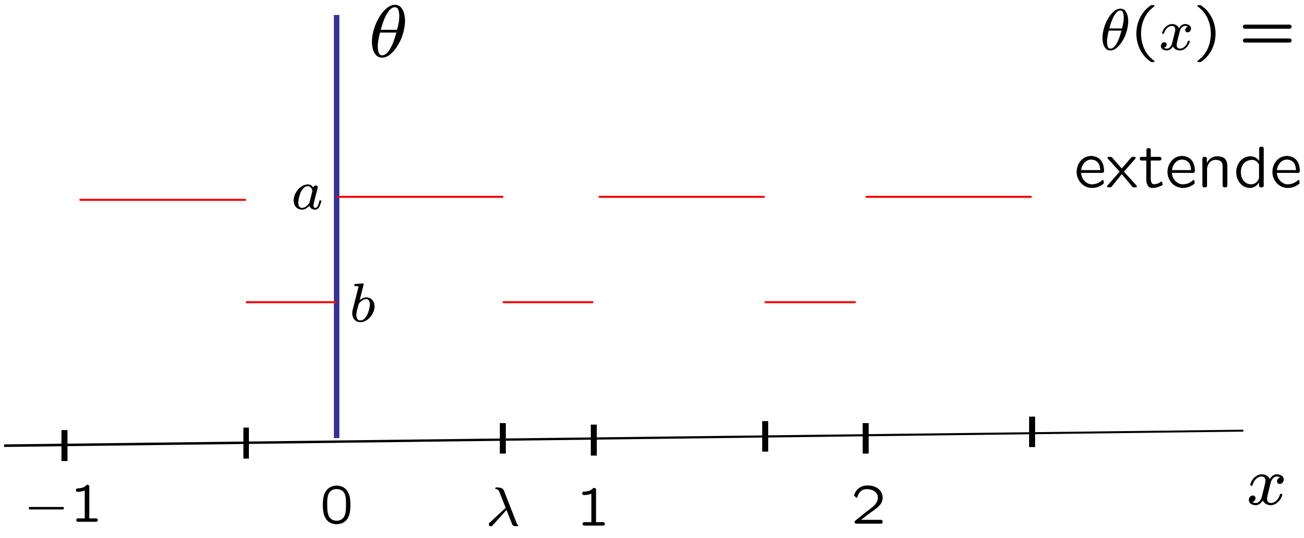
where $\frac{1}{p} + \frac{1}{p'} = 1$.

The importance of weak convergence for nonlinear PDE comes from the fact that if $1 < p \leq \infty$ then any bounded sequence in L^p has a weakly convergent subsequence (weak* if $p = \infty$).

If the bounded sequence is a sequence of approximating solutions to the PDE (e.g. coming from some numerical method, or a minimizing sequence for a variational problem), then the weak limit is a candidate solution.

But then we need somehow to pass to the limit in nonlinear terms using weak convergence.

Example: Rademacher functions.



$$\theta(x) = \begin{cases} a & \text{if } 0 < x \leq \lambda \\ b & \text{if } \lambda < x \leq 1 \end{cases}$$

extended periodically to $\mathbb{R}$.

Exercise. Define $\theta^{(j)}(x) = \theta(jx)$.

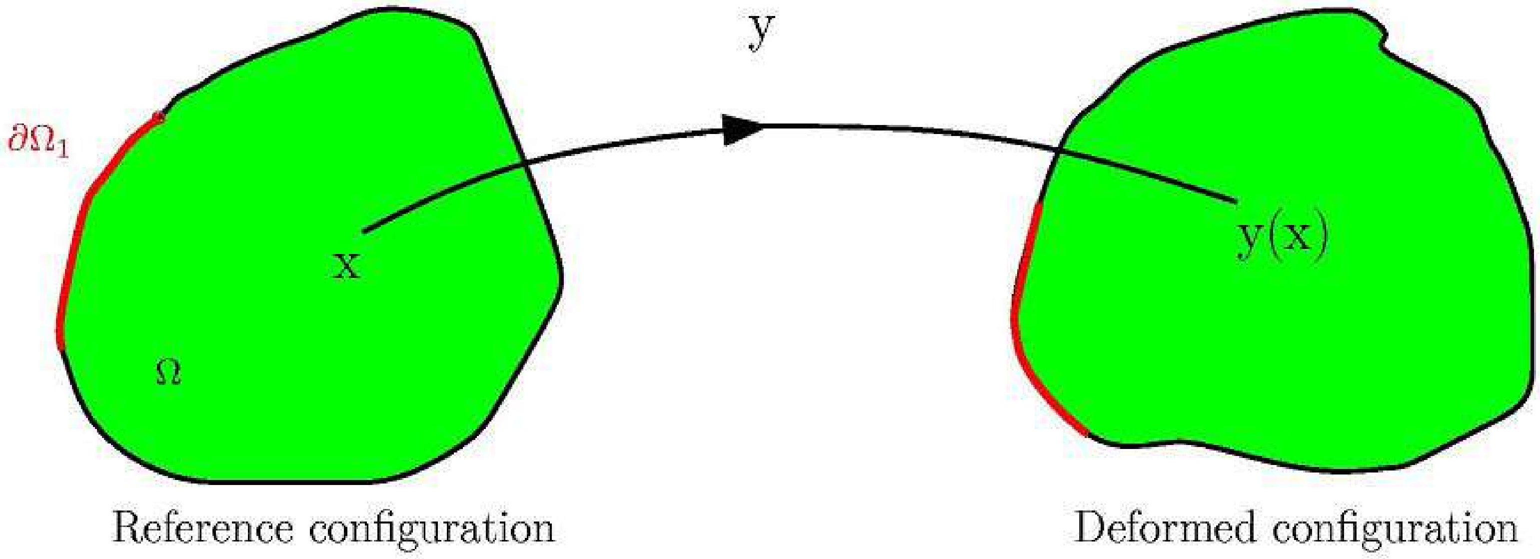
(i) Prove that $\theta^{(j)} \overset{*}{\rightharpoonup} \lambda a + (1-\lambda)b$ in $L^\infty(0,1)$

(ii) Deduce that if $f : \mathbb{R} \to \mathbb{R}$ is continuous and such that $u^{(j)} \overset{*}{\rightharpoonup} u$ in L^∞ implies $f(u^{(j)}) \overset{*}{\rightharpoonup} f(u)$ in L^∞ then f is *affine*, i.e. $f(v) = \alpha v + \beta$ for constants α, β.

