Reduction of the symmetry group

It is convenient to consider a simplified theory in which we only consider those $\boldsymbol{\mu}$ that generate elements of the point group, thus ignoring large lattice invariant shears that are typically associated with plasticity.

Theorem. (Ericksen-Pitteri neighbourhood) Given a Bravais lattice $\mathbf{B} \in GL^+(3,\mathbb{R})$ there is an open neighbourhood $\mathcal{N}$ of $SO(3)$ in $GL^+(3,\mathbb{R})$ such that
(i) $SO(3)\mathcal{N} = \mathcal{N}$
(ii) if $\boldsymbol{\mu} \in GL^+(3,\mathbb{Z})$ then either $\mathcal{N}\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} = \mathcal{N}$ (in which case $\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \in P(\mathbf{B})$), or $\mathcal{N}\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \cap \mathcal{N} = \emptyset$.

Thus, if we restrict $\psi(\mathbf{A},\theta)$ to $\mathcal{N}$ then the symmetry group of ψ is reduced to

$$P^{+}(\mathbf{B}) = P(\mathbf{B}) \cap SO(3) = \mathcal{S} \cap SO(3).$$

Proof. We claim that a suitable neighbourhood is given by

$$\mathcal{N}_\varepsilon = \{\mathbf{A} : |\mathbf{A}^T\mathbf{A} - \mathbf{1}| < \varepsilon\}$$

for $\varepsilon > 0$ sufficiently small.

Note that $SO(3)\mathcal{N}_\varepsilon = \mathcal{N}_\varepsilon SO(3) = \mathcal{N}_\varepsilon$, since if $\mathbf{Q} \in SO(3)$

$$|(\mathbf{AQ})^T\mathbf{AQ} - \mathbf{1}| = |\mathbf{Q}^T(\mathbf{A}^T\mathbf{A} - \mathbf{1})\mathbf{Q}| = |\mathbf{A}^T\mathbf{A} - \mathbf{1}|.$$

Suppose for contradiction that the result is false for $\varepsilon = j^{-1}$, $j = 1, 2 \ldots$. Then for each j there exists $\boldsymbol{\mu}^{(j)}$ with $\mathbf{B}\boldsymbol{\mu}^{(j)}\mathbf{B}^{-1} \notin P(\mathbf{B})$ and $\mathbf{C}^{(j)} = \mathbf{D}^{(j)}\mathbf{B}\boldsymbol{\mu}^{(j)}\mathbf{B}^{-1} \in \mathcal{N}_{1/j}$.

We can assume that $\mathbf{C}^{(j)} \to \mathbf{R}, \mathbf{D}^{(j)} \to \tilde{\mathbf{R}}, \boldsymbol{\mu}^{(j)} \to \boldsymbol{\mu}$, where $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$, and hence $\mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \in P(\mathbf{B})$. But $\boldsymbol{\mu}^{(j)} \to \boldsymbol{\mu}$ implies $\boldsymbol{\mu}^{(j)} = \boldsymbol{\mu}$ for j sufficiently large. Contradiction. $\square$

If we apply this result to the phase transformation case then we can restrict the symmetry group to $P^{+}(\mathbf{B})$ provided $\mathbf{U}(\theta)$ is sufficiently close to $\mathbf{1}$ and θ sufficiently close to θ_c.

Thus, restricting ψ to $\mathcal{N}$, and defining as before

$$K(\theta) = \{\mathbf{A} \in \mathcal{N} : \psi(\mathbf{A}, \theta) = 0\},$$

we assume that

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

where $\mathbf{U}_i(\theta)$ are the distinct matrices $\mathbf{Q}^T\mathbf{U}(\theta)\mathbf{Q}$ for $\mathbf{Q} \in P^c \cap SO(3) = P^{24}$.

