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ILLUSTRATING THE IMPACT OF THE MATHEMATICAL SCIENCES

The Illustrating Mathematics Project

A collection of narratives and graphics will be the central focus of a consensus report that broadly describes the fundamental role of the mathematical sciences in the U.S. economy, national security, health and medicine, and other science, engineering, and technology domains. Visit https://www.nationalacademies.org/our-work/illustrating-the-impact-of-the-mathematical-sciences for more information.

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and is made possible with support from
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ILLUSTRATING MATHEMATICS

2020 Webinar Series, 3-4pm ET

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February 25, 2020: *From Solving to Seeing*

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ILLUSTRATING MATHEMATICS
Supercompatibility and the Design of Materials

Richard James,
University of Minnesota

Robert Kohn,
New York University

Irene Fonseca,
Carnegie Mellon University
(moderator)

Supercompatibility and the design of materials

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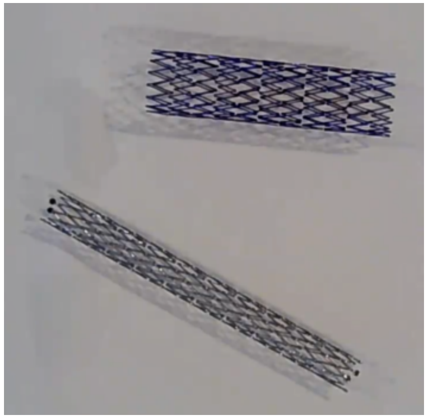
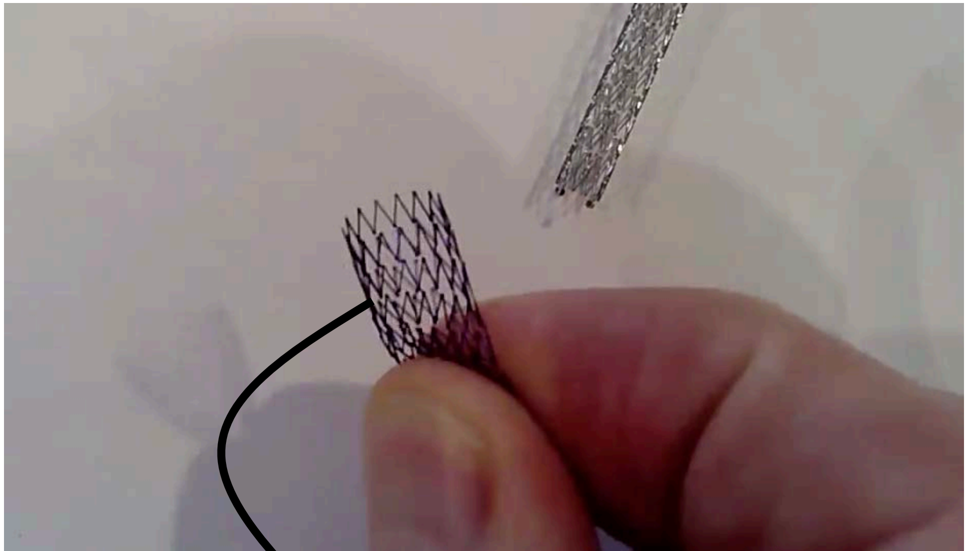
The reversibility of phase transformations

Click here to watch a demonstration of Nickel-Titanium Stents.



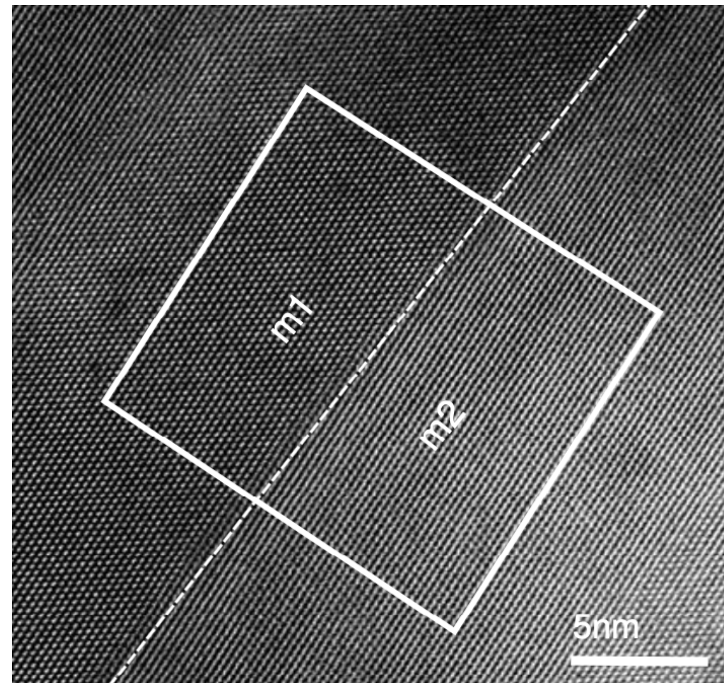
Click here to watch demonstration of -15°C Tin phase transformation.