We say that $y^{(j)} \rightharpoonup y$ in $W^{1,p}$ if $y^{(j)} \rightharpoonup y$ in L^p and $Dy^{(j)} \rightharpoonup Dy$ in L^p ($\rightharpoonup$ replaced by $\overset{*}{\rightharpoonup}$ if $p = \infty$).

Question: for what continuous $f : M^{3\times 3} \to \mathbb{R}$ does $y^{(j)} \overset{*}{\rightharpoonup} y$ in $W^{1,\infty}$ imply $f(Dy^{(j)}) \overset{*}{\rightharpoonup} f(Dy)$ in L^∞?

Answering this turns out to be a key to proving the existence of minimizers for a realistic class of materials.



$\Omega \subset \mathbb{R}^3$ bounded domain with Lipschitz boundary $\partial\Omega$, $\partial\Omega_1 \subset \partial\Omega$ relatively open, $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$.

We want to minimize

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

in the set of admissible mappings

$\mathcal{A} = \{y \in W^{1,1} : \det Dy(x) > 0 \text{ a.e., } y|_{\partial\Omega_1} = \bar{y}\}.$

(Note that we have replaced the invertibility condition by the local condition $\det Dy(x) > 0$ a.e., which is easier to handle.)

So far we have assumed that

(H1) $\psi : M^{3\times 3}_{+} \to [0, \infty)$ is C^1,

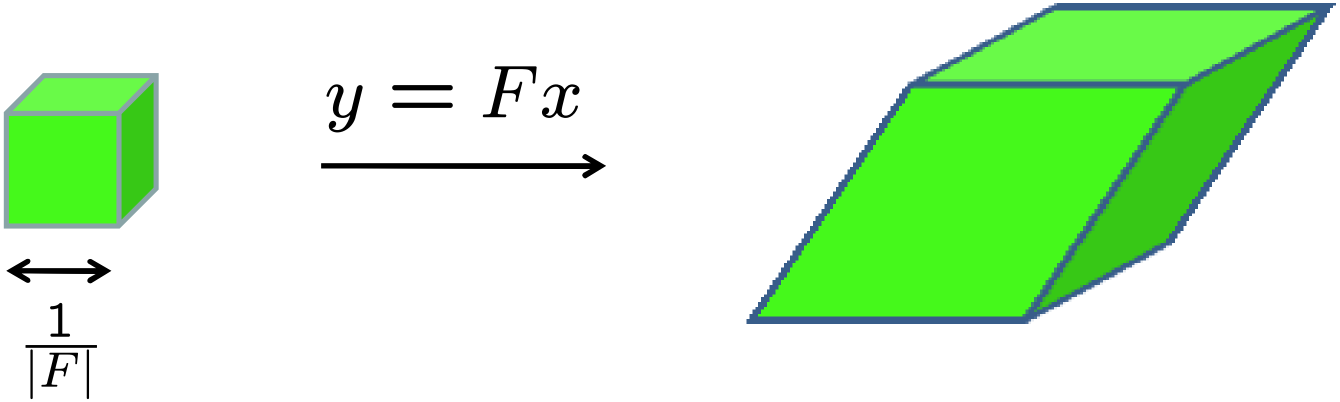
(H2) $\psi(F) \to \infty$ as $\det F \to 0+$,

so that setting $\psi(F) = \infty$ if $\det F \leq 0$, we have that $\psi : M^{3\times 3} \to [0, \infty]$ is continuous, and that ψ is *frame-indifferent*, i.e.

(H3) $\psi(RF) = \psi(F)$ for all $R \in \mathrm{SO}(3), F \in M^{3\times 3}$.

(In fact (H3) plays no direct role in the existence theory.)

Growth condition



$$\lim_{|F|\to\infty} \frac{\psi(F)}{|F|^3} = \infty$$

says that you can't get a finite line segment from an infinitesimal cube with finite energy.

We will use growth conditions a little weaker than this. Note that if

$$\psi(F) \geq C(1 + |F|^{3+\varepsilon})$$

for some $\varepsilon > 0$ then any deformation with finite elastic energy

$$\int_\Omega \psi(Dy(x))\, dx$$

and satisfying suitable boundary conditions is in $W^{1,3+\varepsilon}$ and so is continuous by the Sobolev embedding theorem.

