The case of two wells

We take

$$K = SO(3)\mathbf{U}_1 \cup SO(3)\mathbf{U}_2,$$

$$\mathbf{U}_1 = \mathrm{diag}\,(\eta_1, \eta_2, \eta_3), \quad \mathbf{U}_2 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_3),$$

and $\eta_2 > \eta_1 > 0$, $\eta_3 > 0$ (e.g. tetragonal to orthorhombic, or special orthorhombic to monoclinic transformations).

The advantage of this case is that it is the only one for which K^{qc} is known.

Theorem (B/James 92) K^{qc} consists of the matrices $\mathbf{A} \in GL^{+}(3, \mathbb{R})$ such that

$$\mathbf{A}^T\mathbf{A} = \begin{pmatrix} a & c & 0 \\ c & b & 0 \\ 0 & 0 & \eta_3^2 \end{pmatrix},$$

where $a > 0, b > 0, a + b + |2c| \leq \eta_1^2 + \eta_2^2,\ ab - c^2 = \eta_1^2\eta_2^2$.

In addition (B/James 91), if $D\mathbf{y}(\mathbf{x}) \in K^{\mathrm{qc}}$ a.e. then $\mathbf{y}$ is a plane strain, i.e.

$$\mathbf{y}(\mathbf{x}) = \mathbf{Q}(y_1(\mathbf{x}), y_2(\mathbf{x}), \eta_3 x_3 + a),$$

where $y_{1,3} = y_{2,3} = 0,\ \mathbf{Q} \in SO(3)$ and $a \in \mathbb{R}$.

Theorem

$$\mathcal{E} = \begin{cases} \emptyset & \text{if } \eta_3 \neq \sqrt{\eta_1 \eta_2} \\ SO(3)\eta_3 & \text{if } \eta_3 = \sqrt{\eta_1 \eta_2} \end{cases}$$

Proof. Suppose $\mathbf{D} = \text{diag}\,(d_1, d_2, d_3) \in \mathcal{E}$. Then for any $\mathbf{R} \in SO(3)$ we have $\mathbf{DR} \in \mathcal{E}$, and so there exist a, b, c with $a > 0$, $b > 0$, $ab - c^2 = \eta_1^2 \eta_2^2$, $a + b + |2c| \leq \eta_1^2 + \eta_2^2$ and

$$\begin{pmatrix} a & c & 0 \\ c & b & 0 \\ 0 & 0 & \eta_3^2 \end{pmatrix} = \mathbf{R} \begin{pmatrix} d_1^2 & 0 & 0 \\ 0 & d_2^2 & 0 \\ 0 & 0 & d_3^2 \end{pmatrix} \mathbf{R}^T.$$

Hence $d_1 = d_2 = d_3 = \eta_3$ and both sides equal $\eta_3^2 \mathbf{1}$, so that we must have $a = b = \eta_3^2, c = 0$. Thus $\eta_3 = \sqrt{\eta_1 \eta_2}$, when indeed $2\eta_3^2 + 0 \leq \eta_1^2 + \eta_2^2$.

(For particular grain geometries and rotations there could be additional zero-energy microstructures.)

Now consider the set

$$\mathcal{E}_{2D} = \bigcap_{\mathbf{R}\in SO(3),\, \mathbf{R}\mathbf{e}_3 = \pm\mathbf{e}_3} K^{qc}\mathbf{R}.$$

Theorem

$\mathbf{A} \in \mathcal{E}_{2D}$ iff $\mathbf{A} = \mathbf{R}\mathbf{D}\tilde{\mathbf{R}}$, where $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$, $\tilde{\mathbf{R}}\mathbf{e}_3 = \pm\mathbf{e}_3$,

$$\mathbf{D} = \begin{pmatrix} v_1 & 0 & 0 \\ 0 & v_2 & 0 \\ 0 & 0 & \eta_3 \end{pmatrix},$$

and $v_1 > 0, v_2 > 0$, $v_1 v_2 = \eta_1\eta_2$, $|v_i| \le \sqrt{\frac{\eta_1^2+\eta_2^2}{2}}$.

(See Kohn & Niethammer (2000) and the book of Dolzmann (2003).)