Back to NiTi



x 5000

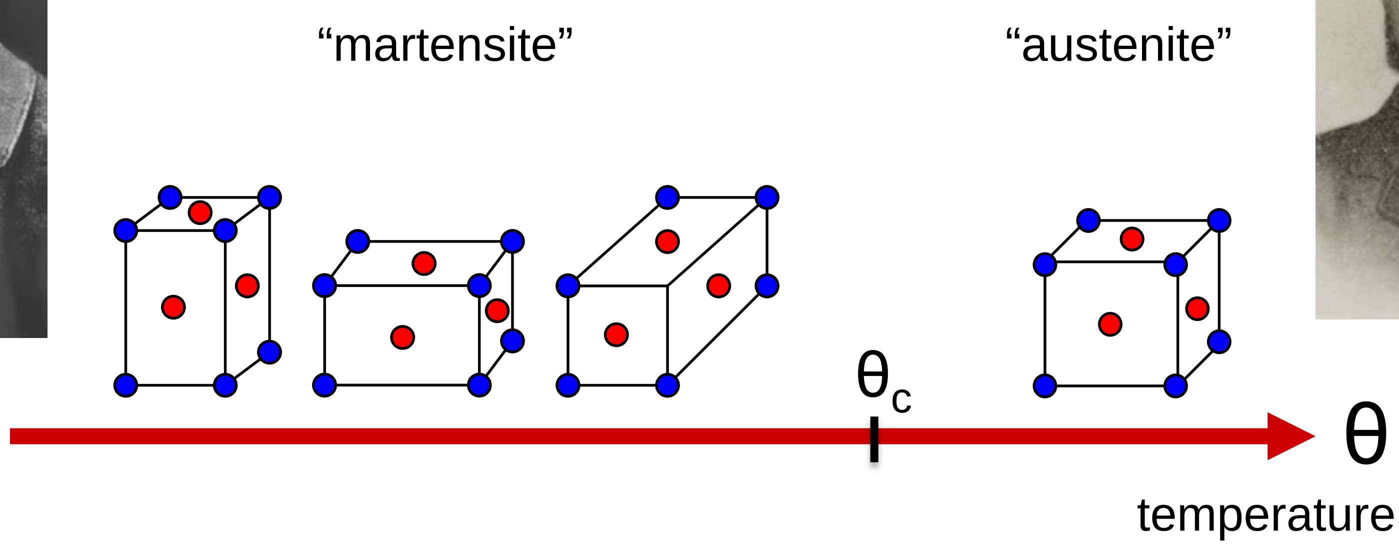
x 50



Adolph Karl
Gottfried Martens

Phase transformations

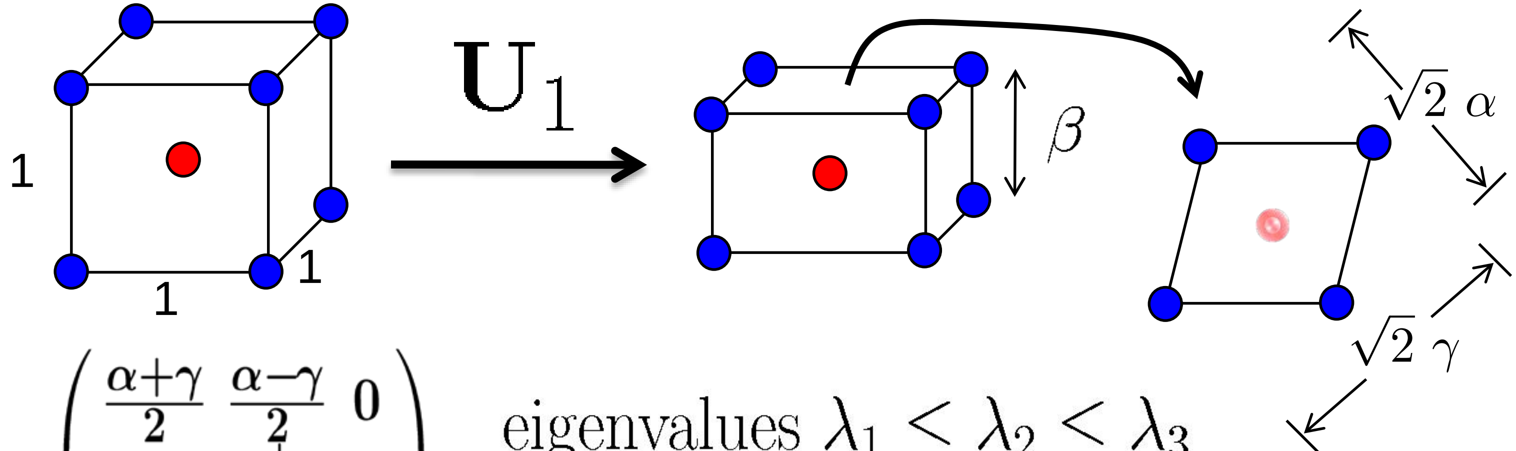
Sir William Chandler
Roberts-Austin



➔ more precisely, change of crystal structure, no diffusion:
martensitic phase transformations

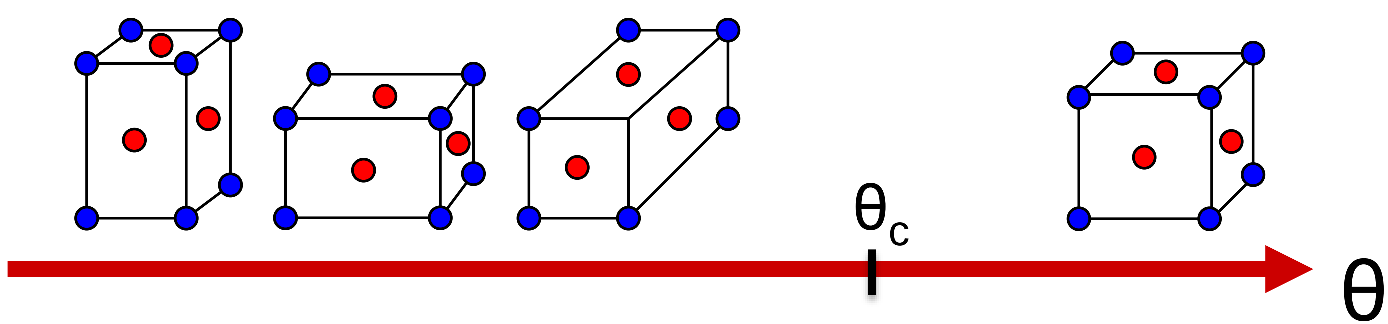
Transformation matrix

(Transformation stretch matrix)

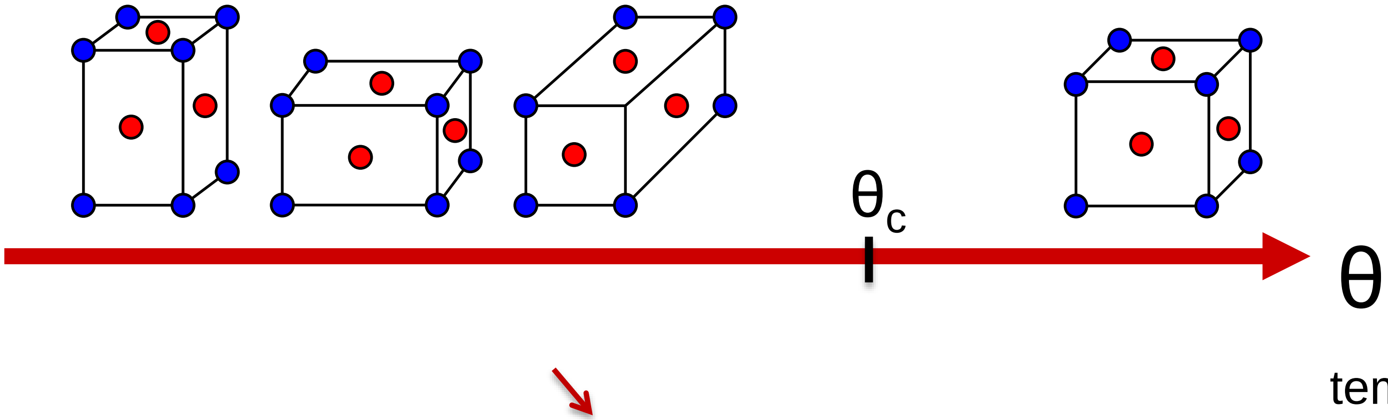


$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

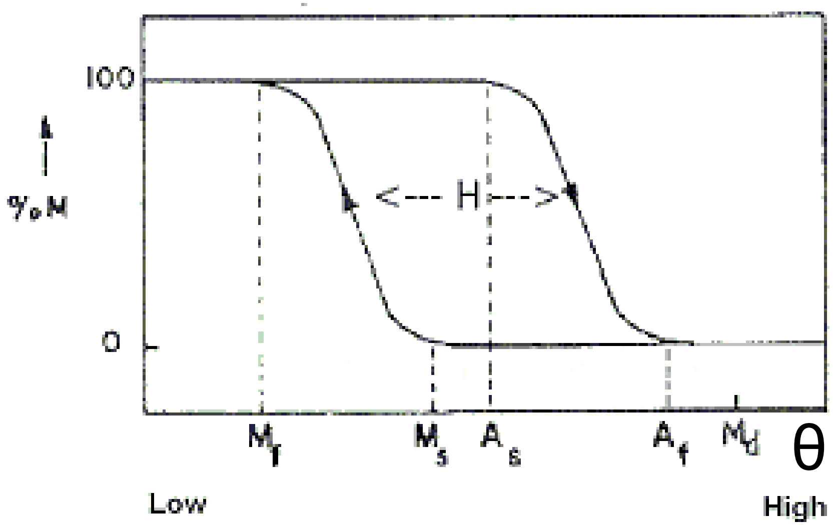
eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$