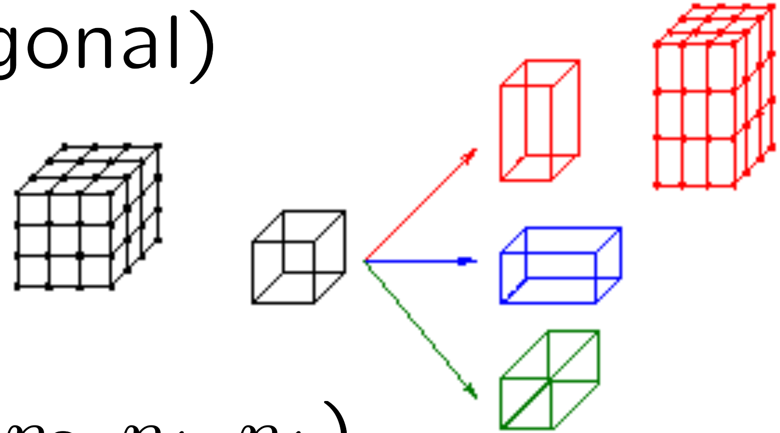
M is the number of *martensitic variants*. If we let

$$G_i = \{\mathbf{Q} \in P^c : \mathbf{Q}^T\mathbf{U}(\theta)\mathbf{Q} = \mathbf{U}_i(\theta)\}$$

then $|G_i|$ is independent of i and so M divides 24.

Example 1. (cubic-to-tetragonal)

(e.g. InTl, NiAl, NiMn, $BaTiO_3$)



$$\mathbf{U}(\theta) = \text{diag}\,(\eta_2, \eta_1, \eta_1),$$

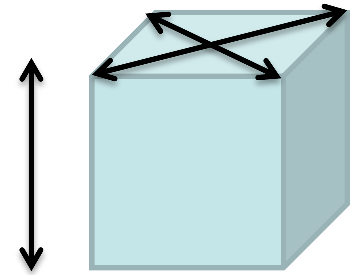
where $\eta_1 = \eta_1(\theta) > 0$, $\eta_2 = \eta_2(\theta) > 0$, $\eta_1 \neq \eta_2$.

Then $M = 3$ and

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

$$\mathbf{U}_3(\theta) = \text{diag}\,(\eta_1, \eta_1, \eta_2).$$

Example 2. (cubic-to-orthorhombic)
(e.g. CuAlNi)

