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Transformations de phase, compatibilité et microstructure

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Unlike more familiar phase transformations such as

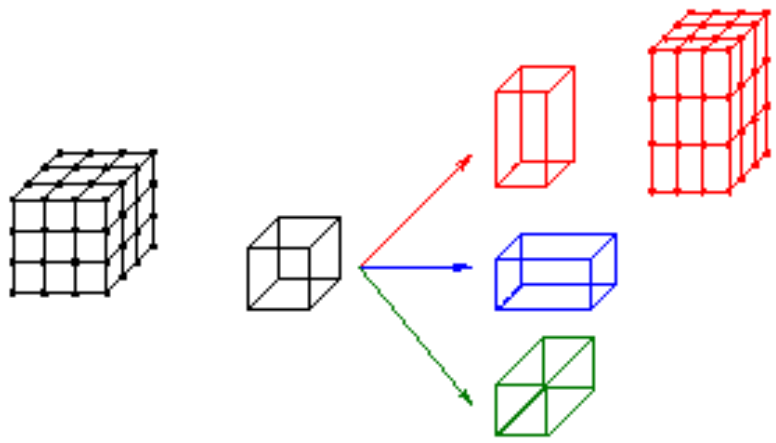
$$\text{ice} \longrightarrow \text{water} \longrightarrow \text{steam}$$

martensitic phase transformations in crystals (metals and alloys) involve a diffusionless *change of shape* of the underlying crystal lattice at some critical temperature.

e.g. cubic to tetragonal

austenite

$\theta > \theta_c$

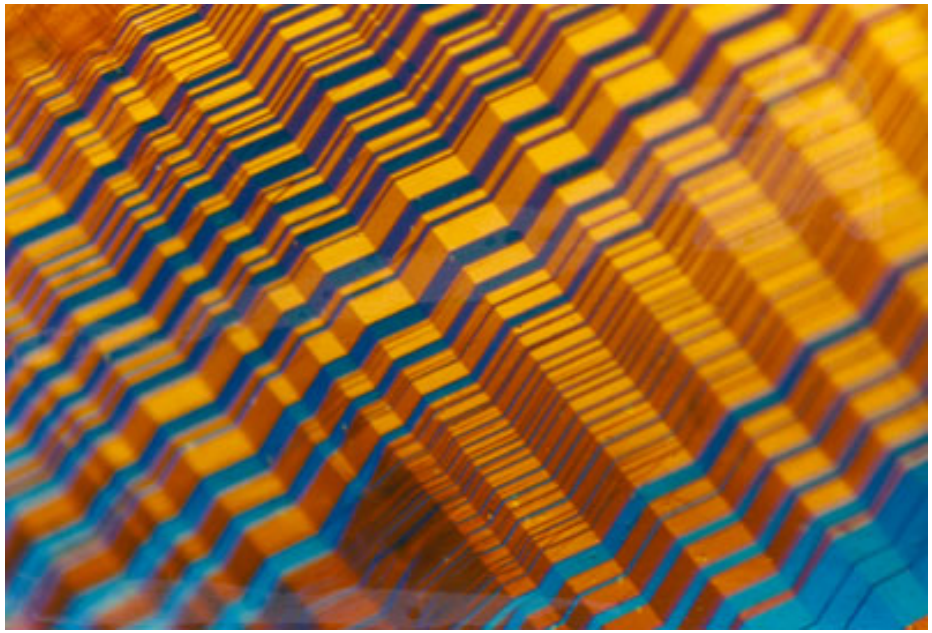


three *variants* of low temperature phase.

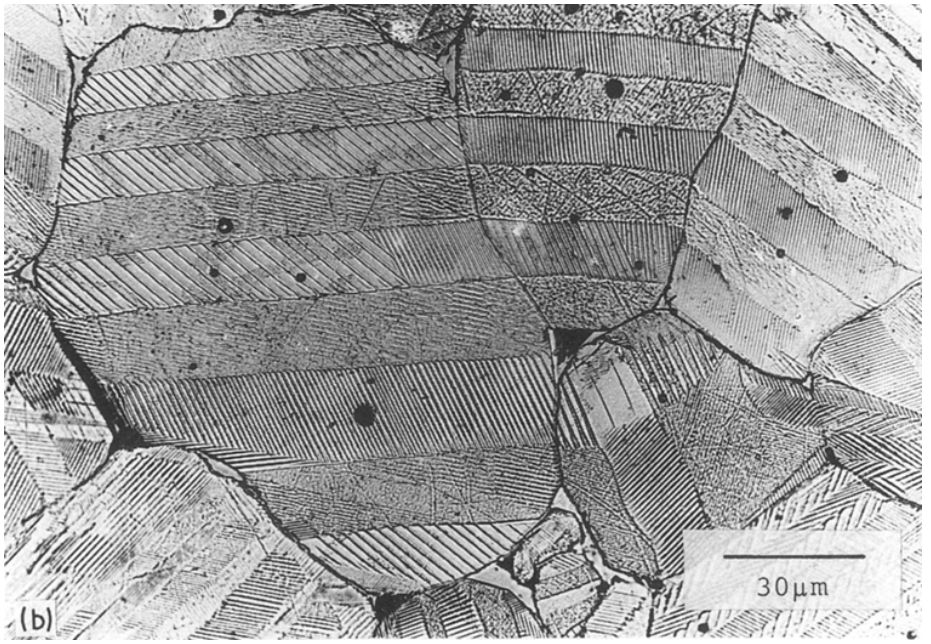
$\theta < \theta_c$

martensite

The requirement that the different variants fit together geometrically (compatibility) leads to characteristic patterns of *microstructure* that are important for determining the macroscopic properties of the material.