Hysteresis loops

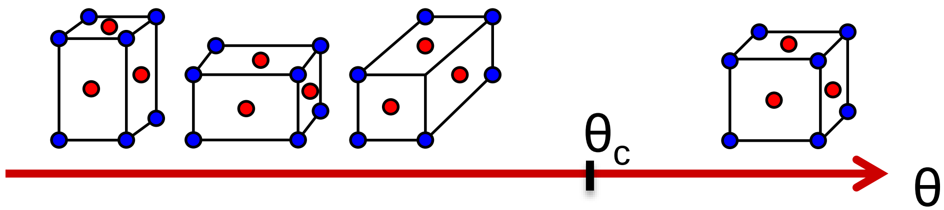


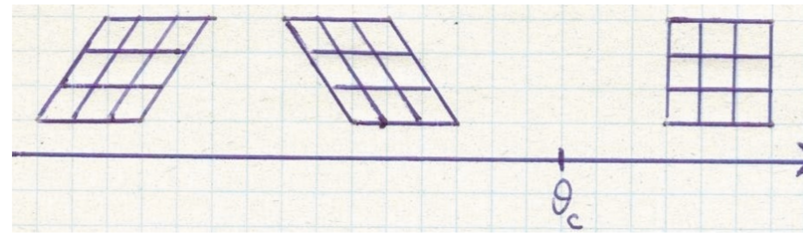
Thermal hysteresis



Essential mechanisms

Microscopic mechanisms of **superelasticity** and **shape-memory** involve a symmetry-breaking phase transformation

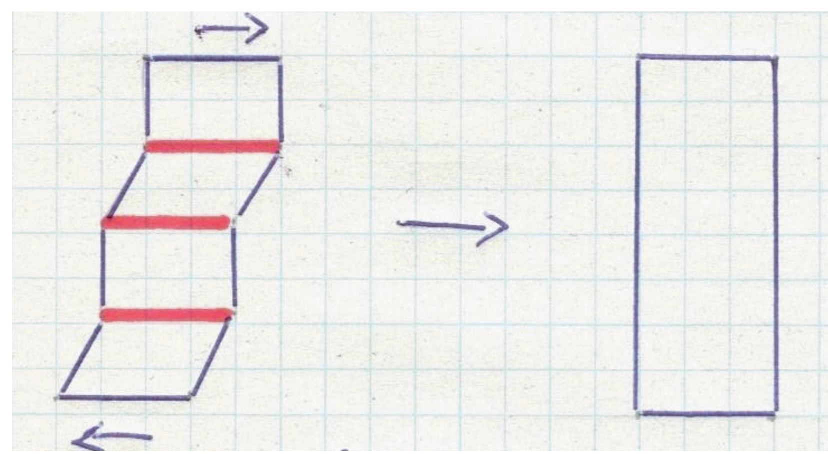




- at temp $\theta > \theta_c$ there is a single preferred lattice structure
- $\theta < \theta_c$ there are several (symmetry-related) preferred structures

Superelastic behavior ($\theta > \theta_c$)

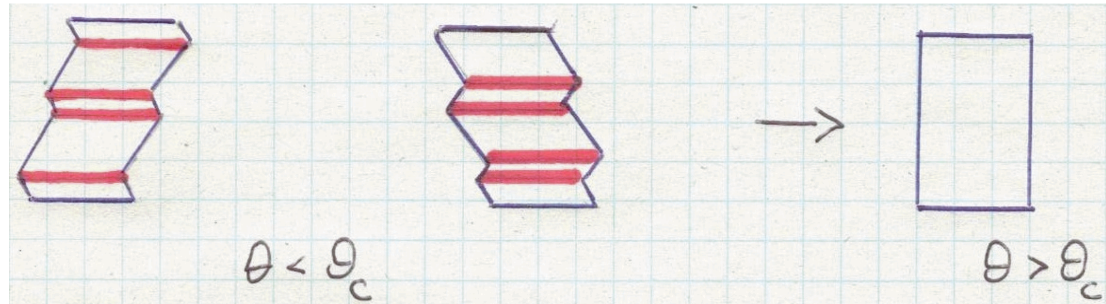
- loading nucleates martensite & moves phase boundaries
- unloading $\Longrightarrow$ return to austensite



Essential mechanisms

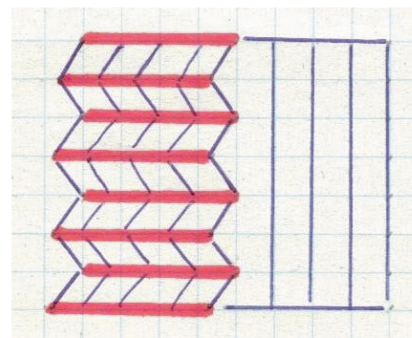
Shape-memory behavior ($\theta < \theta_c$)

- deformation (without stress) by mixing martensite variants
- heating restores lattice to austenite



Microstructure

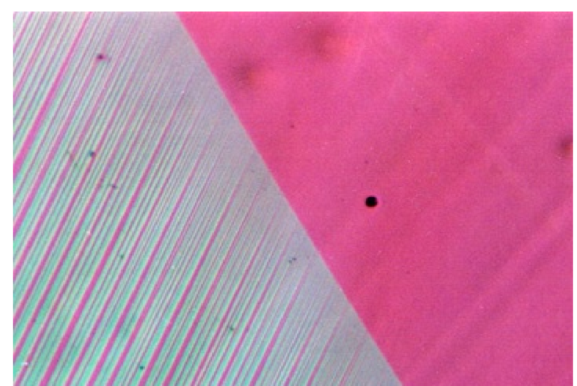
- permits mixture of martensite variants to mimic austenite
- but: transition layer isn't stress-free



$\theta = \theta_c$

Warning: 2D schematic oversimplifies

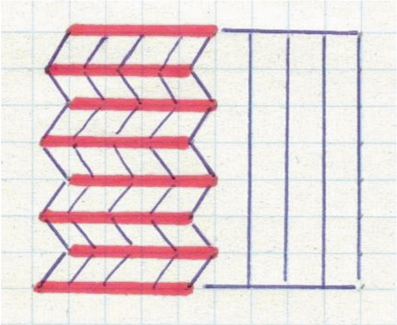
- in reality there are many variants of martensite
- microstructure predominates, except in special circumstances