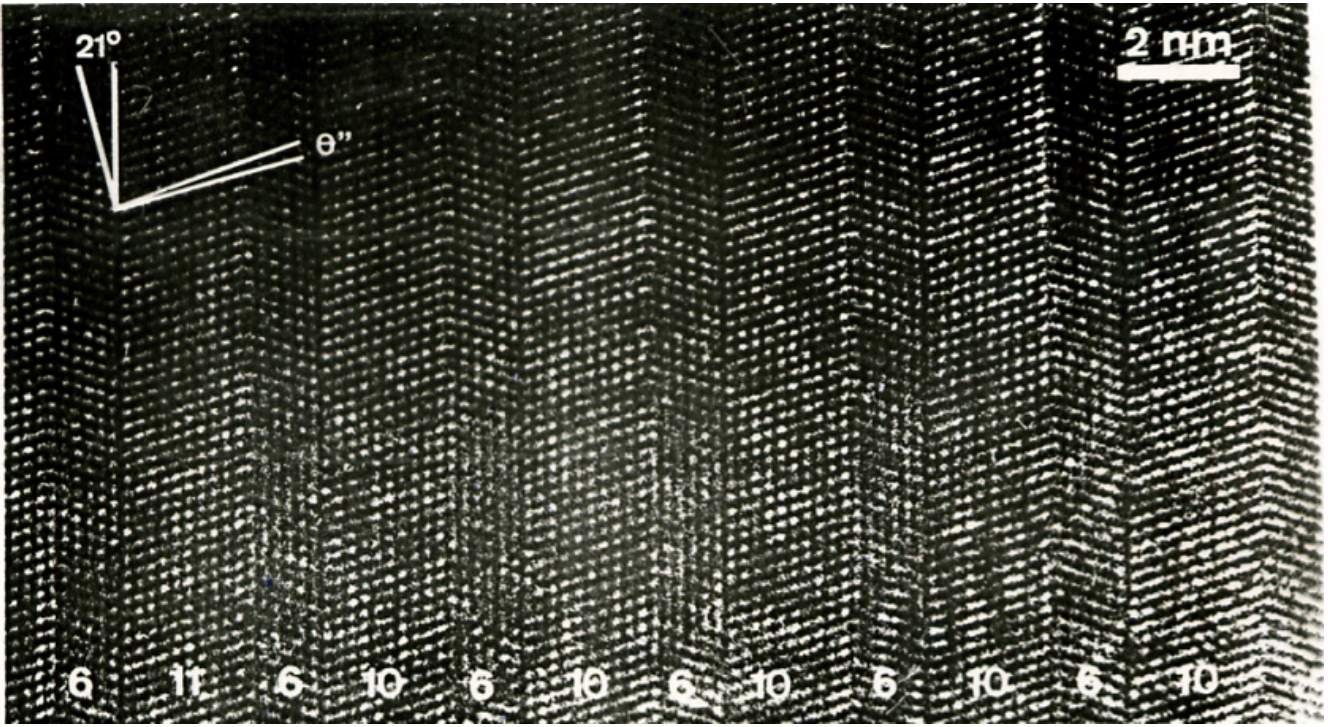


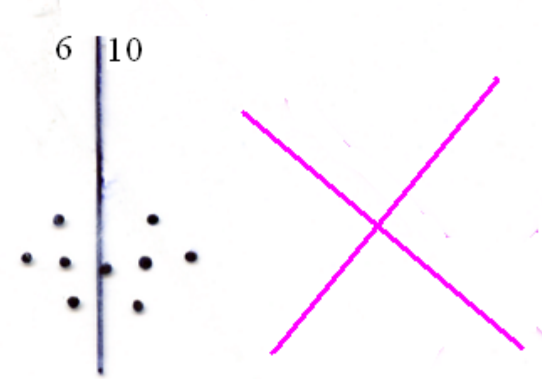
$$\mathbf{U}(\theta) = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \alpha = \alpha(\theta) > 0, \beta = \beta(\theta) > 0, \; \gamma = \gamma(\theta) > 0$$

$M = 6$

$$\mathbf{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \mathbf{U}_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad \mathbf{U}_3 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix},$$

$$\mathbf{U}_4 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\gamma-\alpha}{2} \\ 0 & \beta & 0 \\ \frac{\gamma-\alpha}{2} & 0 & \frac{\alpha+\gamma}{2} \end{pmatrix}, \quad \mathbf{U}_5 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} \\ 0 & \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}, \quad \mathbf{U}_6 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} \\ 0 & \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} \end{pmatrix}.$$