Convexity conditions

The key difficulty is that ψ is never convex

(Recall that ψ is convex if

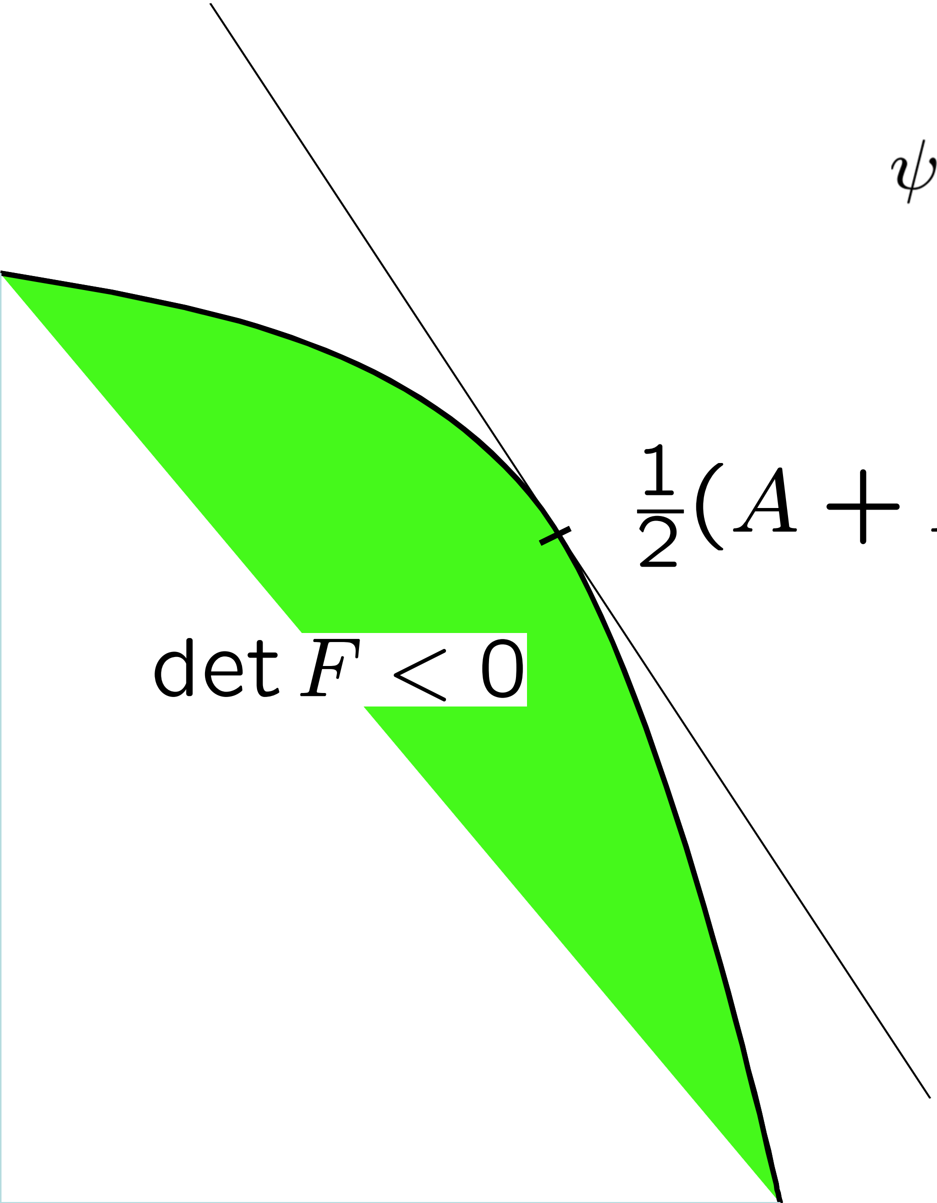
$$\psi(\lambda F + (1-\lambda)G) \leq \lambda\psi(F) + (1-\lambda)\psi(G)$$

for all F, G and $0 \leq \lambda \leq 1$.)

Reasons

1. Convexity of ψ is inconsistent with (H2) because $M_+^{3\times3}$ is not convex.

Remark: $M_{+}^{3\times 3}$ is not simply-connected.



$A = \mathrm{diag}\,(1,1,1)$

$$\psi(\tfrac{1}{2}(A+B)) = \infty$$
$$> \tfrac{1}{2}\psi(A) + \tfrac{1}{2}\psi(B)$$

$\frac{1}{2}(A+B) = \mathrm{diag}\,(0,0,1)$

$\det F < 0$

$\det F > 0$

$B = \mathrm{diag}\,(-1,-1,1)$

2. If ψ is convex, then any equilibrium solution (solution of the EL equations) is an absolute minimizer of the elastic energy

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

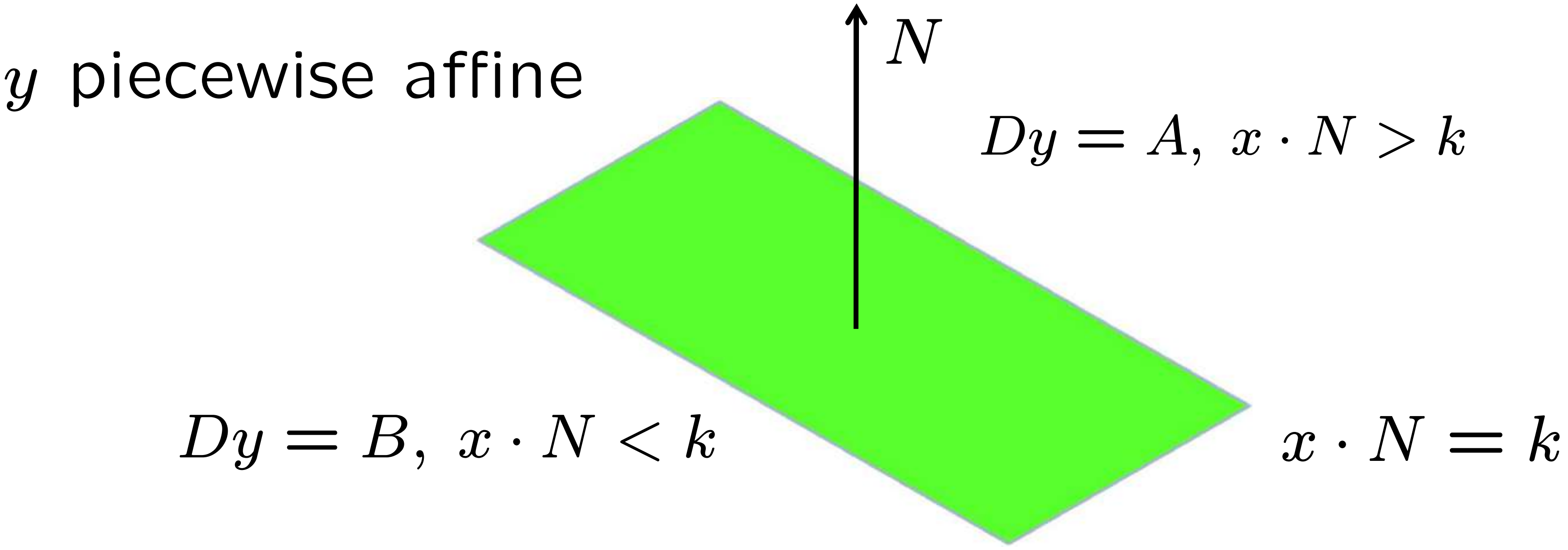
Proof.

$$I(z) = \int_\Omega \psi(Dz)\,dx \geq$$
$$\int_\Omega [\psi(Dy) + D\psi(Dy)\cdot(Dz - Dy)]\,dx = I(y).$$

This contradicts common experience of nonunique equilibria, e.g. buckling.