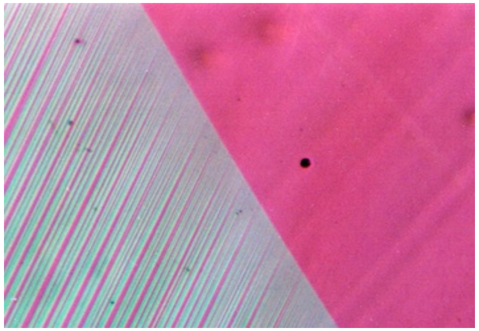


Mathematical description

Use the framework of nonlinear elasticity: let $\mathbf{x} \mapsto \mathbf{y}(\mathbf{x})$ take austenite (high symmetry) lattice to actual configuration

- $\mathbf{y}(\mathbf{x})$ is continuous but only piecewise smooth
- preferred values of $\nabla\mathbf{y}$ are set by the phase transformation



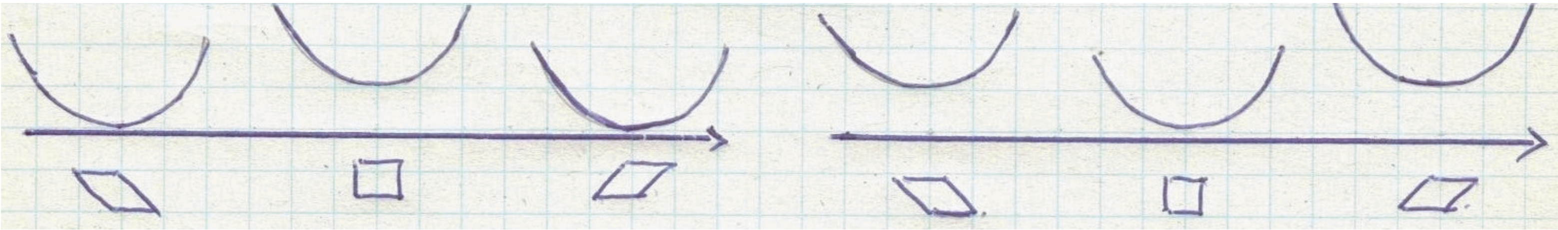


Predicting structure is a problem in the **calculus of variations**:

$$\min_{\text{bdry conds}} \int_{\text{ref domain}} \varphi(\nabla \mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x} \;+\; \text{energy of the loading device}$$

where φ is a multiwell energy density, with local minima at the preferred structures:

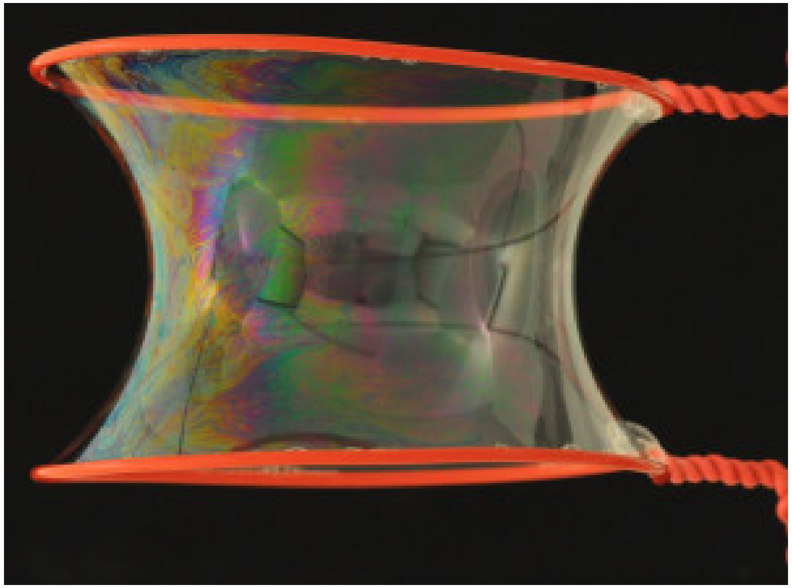
$\varphi(\nabla \mathbf{y}, \theta),\ \theta < \theta_c$ $\qquad$ $\varphi(\nabla \mathbf{y}, \theta),\ \theta > \theta_c$



A different kind of variational problem

In many familiar examples a solution exists. Goals for analysis include

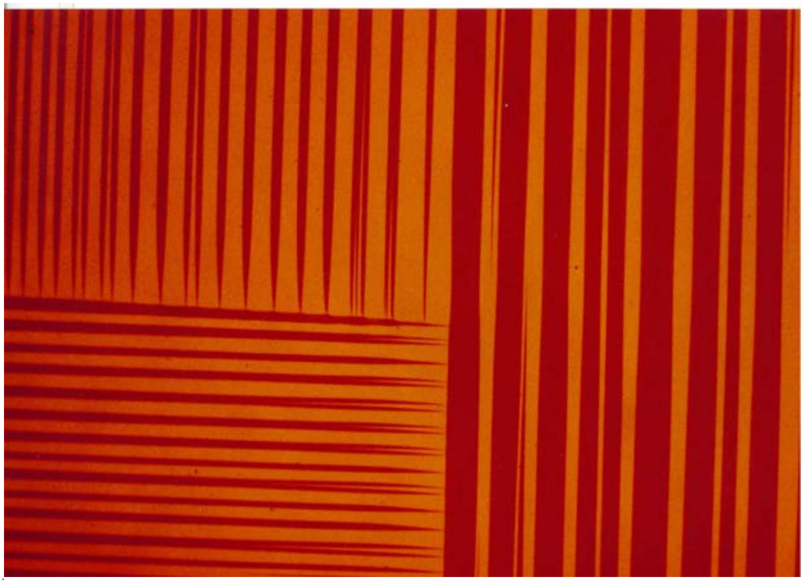
- finding it numerically
- understanding its singularities



mathematicalgarden.wordpress.com

Ours is different: a solution may not exist, if microstructure is needed. Goals include