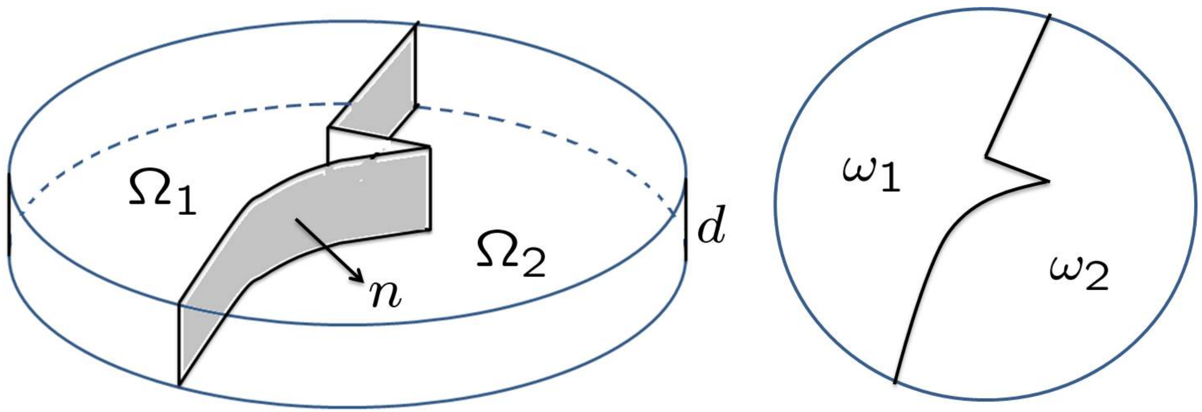
There are nontrivial deformations $\mathbf{y}$ with $D\mathbf{y}(\mathbf{x}) \in \mathcal{E}_{2D}$ a.e. $\mathbf{x} \in \Omega$, such as

$$\mathbf{y}(\mathbf{x}) = (\sqrt{\eta_1\eta_2}\,x_1, \sqrt{\eta_1\eta_2}\,x_2, \eta_3 x_3) + \varepsilon g(\mathbf{x}\cdot\mathbf{e}^{\perp})\mathbf{e},$$

where $|\mathbf{e}| = |\mathbf{e}^{\perp}| = 1, \mathbf{e}^{\perp}\cdot\mathbf{e} = \mathbf{e}\cdot\mathbf{e}_3 = 0$, $|g'| \le M < \infty$ and $|\varepsilon|$ sufficiently small.

Such deformations nontrivially deform the grain boundaries (it would be interesting to have experimental results on grain boundary deformation resulting from martensitic transformations).

Zero-energy microstructures for a bicrystal



Energy wells $K = \mathrm{SO}(3)\mathbf{U}_1 \cup \mathrm{SO}(3)\mathbf{U}_2$

$\mathbf{U}_1 = \mathrm{diag}\,(\eta_2, \eta_1, \eta_3), \mathbf{U}_2 = \mathrm{diag}\,(\eta_1, \eta_2, \eta_3),$

$\eta_2 > \eta_1 > 0, \eta_3 > 0$

Grain 1

$\Omega_1 = \omega_1 \times (0, d)$

$\mathrm{supp}\,\nu_x \subset K$ a.e. $x \in \Omega_1$

Grain 2

$\Omega_2 = \omega_2 \times (0, d)$

$\mathrm{supp}\,\nu_{\mathbf{x}} \subset K\mathbf{R}(\alpha)$ a.e. $\mathbf{x} \in \Omega_2$