Rank-one matrices and the Hadamard jump condition

y piecewise affine

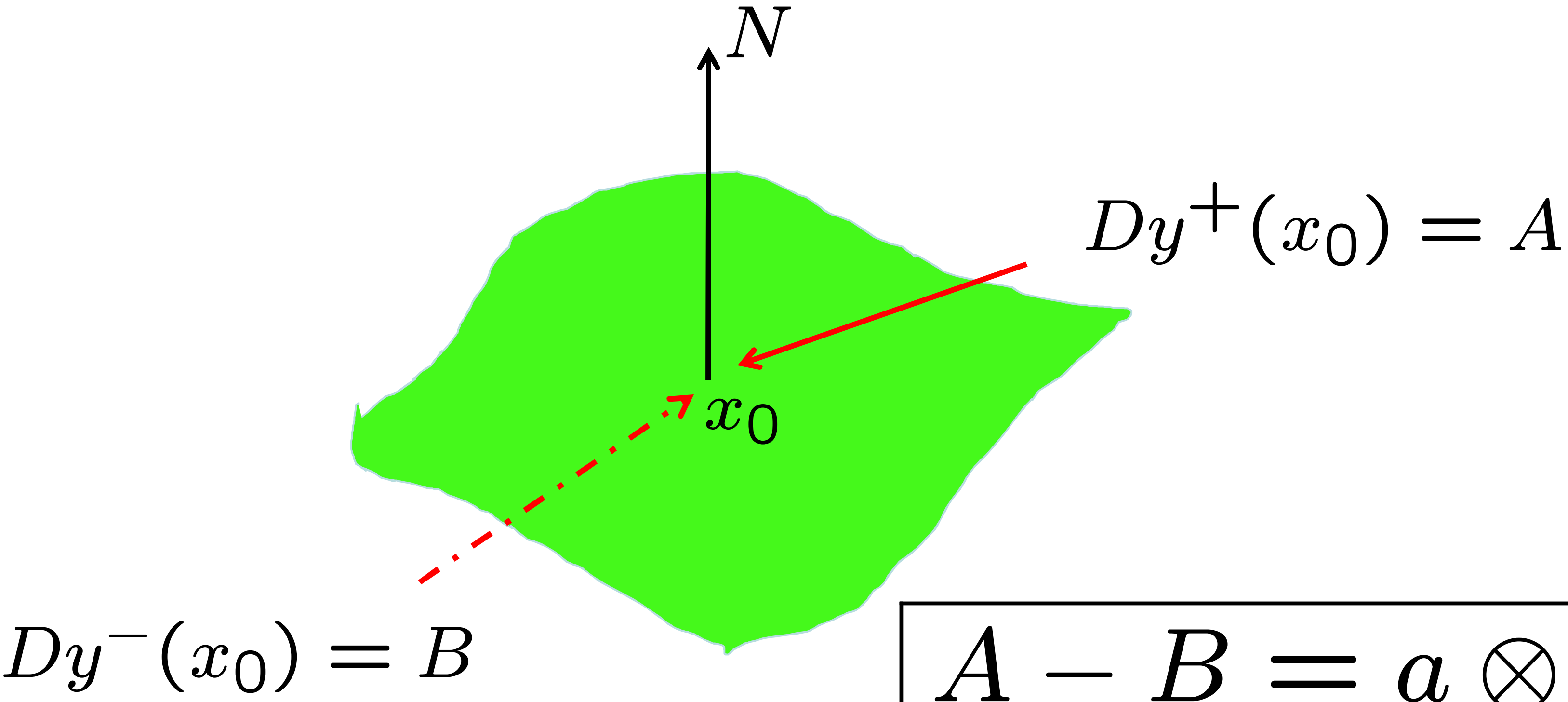


Let $C = A - B$. Then $Cx = 0$ if $x \cdot N = 0$. Thus $C(z - (z \cdot N)N) = 0$ for all z, and so $Cz = (CN \otimes N)z$. Hence

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

Hadamard jump condition

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



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

Exercise: prove this by blowing up around x using $y_\varepsilon(x) = \varepsilon y(\frac{x-x_0}{\varepsilon})$.

(See later for generalizations when y not piecewise C^1.)

Rank-one convexity

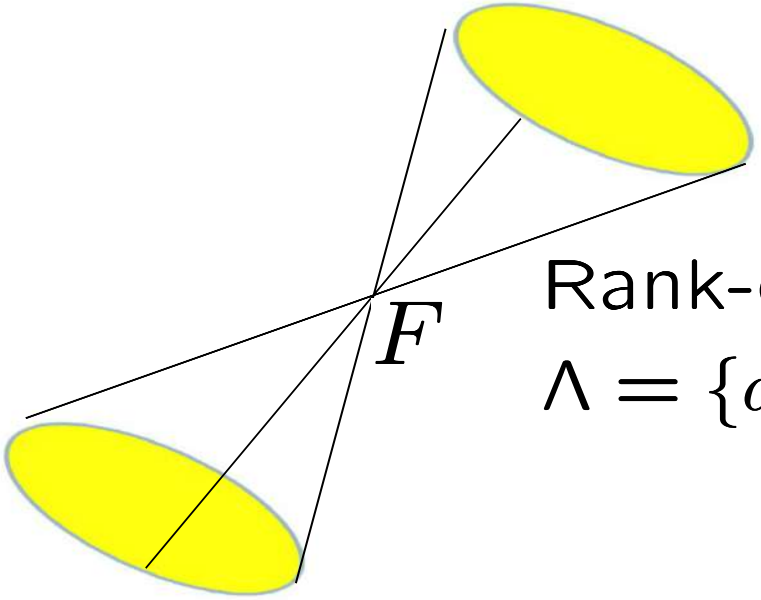
ψ is *rank-one convex* if the map $t \mapsto \psi(F + ta \otimes N)$ is convex for each $F \in M^{3\times 3}$ and $a \in \mathbb{R}^3, N \in \mathbb{R}^3$.