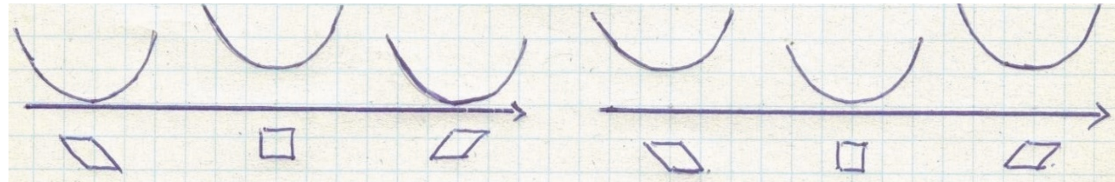
- understanding when microstructure is needed
- learning how interfacial energy sets the character and scale of phase mixtures



courtesy C. Chu

Free energy and energy wells

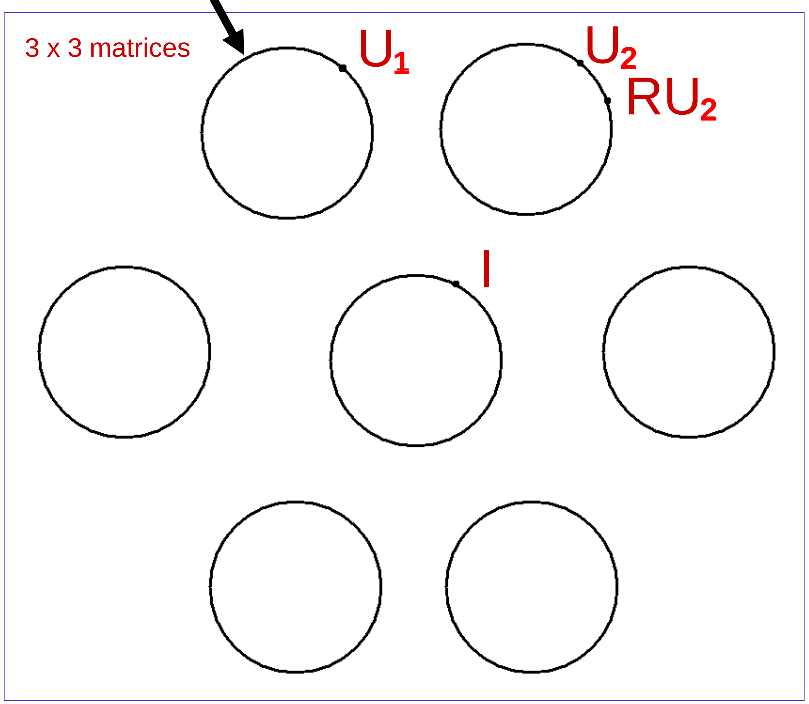
$\varphi(\nabla \mathbf{y}, \theta),\ \theta < \theta_c$ $\qquad$ $\varphi(\nabla \mathbf{y}, \theta),\ \theta > \theta_c$



$$\min_{BC} \int_\Omega \varphi(\nabla \mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x}$$

$$\theta = \theta_c$$

minimizers...



$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

$$\mathbf{U}_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

$$\mathbf{U}_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix}$$

$$\mathbf{U}_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix}$$

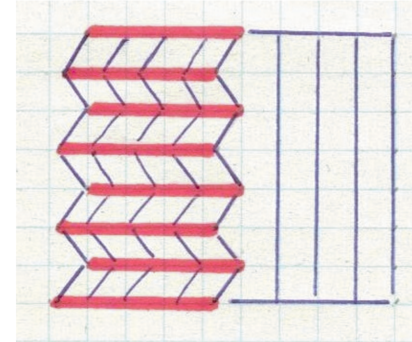
$$\mathbf{U}_5 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}$$