CuAlNi single crystal: Chu/James



$BaTiO_3$ polycrystal: G. Arlt 1990

The aim of the course is to try to understand such microstructures, using the following ingredients:

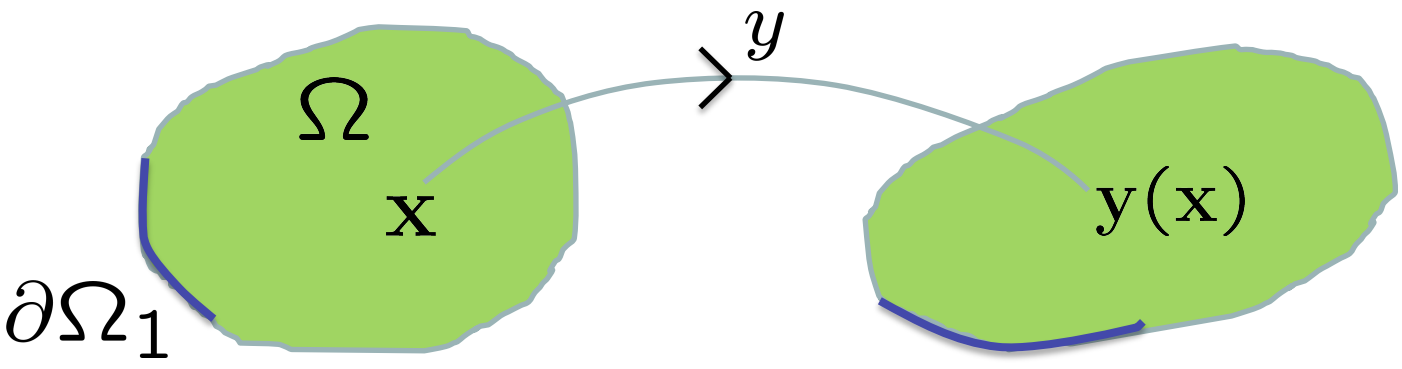
(i) A description of crystal lattices,

(ii) A related nonlinear elasticity model,

(iii) An analysis of possible interfaces and microstructures,

(iv) Techniques of the multi-dimensional calculus of variations (quasiconvexity ...).

Brief review of nonlinear elastostatics



Reference configuration Deformed configuration

Assume material is homogeneous and occupies a bounded (Lipschitz) domain $\Omega \subset \mathbb{R}^3$ in a reference configuration.

Elastic free energy at constant temperature θ

$$I_\theta(\mathbf{y}) = \int_\Omega \psi(D\mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x}.$$

free-energy density

Properties of free-energy density: $\psi(\mathbf{A}, \theta)$ defined for $\mathbf{A} \in D(\psi), \theta \in I$, where $D(\psi)$ is an open subset of

$$GL^{+}(3, \mathbb{R}) = \{\mathbf{A} \in M^{3\times 3} : \det \mathbf{A} > 0\}.$$

(i) (frame-indifference)

$\psi(\mathbf{QA}, \theta) = \psi(\mathbf{A}, \theta)$ for all $\mathbf{Q} \in SO(3), \mathbf{A} \in D(\psi), \theta \in I$

(ii) (material symmetry)

$\psi(\mathbf{AM}, \theta) = \psi(\mathbf{A}, \theta)$ for all $\mathbf{M} \in \mathcal{S}, \mathbf{A} \in D(\psi), \theta \in I$,
where $\mathcal{S}$ is a subgroup of the set of unimodular matrices
$SL(3) = \{\mathbf{A} \in M^{3\times 3} : \det \mathbf{A} = 1\}$.

For consistency, we need $SO(3)\, D(\psi)\, \mathcal{S} = D(\psi)$.

Energy minimization problem

Minimize

$$I_\theta(\mathbf{y}) = \int_\Omega \psi(D\mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x}$$

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

$$\mathbf{y}|_{\partial\Omega_1} = \bar{\mathbf{y}}.$$

In order that we can be assured that a minimizer exists we typically need that in addition $\psi(\cdot, \theta)$ is quasiconvex and coercive. However we will see that for elastic crystals neither condition is generally satisfied.