(Same definition for $M^{m\times n}$.)

Equivalently ψ is rank-one convex if

$$\psi(\lambda F + (1-\lambda)G) \leq \lambda\psi(F) + (1-\lambda)\psi(G)$$

if $F, G \in M^{3\times 3}$ with $F - G = a \otimes N$ and $\lambda \in (0, 1)$.



Rank-one cone

$\Lambda = \{a \otimes N : a, N \in \mathbb{R}^3\}$

Rank-one convexity is consistent with (H2) because $\det(F + ta \otimes N)$ is linear in t, so that $M_+^{3\times 3}$ is rank-one convex (i.e. if $F, G \in M_+^{3\times 3}$ with $F - G = a \otimes N$ then $\lambda F + (1-\lambda)G \in M_+^{3\times 3}$.)

If $\psi \in C^2(M_+^{3\times 3})$ then ψ is rank-one convex iff

$$\frac{d^2}{dt^2}\psi(F + ta \otimes N)|_{t=0} \geq 0,$$

for all $F \in M_+^{3\times 3}, a, N \in \mathbb{R}^3$, or equivalently

$$D^2\psi(F)(a \otimes N, a \otimes N) = \frac{\partial^2 \psi(F)}{\partial F_{i\alpha} \partial F_{j\beta}} a_i N_\alpha a_j N_\beta \geq 0,$$

(Legendre-Hadamard condition).

Quasiconvexity (C.B. Morrey,1952)

Let $\psi : M^{m\times n} \to [0,\infty]$ be continuous. ψ is said to be *quasiconvex at* $F \in M^{m\times n}$ if the inequality

$$\int_\Omega \psi(F + D\varphi(x))\,dx \geq \int_\Omega \psi(F)\,dx$$

definition independent of Ω

holds for any $\varphi \in W_0^{1,\infty}(\Omega;\mathbb{R}^m)$, and is *quasiconvex* if it is quasiconvex at every $F \in M^{m\times n}$.

Could replace by $C_0^\infty(\Omega;\mathbb{R}^m)$

Here $\Omega \subset \mathbb{R}^n$ is any bounded open set with Lipschitz boundary, and $W_0^{1,\infty}(\Omega;\mathbb{R}^m)$ is the set of those $y \in W^{1,\infty}(\Omega;\mathbb{R}^m)$ which are zero on $\partial\Omega$ (in the sense of trace).

Setting $m = n = 3$ we see that ψ is quasiconvex if for any $F \in M^{3\times 3}$ the pure displacement problem to minimize

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

subject to the linear boundary condition

$$y(x) = Fx,\ x \in \partial\Omega,$$

has $y(x) = Fx$ as a minimizer.

Theorem

If ψ is continuous and quasiconvex then ψ is rank-one convex.

Corollary If $m = 1$ or $n = 1$ then a continuous $\psi : M^{m\times n} \to [0, \infty]$ is quasiconvex iff it is convex.

Proof.

If $m = 1$ or $n = 1$ then rank-one convexity is the same as convexity. If ψ is convex then by Jensen's inequality:

$$\frac{1}{\operatorname{meas}\Omega}\int_\Omega \psi(F + D\varphi)\,dx$$
$$\geq \psi\left(\frac{1}{\operatorname{meas}\Omega}\int_\Omega (F + D\varphi)\,dx\right) = \psi(F).$$

Theorem (van Hove)
Let $\psi(F) = c_{ijkl}F_{ij}F_{kl}$ be quadratic. Then ψ is rank-one convex $\Leftrightarrow$ ψ is quasiconvex.

Proof.

Let ψ be rank-one convex. Since for any $\varphi \in W_0^{1,\infty}$

$$\int_\Omega [\psi(F + D\varphi) - \psi(F)]\, dx = \int_\Omega c_{ijkl}\varphi_{i,j}\varphi_{k,l}\, dx$$

we just need to show that the RHS is ≥ 0.

Extend φ by zero to the whole of $\mathbb{R}^n$ and take Fourier transforms.

By the Plancherel formula

$$\begin{aligned}\int_{\Omega} c_{ijkl}\varphi_{i,j}\varphi_{k,l}\,dx &= \int_{\mathbb{R}^n} c_{ijkl}\varphi_{i,j}\varphi_{k,l}\,dx \\ &= 4\pi^2\int_{\mathbb{R}^n}\mathrm{Re}\,[c_{ijkl}\widehat{\varphi}_i\xi_j\bar{\widehat{\varphi}}_k\xi_l]\,d\xi \\ &\geq 0\end{aligned}$$

as required.

Null Lagrangians

When does equality hold in the quasiconvexity condition? That is, for what L is

$$\int_\Omega L(F + D\varphi(x))\,dx = \int_\Omega L(F)\,dx$$

for all $\varphi \in W_0^{1,\infty}(\Omega;\mathbb{R}^m)$? We call such L *quasiaffine*.

Theorem (Landers, Morrey, Reshetnyak ...)
If $L : M^{3\times 3} \to \mathbb{R}$ is continuous then the following are equivalent:

(i) L is quasiaffine.