$$\mathbf{U}_6 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}$$

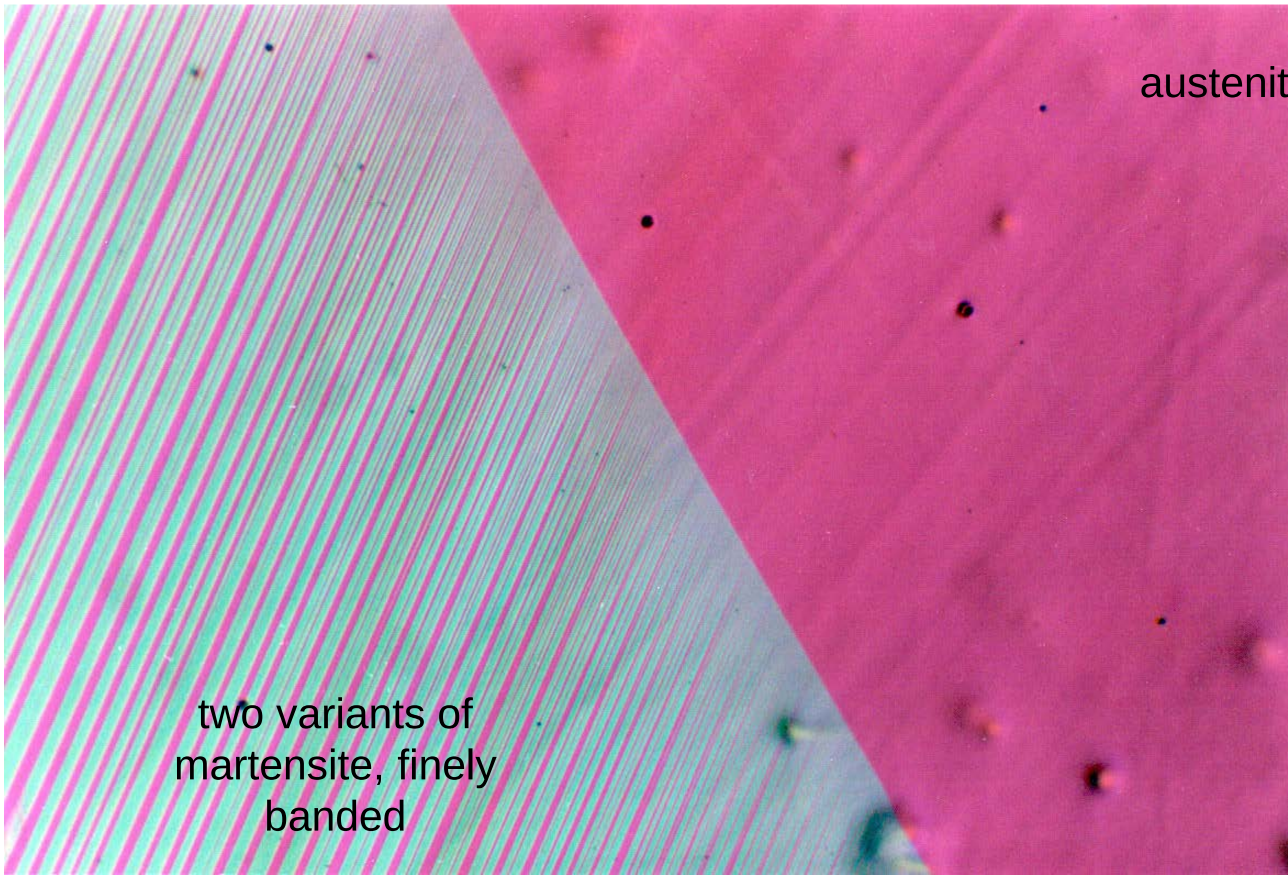
Cu_{69}
$Al_{27.5}$
$Ni_{3.5}$

$\alpha = 1.0619$
$\beta = 0.9178$
$\gamma = 1.0230$

The austenite/martensite interface



The typical mode of transformation when $\lambda_2 \neq 1$



A suggestion from mathematics

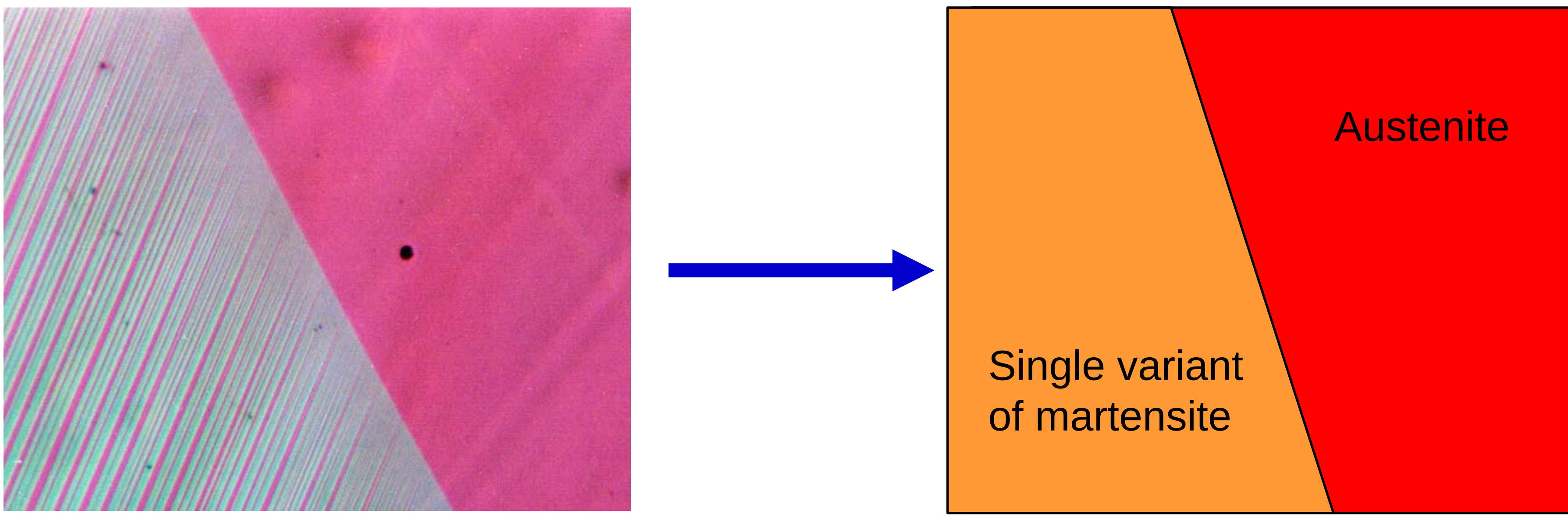
The lattice parameters α, β, γ depend on composition

for example

$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

$$\text{eigenvalues } \lambda_1 \leq \lambda_2 \leq \lambda_3$$

Can we tune the composition of the material
so that a single variant of martensite is compatible
with austenite?

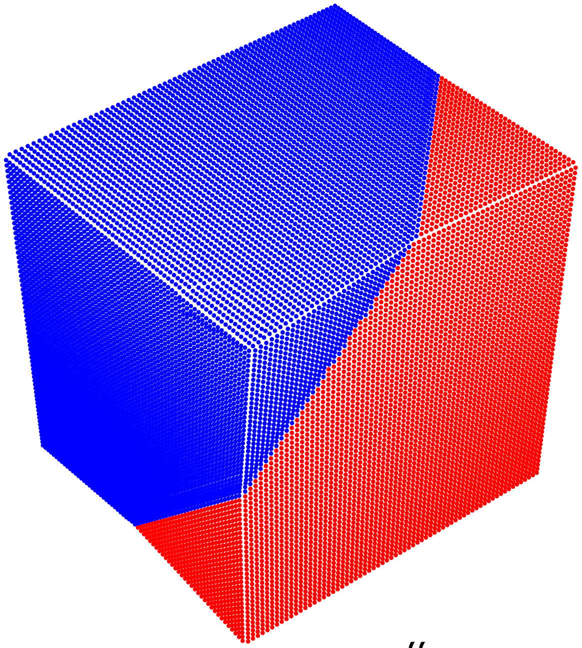


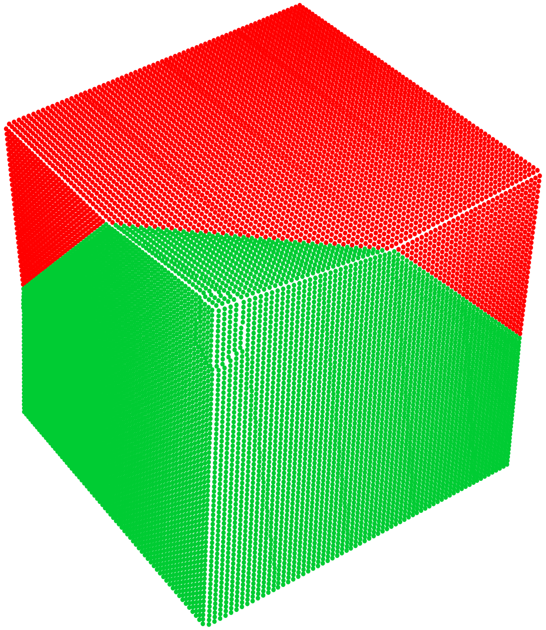
Lemma $\lambda_2 = 1$ *is necessary and sufficient that there is* $\mathbf{R} \in \mathrm{SO}(3)$ *such that* $\mathbf{R}\mathbf{U}_1 - \mathbf{I} = \mathbf{a} \otimes \mathbf{n}$.