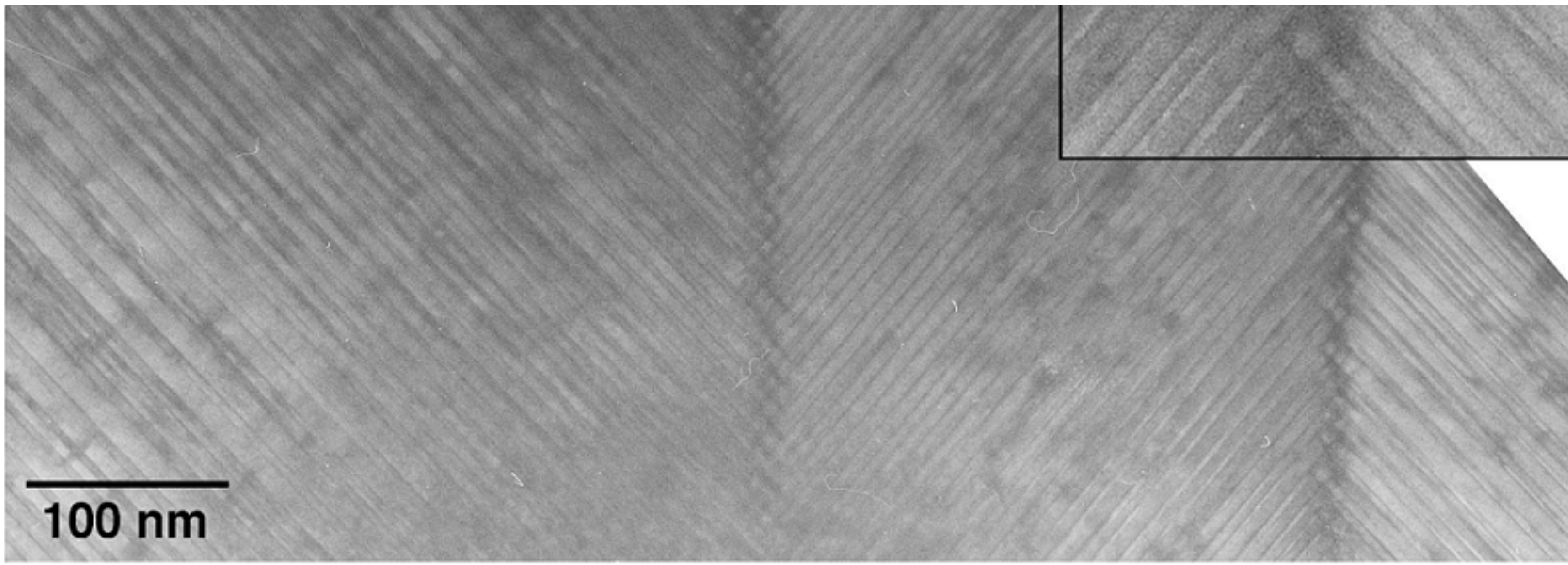




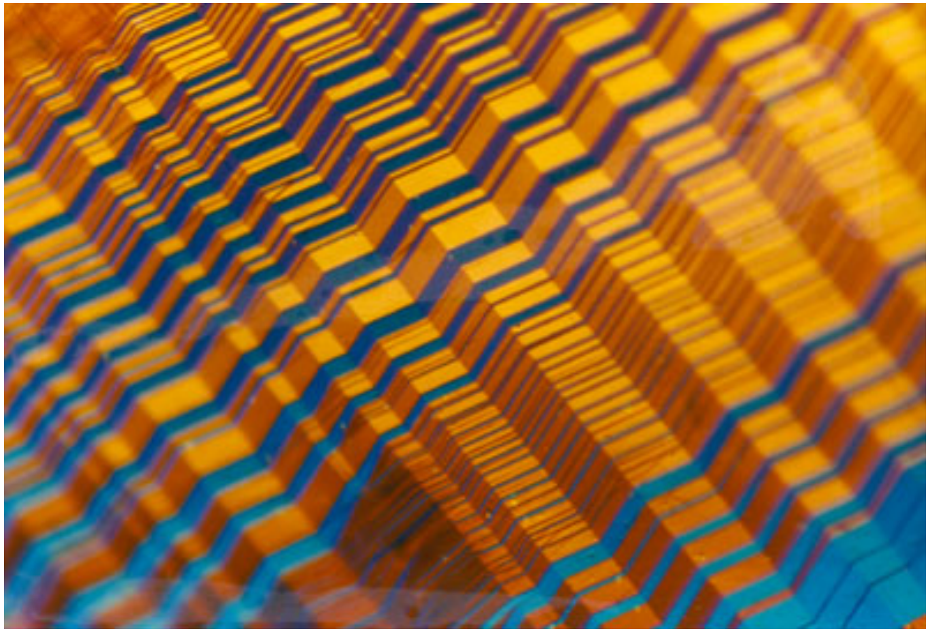
Atomistically sharp interfaces for cubic to tetragonal transformation in NiMn