(ii) L is a (smooth) *null Lagrangian*, i.e. the Euler-Lagrange equations $\operatorname{Div} D_F L(Du) = 0$ hold for *all* smooth u.

(iii) $L(F) = \text{const.} + C \cdot F + D \cdot \operatorname{cof} F + e \det F$.

(iv) $u \mapsto L(Du)$ is sequentially weakly continuous from $W^{1,p} \to L^1$ for sufficiently large p ($p > 3$ will do).

Proof that $u \mapsto \text{cof}\, Du$ is sequentially weakly continuous.

Consider, for example, $J(Du) = u_{1,1}u_{2,2} - u_{1,2}u_{2,1}$.

Let $u^{(j)} \rightharpoonup u$ in $W^{1,p}$, $p > 2$. Then $J(Du^{(j)})$ is bounded in $L^{p/2}$ and so we can suppose that $J(Du^{(j)}) \rightharpoonup \chi$ in L^1.

Let $\varphi \in C_0^\infty(\Omega)$. For smooth v we have the identity

$$J(Dv) = (v_1 v_{2,2})_{,1} - (v_1 v_{2,1})_{,2}.$$

Thus, approximating $v \in W^{1,2}$ by smooth mappings we find that

$$\int_\Omega J(Dv)\varphi\, dx = \int_\Omega [v_1 v_{2,1}\varphi_{,2} - v_1 v_{2,2}\varphi_{,1}]\, dx.$$

Setting $v = u^{(j)}$ we get

$$\int_\Omega J(Du^{(j)})\varphi\,dx = \int_\Omega [u_1^{(j)} u_{2,1}^{(j)} \varphi_{,2} - u_1^{(j)} u_{2,2}^{(j)} \varphi_{,1}]\,dx.$$

$$\begin{array}{ccccc} \Big\downarrow {\scriptstyle L^1} & \Big\downarrow {\scriptstyle L^{p'}} & \Big\downarrow {\scriptstyle L^p} & \Big\downarrow {\scriptstyle L^{p'}} & \Big\downarrow {\scriptstyle L^p} \\ \chi & u_1 & u_{2,1} & u_1 & u_{2,2} \end{array}$$

So

$$\begin{aligned} \int_\Omega \chi\varphi\,dx &= \int_\Omega [u_1 u_{2,1}\varphi_{,2} - u_1 u_{2,2}\varphi_{,1}]\,dx \\ &= \int_\Omega J(Du)\varphi\,dx. \end{aligned}$$

Hence $\chi = J(Du)$ as required.

Polyconvexity

Definition

ψ is *polyconvex* if there exists a convex function $g : M^{3\times 3} \times M^{3\times 3} \times \mathbb{R} \to (-\infty, \infty]$ such that

$$\psi(F) = g(F, \mathrm{cof}\, F, \det F) \text{ for all } F \in M^{3\times 3}.$$

Theorem

Let ψ be polyconvex, with g lower semicontinuous. Then ψ is quasiconvex.

Proof. Writing $\mathbf{J}(F) = (F, \mathrm{cof}\, F, \det F)$ and

$$⨍_\Omega f\, dx = \frac{1}{\mathrm{meas}\,\Omega} \int_\Omega f\, dx,$$

$$\begin{aligned} ⨍_\Omega \psi(F + D\varphi(x))\, dx &= ⨍_\Omega g(\mathbf{J}(F + D\varphi(x)))\, dx \\ &\overset{\text{Jensen}}{\geq} g\left(⨍_\Omega \mathbf{J}(F + D\varphi)\, dx\right) \\ &= g(\mathbf{J}(F)) \\ &= \psi(F). \end{aligned}$$

Remark

There are quadratic rank-one convex ψ that are not polyconvex. Such ψ cannot be written in the form

$$\psi(F) = Q(F) + \sum_{l=1}^{N} \alpha_l J_2^{(l)}(F),$$

where $Q \geq 0$ is quadratic and the $J_2^{(l)}$ are 2×2 minors (Terpstra, D. Serre).

Examples and counterexamples

We have shown that

$$\psi\ \text{convex} \overset{\not\Leftarrow \quad \psi=\det}{\Rightarrow} \psi\ \text{polyconvex} \overset{\not\Leftarrow\ \text{Zhang}}{\Rightarrow} \psi\ \text{quasiconvex}$$

$$\underset{\not\Leftarrow\ \text{Šverák}}{\Rightarrow} \psi\ \text{rank-one convex.}$$

The reverse implications are all false.

So is there a tractable characterization of quasiconvexity? This is the main road-block of the subject.

Theorem (Kristensen 1999)
There is no local condition equivalent to quasiconvexity (for example, no condition involving ψ and any number of its derivatives at an arbitrary matrix F).

This might lead one to think that it is not possible to characterize quasiconvexity. On the other hand Kristensen also proved

Theorem (Kristensen)
Polyconvexity is not a local condition.

For example, one might contemplate a characterization of the type

ψ quasiconvex $\Leftrightarrow$ ψ is the supremum of a family of special quasiconvex functions (including null Lagrangians).

Quasiconvexity is essentially both necessary and sufficient for the existence of minimizers (for the sufficiency under suitable growth conditions on ψ).

However, as well as being a practically unverifiable condition, the existence theorems based on quasiconvexity (still) do not really apply to elasticity because they assume that ψ is everywhere finite, whereas this is contradicted by (H2).

However we will show that it is possible to prove the existence of minimizers for mixed boundary value problems if we assume ψ is polyconvex and satisfies (H2) and appropriate growth conditions. Furthermore the hypotheses are satisfied by various commonly used models of natural rubber and other materials (but not, as we see later, for materials undergoing martensitic phase transformations).