for example

$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$

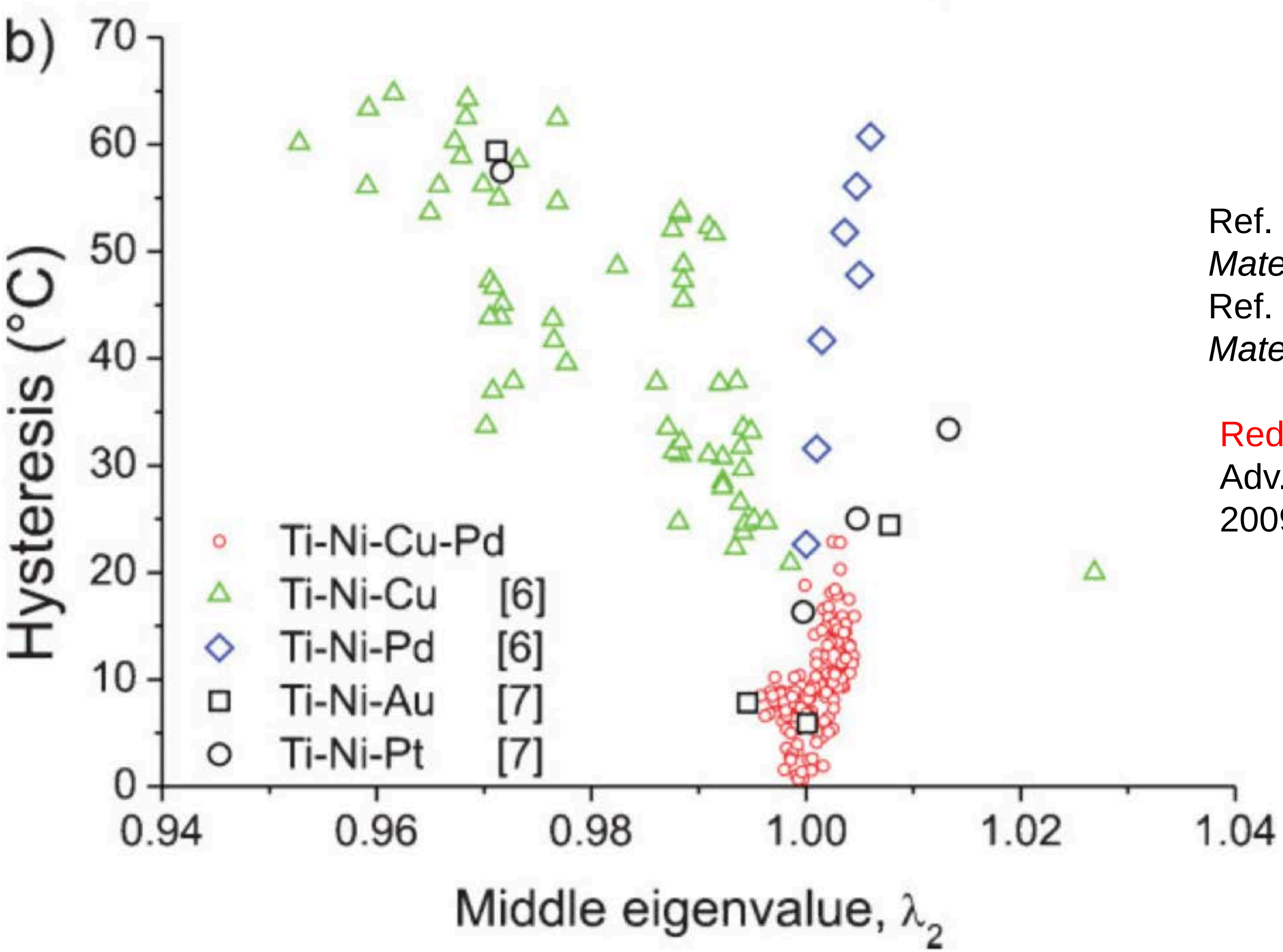




"supercompatibility"

Complete removal of stressed transition layers between phases

Hysteresis vs λ_2



Ref. 6 J. Cui et al. *Nature Materials*, **5**, 286 (2006), Ref. 7 Z. Zhang et al., *Acta Materialia* (2009)

Red: Zarnetta et al., Adv. Funct. Matls, 2009

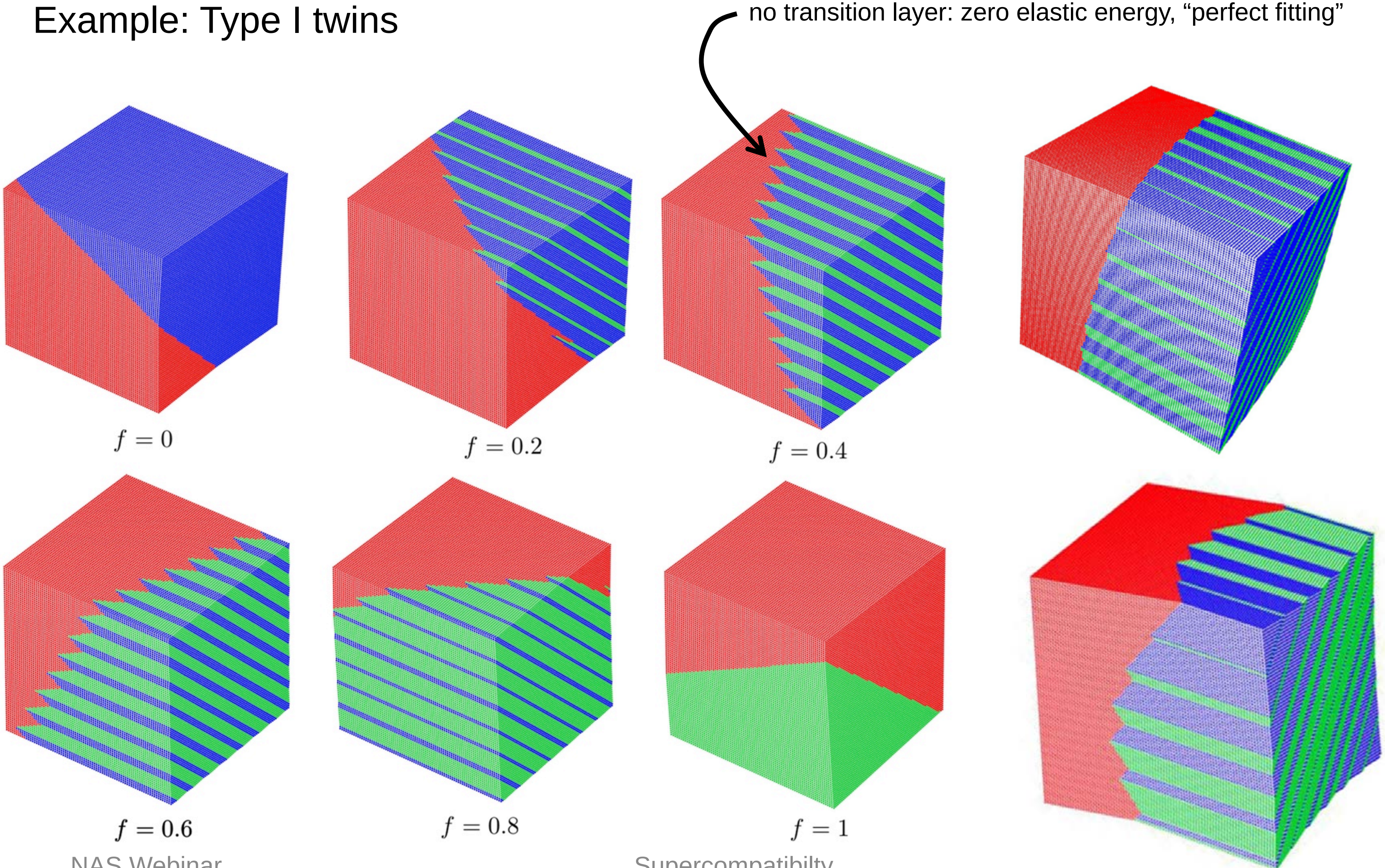
The cofactor conditions

cofactor conditions

$$\lambda_2 = 1$$
$$\mathbf{a} \cdot \mathbf{U}_1 \mathrm{cof}(\mathbf{U}_1^2 - \mathbf{I})\mathbf{n} = 0$$
$$\mathrm{tr}\mathbf{U}_1^2 - \det \mathbf{U}_1^2 - \frac{1}{4}|\mathbf{a}|^2|\mathbf{n}|^2 - 2 \geq 0$$