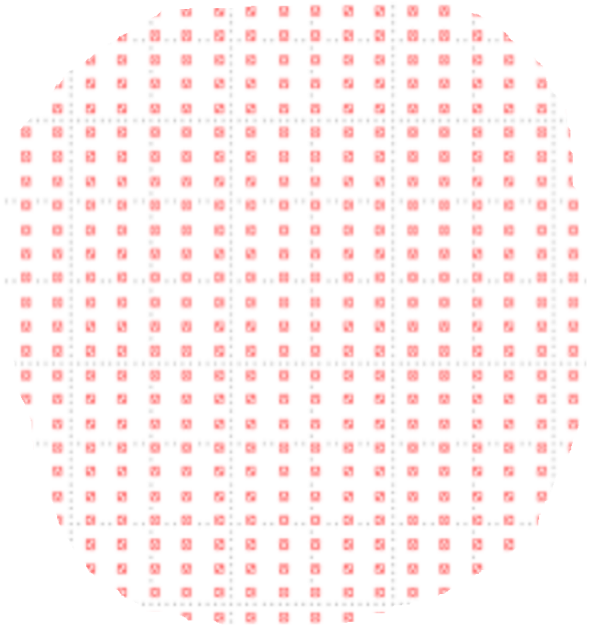
Bravais lattices

A Bravais lattice is an infinite lattice of points in $\mathbb{R}^3$ generated by linear combinations with integer coefficients of three linearly independent basis vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$.

Setting $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3) \in GL(3, \mathbb{R})$ we write the corresponding Bravais lattice as

$$\mathcal{L}(\mathbf{B}) = \{m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 : m_i \in \mathbb{Z}\}.$$

Notice that if $\mathbf{B} = (B_{ij})$ then $B_{ij} = \mathbf{b}_j \cdot \mathbf{e}_i$, where $\mathbf{e}_i$ is the unit vector in the i^{th} coordinate direction.



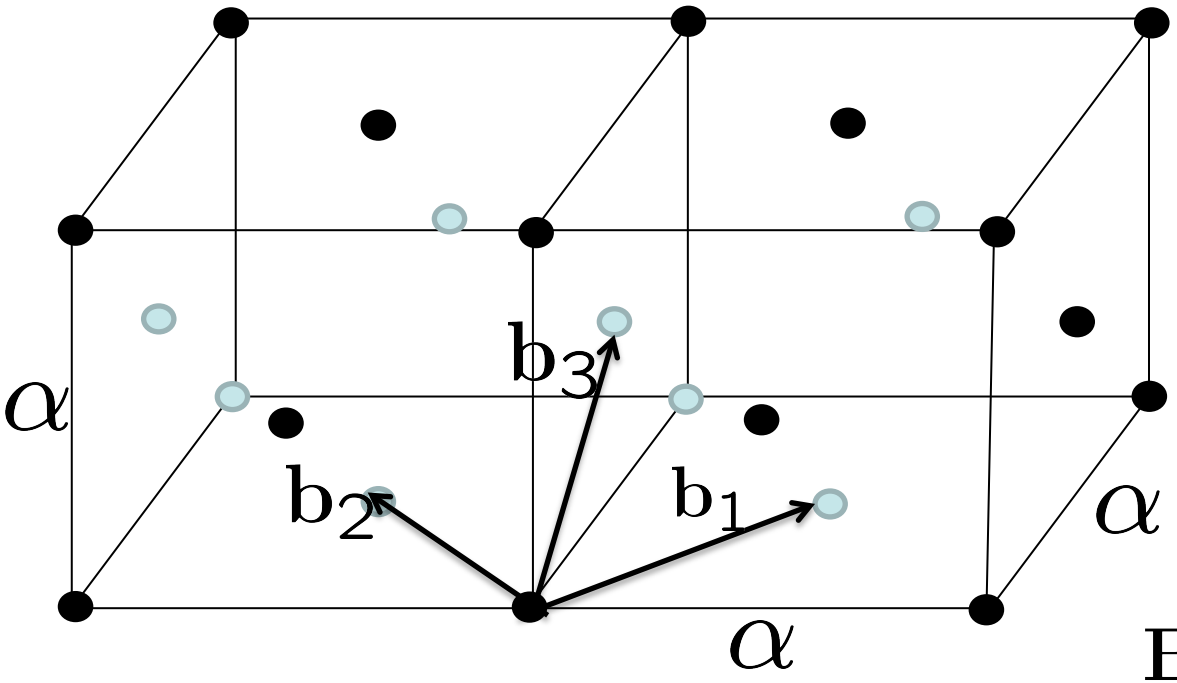
We think of a single crystal as consisting of a part of a Bravais lattice consisting of many points, each point representing an atomic position.

Typical alloys are *solid solutions* of different elements, so that each lattice site has a probability of being occupied by a particular element according to the overall composition.

Some crystals form *multilattices* which are finite unions of translates of a Bravais lattice. We will not consider these.

Examples of Bravais lattices.

1. Face-centred cubic (fcc)



$$\mathbf{B} = \alpha \mathbf{Q} \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} \end{pmatrix},$$

$$\mathbf{Q} \in O(3)$$

Equivalently

$$\mathbf{B}^T\mathbf{B} = \frac{\alpha^2}{4} \begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

Note that any atom can be taken as the origin.