Theorem (Müller, Qi &Yan 1994, following JB 1977)
Suppose that ψ satisfies (H1), (H2) and
(H4) $\psi(F) \geq c_0(|F|^2+|\mathrm{cof}\, F|^{3/2})-c_1$ for all $F \in M^{3\times 3}$, where $c_0 > 0$,
(H5) ψ is *polyconvex*, i.e. $\psi(F) = g(F, \mathrm{cof}\, F, \det F)$ for all $F \in M^{3\times 3}$ for g continuous and convex.
Let

$$I(y) = \int_\Omega \psi(Dy(x))\, dx.$$

Assume that there exists some y in

$$\mathcal{A} = \{y \in W^{1,1}(\Omega; \mathbb{R}^3) : y|_{\partial\Omega_1} = \bar{y}\}$$

with $I(y) < \infty$, where $\mathcal{H}^2(\partial\Omega_1) > 0$ and $\bar{y} : \partial\Omega_1 \to \mathbb{R}^3$.
Then there exists a global minimizer y^* of I in $\mathcal{A}$.

The theorem applies to the Ogden materials:

$$\Phi = \sum_{i=1}^{N} \alpha_i(v_1^{p_i} + v_2^{p_i} + v_3^{p_i} - 3) + \sum_{i=1}^{M} \beta_i((v_2v_3)^{q_i} + (v_3v_1)^{q_i} + (v_1v_2)^{q_i} - 3) + h(v_1v_2v_3)$$

where $\alpha_i, \beta_i, p_i, q_i$ are constants and h is convex, $h(\delta) \to \infty$ as $\delta \to 0+$, $\frac{h(\delta)}{\delta} \to \infty$ as $\delta \to \infty$, under appropriate conditions on the constants.

Sketch of proof

Let's make the slightly stronger hypothesis that

$$g(F,H,\delta) \geq c_0(|F|^p + |H|^{p'} + |\delta|^q) - c_1,$$

for all $F \in M^{3\times 3}$, where $p \geq 2$, $\frac{1}{p} + \frac{1}{p'} = 1$, $c_0 > 0$ and $q > 1$.

Let $l = \inf_{y\in\mathcal{A}} I(y) < \infty$ and let $y^{(j)}$ be a minimizing sequence for I in $\mathcal{A}$, so that

$$\lim_{j\to\infty} I(y^{(j)}) = l.$$

Then we may assume that for all j

$$\begin{aligned} l+1 \geq \quad & I(y^{(j)}) \\ \geq \quad & \int_\Omega \Big(c_0[|Dy^{(j)}|^p + |\mathrm{cof}\, Dy^{(j)}|^{p'} \\ & \qquad + |\det Dy^{(j)}|^q] - c_1 \Big)\, dx. \end{aligned}$$

Lemma

There exists a constant $d > 0$ such that

$$\int_\Omega |z|^p dx \leq d \left(\int_\Omega |Dz|^p dx + \left| \int_{\partial\Omega_1} z\, dA \right|^p \right)$$

for all $z \in W^{1,p}(\Omega; \mathbb{R}^3)$.

By the Lemma $y^{(j)}$ is bounded in $W^{1,p}$ and so we may assume $y^{(j)} \rightharpoonup y^*$ in $W^{1,p}$ for some y^*.

But also we have that $\operatorname{cof} Dy^{(j)}$ is bounded in $L^{p'}$ and that $\det Dy^{(j)}$ is bounded in L^q. So we may assume that $\operatorname{cof} Dy^{(j)} \rightharpoonup H$ in $L^{p'}$ and that $\det Dy^{(j)} \rightharpoonup \delta$ in L^q.

By the results on the weak continuity of minors we deduce that $H = \operatorname{cof} Dy^*$ and $\delta = \det Dy^*$.

Let $u^{(j)} = (Dy^{(j)}, \text{cof}\, Dy^{(j)}, \det Dy^{(j)})$, $u = (Dy^*, \text{cof}\, Dy^*, \det Dy^*))$. Then

$$u^{(j)} \rightharpoonup u \text{ in } L^1(\Omega; \mathbb{R}^{19}).$$

But g is convex, and so (e.g. using Mazur's theorem),

$$\begin{aligned} I(y^*) = \int_\Omega g(u)\, dx &\leq \liminf_{j\to\infty} \int_\Omega g(u^{(j)})\, dx \\ &= \lim_{j\to\infty} I(y^{(j)}) = l. \end{aligned}$$

But $y^{(j)}|_{\partial\Omega_1} = \bar{y} \rightharpoonup y^*|_{\partial\Omega_1}$ in $L^1(\partial\Omega_1; \mathbb{R}^3)$ and so $y^* \in \mathcal{A}$ and y^* is a minimizer.

3. Martensitic phase transformations

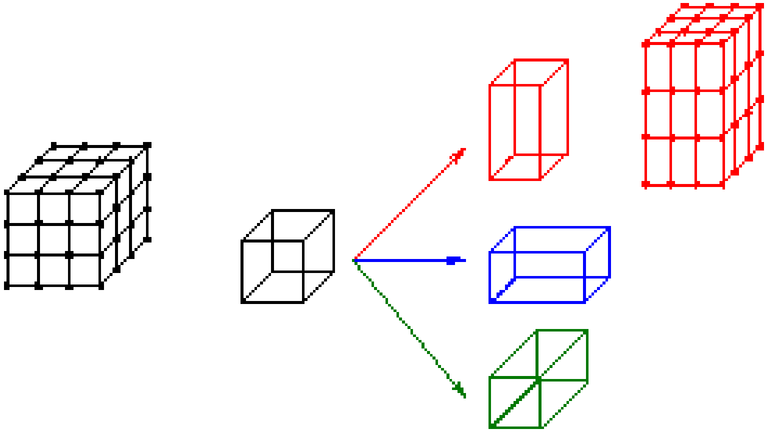
These involve a change of shape of the crystal lattice of some alloy at a critical temperature.