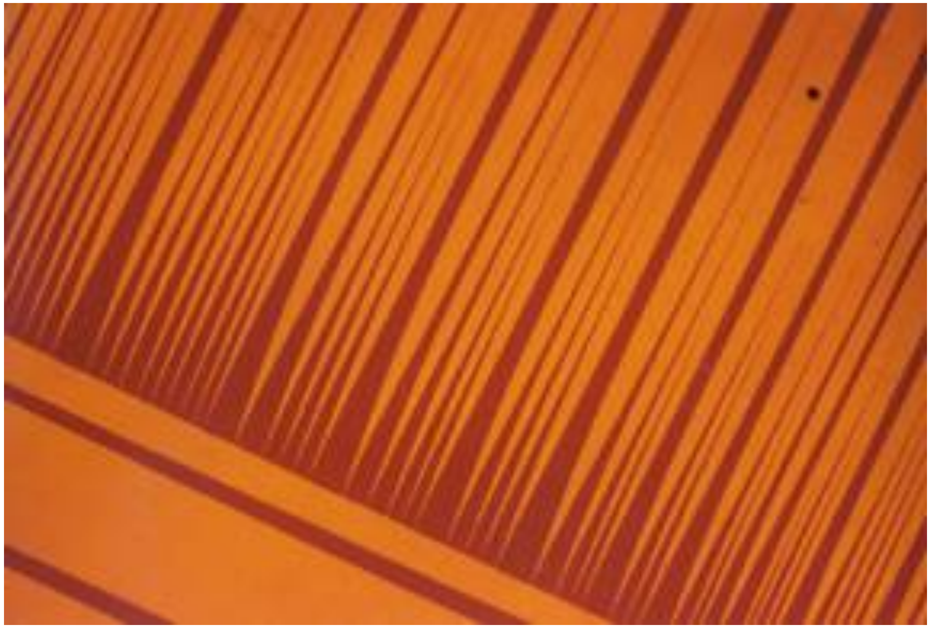
Baele, van Tenderloo, Amelinckx

Macrotwins in $Ni_{65}Al_{35}$ involving two tetragonal variants (Boullay/Schryvers)



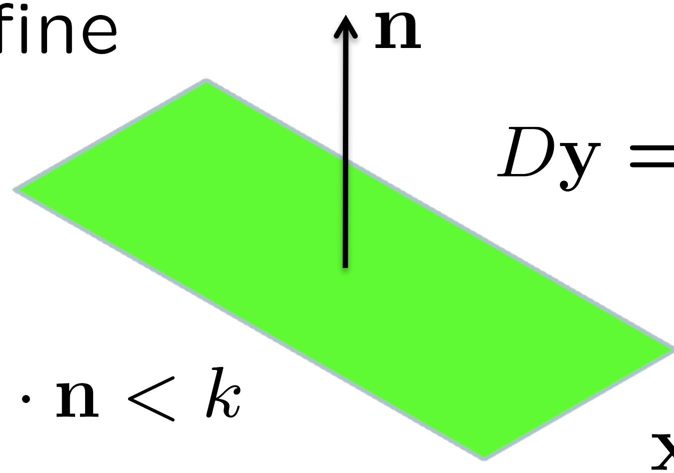
Martensitic microstructures in CuAlNi (Chu/James)





The Hadamard jump condition

$\mathbf{y}$ piecewise affine



Let $\mathbf{C} = \mathbf{A} - \mathbf{B}$. Then $\mathbf{C}\mathbf{x} = \mathbf{0}$ if $\mathbf{x}\cdot\mathbf{n} = 0$. Thus $\mathbf{C}(\mathbf{z} - (\mathbf{z}\cdot\mathbf{n})\mathbf{n}) = \mathbf{0}$ for all $\mathbf{z}$, and so $\mathbf{C}\mathbf{z} = (\mathbf{C}\mathbf{n}\otimes\mathbf{n})\mathbf{z}$.

Hence $$\boxed{\mathbf{A} - \mathbf{B} = \mathbf{a}\otimes\mathbf{n}}$$ Hadamard jump condition