$\mathbf{R}(\alpha)\mathbf{e}_3 = \mathbf{e}_3$

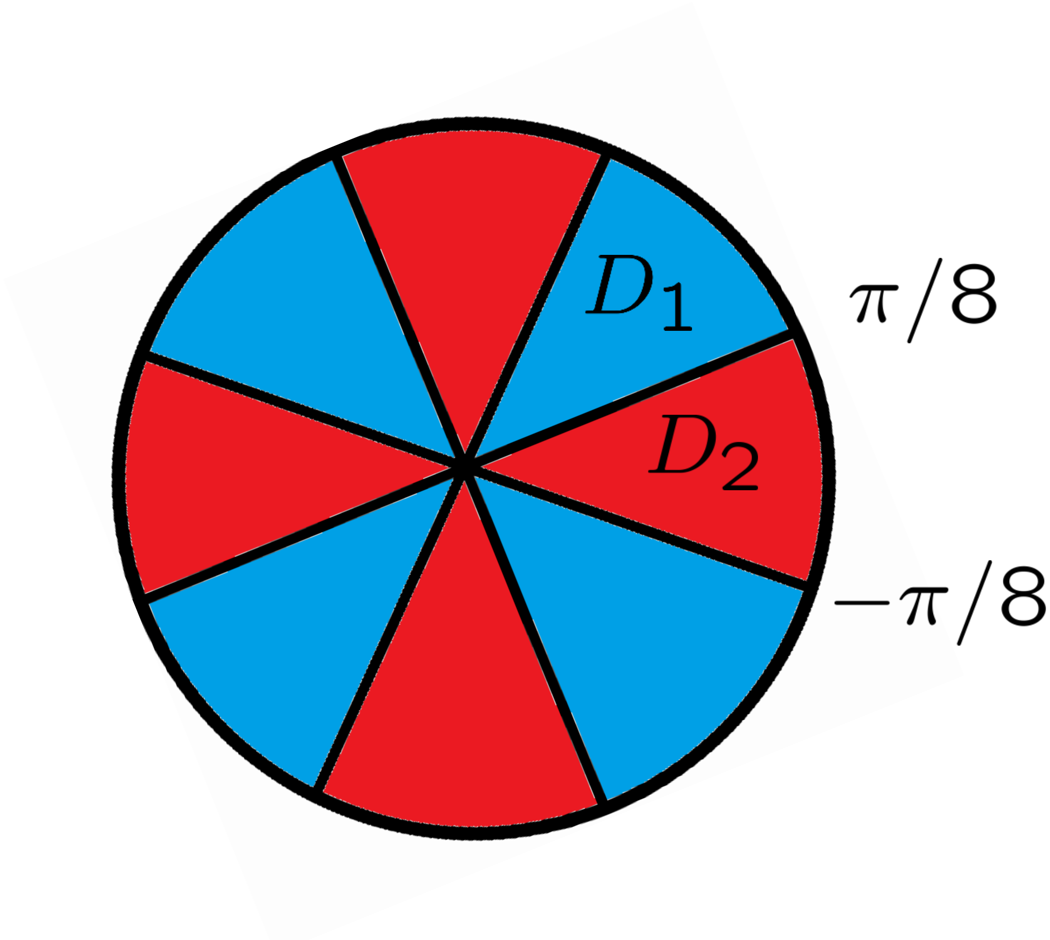
Question: Is it true that every zero-energy microstructure is nontrivial (i.e. not a pure phase $\nu_{\mathbf{x}} = \delta_{\mathbf{A}}$) in each of the grains?

(If the interface between the grains were not vertical, so that it had the form $x_3 = g(x_1, x_2)$ for some open set of (x_1, x_2), we cannot have a pure phase in one of the grains because a short calculation shows that it violates the microstructure being a plane strain in the other grain.)

Result 1. If the interface is *planar* then whatever its normal n there always exists a zero-energy microstructure which has a pure phase (i.e. $\nu_{\mathbf{x}} = \delta_{\mathbf{A}}$) in one of the grains.

Therefore the interface needs to be curved in order to show that the microstructure has to be nontrivial. Write the normal to the interface as $\mathbf{n} = (\cos\theta, \sin\theta, 0)$.

Result 2. Suppose that $\alpha = \pi/4$. Then it is impossible to have a zero-energy microstructure with a pure phase in one of the grains if the boundary between the grains contains a normal with $\theta \in D_1$ and another normal with $\theta' \in D_2$.



Proofs use:

1. A reduction to 2D using the plane strain result for the two-well problem.

2. The characterization of the quasiconvex hull of two wells.

3. Use of a *generalized Hadamard jump condition* in 2D to show that there has to be a rank-one connection $\mathbf{b} \otimes \mathbf{N}$ between the polyconvex hulls for each grain.

4. Long and detailed calculations.

For the details see, JB & C. Carstensen, *Interaction of martensitic microstructures in adjacent grains*, ICOMAT 2017 Proceedings.