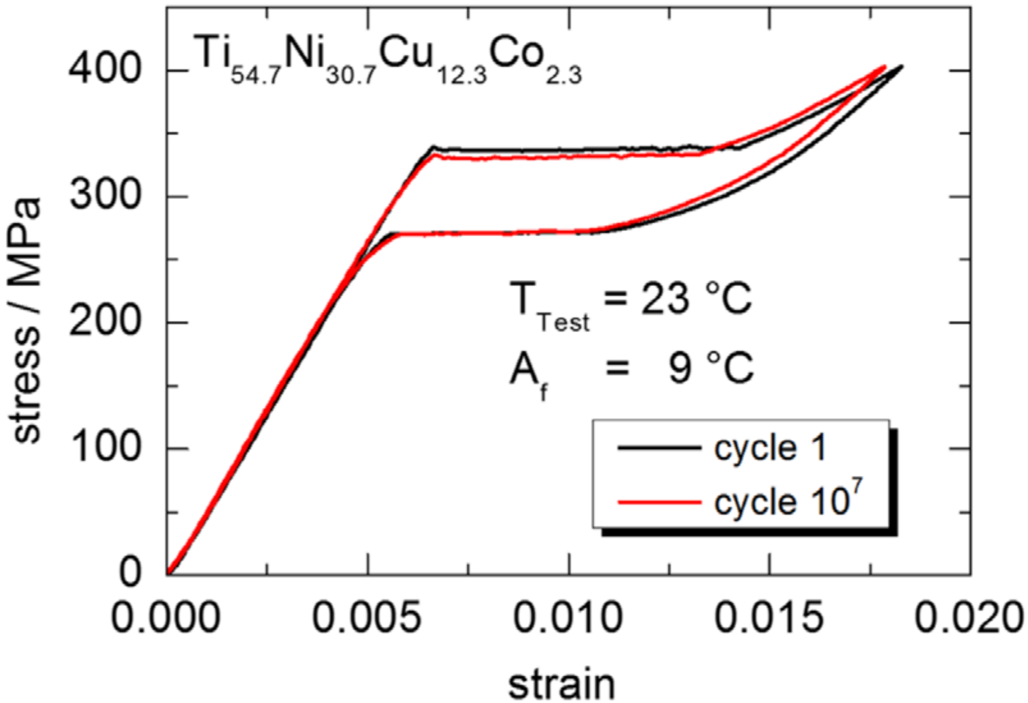
Example: Type I twins

no transition layer: zero elastic energy, "perfect fitting"



Alloy satisfying the cofactor conditions

C. Chluba et al., Science (2015) (Laboratory of Eckhard Quandt, University of Kiel)



Currently, there is a worldwide search for new supercompatible alloys

What other mathematical challenges lie nearby?

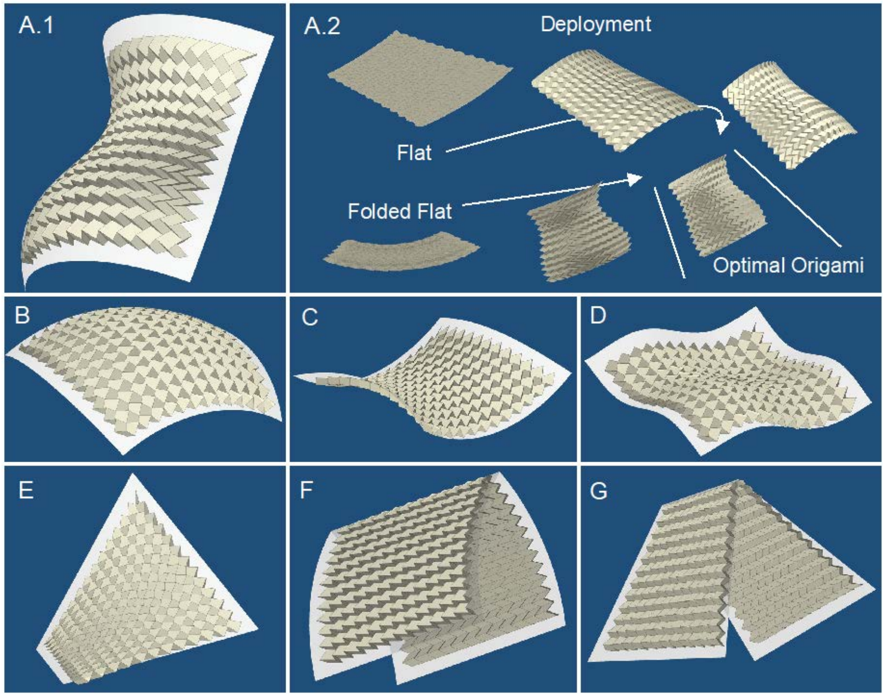
Today's discussion has focused on shape-memory materials, but there are many cross-cutting issues. Here are two:

(1) The deformations possible in a system depend sensitively on its structure

Another example of current interest: **deployable origami** (architectural design, therapeutics, deployable space structures, medical stent design, antenna design , robotics).

Goal: prescribe fold lines on a flat sheet so that

- It has a one-parameter family of (partially) folded configurations, and
- this family passes through a good approximation to a specified surface



See recent work of X. Dang et al, arXiv:2008.02349.

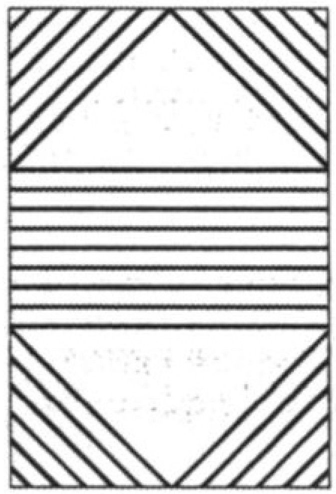
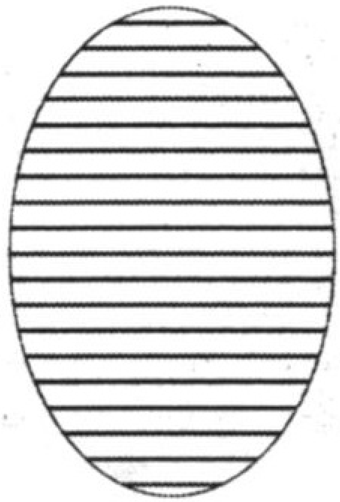
What other mathematical challenges lie nearby?

(2) Patterns and microstructure arising in other variational problems

Geometry-driven wrinkling

- In recent experiments, regions cut from a thin spherical shell were flattened by floating on water (Albarrán et al, arXiv:1806.03718)
- The wrinkling patterns are robust, and they depend on the region's shape
- Recent work by Ian Tobasco explains these patterns (arXiv:1906.02153).



Conclusions

- Shape-memory materials are useful because they sustain large deformation with little damage
- Mathematical understanding of the mechanism revealed that certain non-generic alloys avoid the need for microstructure, leading to less damage and improved behavior
- The theory involves calculus of variations problems with multiwell energies
- This is but one of many areas where the calculus of variations interacts with mechanics, in ways that challenge and enrich both fields

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Please submit questions using the Q&A button in the zoom menu.

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