e.g. cubic to tetragonal

$\theta > \theta_c$

cubic

austenite



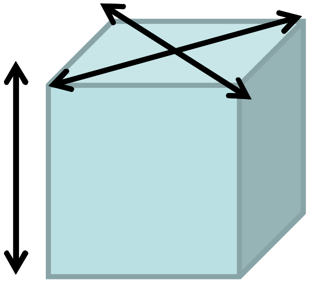
$\theta < \theta_c$

three tetragonal variants of martensite

cubic to

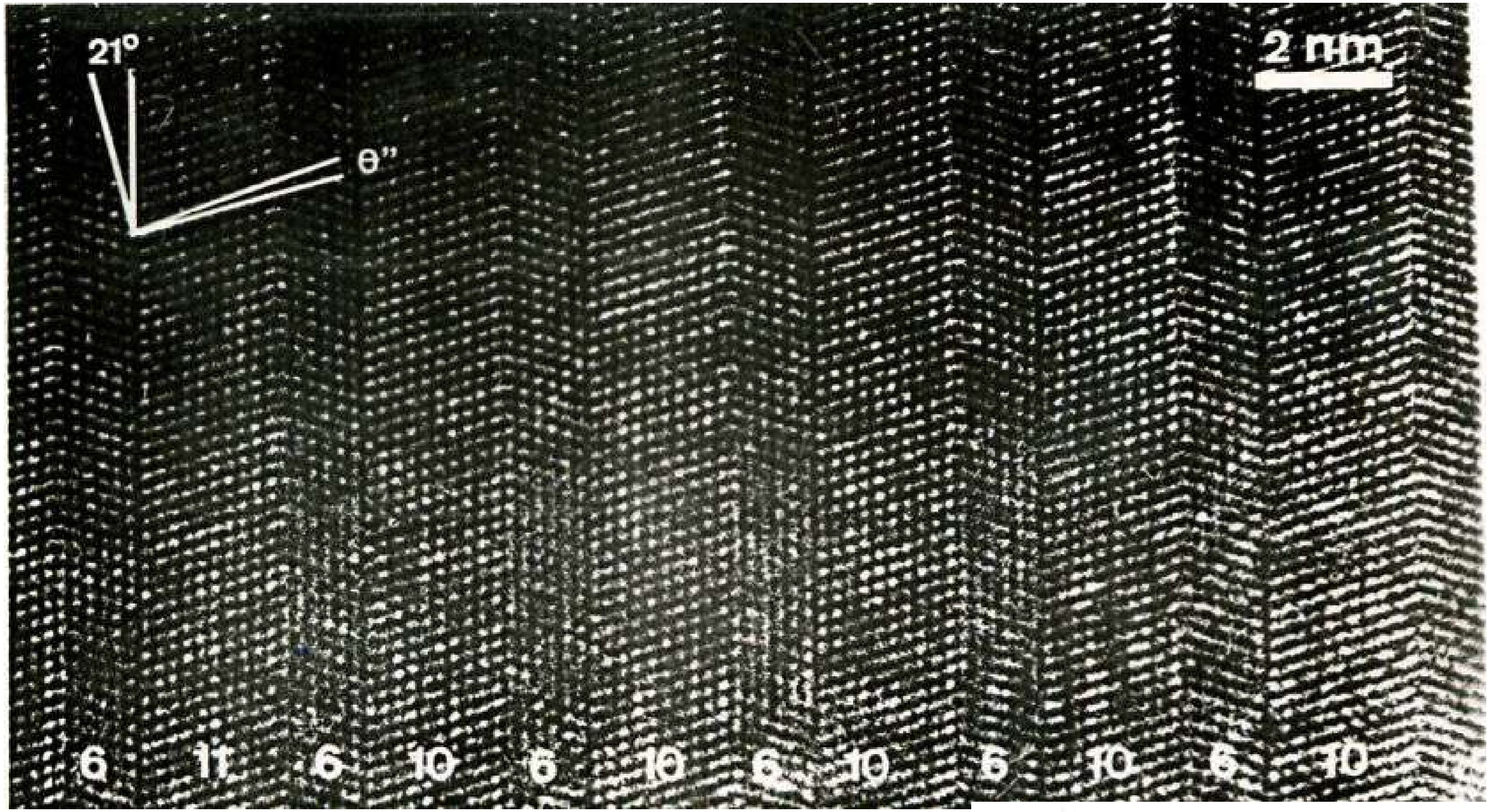
orthorhombic

(e.g. CuAlNi)



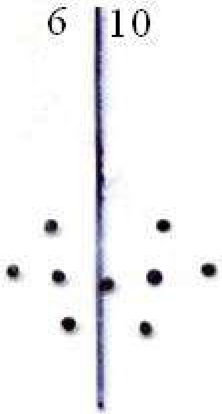
$\theta < \theta_c$

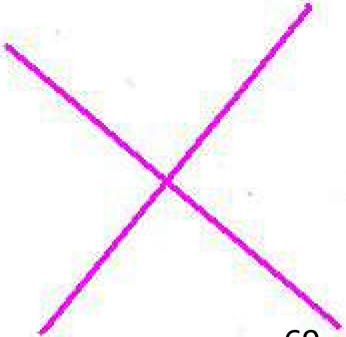
six orthorhombic variants of martensite



Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

Baele, van Tenderloo, Amelinckx





Energy minimization problem for single crystal

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

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 $A \in M_+^{3\times 3}$.

Energy-well structure

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

Assume

austenite

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

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

martensite

The $U_i(\theta)$ are the distinct matrices $QU_1(\theta)Q^T$ for $Q \in P^{24} =$ cubic group.

For cubic to tetragonal $N = 3$ and

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

For cubic to orthorhombic $N = 6$ and

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

By the Hadamard jump condition, interfaces correspond to pairs of matrices A, B with

$$A - B = a \otimes N,$$

where N is the interface normal. At minimum energy $A, B \in K(\theta)$.

From the form of $K(\theta)$, we need to know what the rank-one connections are between two given energy wells $SO(3)U$, $SO(3)V$.