Another possibility is to take $\boldsymbol{\mu} = \mathbf{1} + \mathbf{P} \otimes \mathbf{Q}$ with $\mathbf{P} \cdot \mathbf{Q} = 0$, when we have $\mathbf{M} = \mathbf{1} + \mathbf{BP} \otimes \mathbf{B}^{-T}\mathbf{Q}$ and

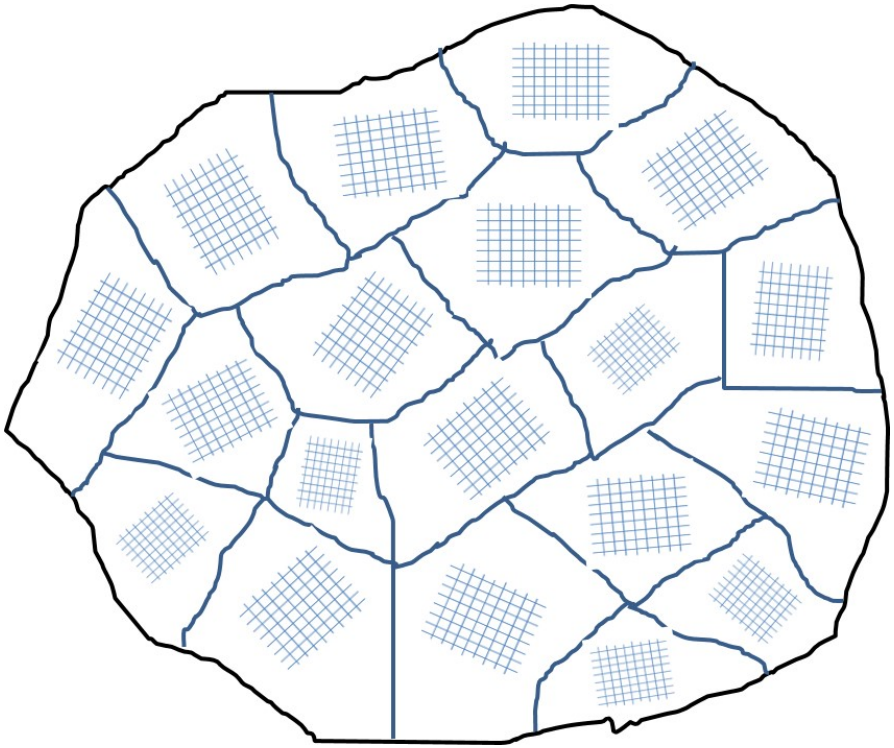
$$\begin{aligned}
\mathbf{M}^T\mathbf{M} - \mathbf{1} &= \mathbf{B}^{-T}\mathbf{Q} \otimes \mathbf{BP} + \mathbf{BP} \otimes \mathbf{B}^{-T}\mathbf{Q} + |\mathbf{BP}|^2 \mathbf{B}^{-T}\mathbf{Q} \otimes \mathbf{B}^{-T}\mathbf{Q} \\
&= (\mathbf{BP} + \frac{1}{2}|\mathbf{BP}|^2 \mathbf{B}^{-T}\mathbf{Q}) \otimes \mathbf{B}^{-T}\mathbf{Q} \\
&\qquad + \mathbf{B}^{-T}\mathbf{Q} \otimes (\mathbf{BP} + \frac{1}{2}|\mathbf{BP}|^2 \mathbf{B}^{-T}\mathbf{Q}),
\end{aligned}$$

so that again $SO(3)$ and $SO(3)\mathbf{M}$ are rank-one connected with normals $\mathbf{B}^{-T}\mathbf{Q}$ and $\mathbf{BP} + \frac{1}{2}|\mathbf{BP}|^2 \mathbf{B}^{-T}\mathbf{Q}$ and $|\mathbf{a}|^2 = |\mathbf{Bp}|^2 |\mathbf{B}^{-T}\mathbf{q}|^2$.

For bcc with $\mathbf{P} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$, $\mathbf{Q} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, we get the normals $\begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix}$ (twinning), $\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$ (slip) with $|\mathbf{a}|^2 = 2$.

Polycrystals

Different orientations of the crystal lattice in each grain.



No diffusion, within the grains, or of the grain boundaries.

Description of grain geometry

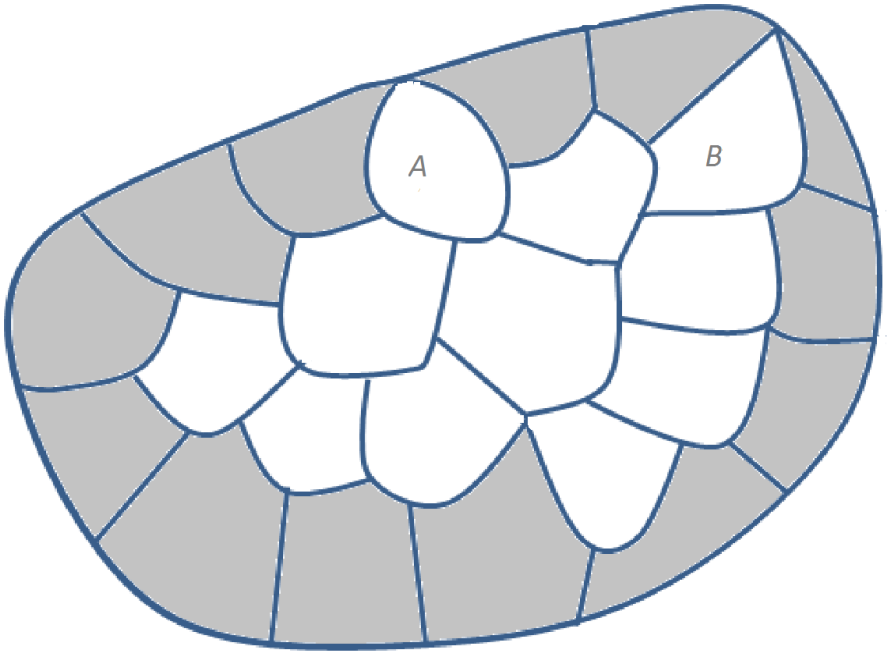
Consider a polycrystal that occupies in a reference configuration a bounded domain (open, connected set) $\Omega \subset \mathbb{R}^3$ composed of a finite number of disjoint grains Ω_j, $j = 1, \ldots, N$, where each Ω_j is a bounded domain with Lipschitz boundary $\partial\Omega_j$, so that

$$\Omega = \text{int} \bigcup_{i=1}^{N} \overline{\Omega}_j.$$

Topology and graphs

Some topological information is encoded in the graph whose vertices are the grains (labelled $1, \ldots, N$) and with edges (i, j) corresponding to grains Ω_i, Ω_j with $\mathcal{H}^2(\partial\Omega_i \cap \partial\Omega_j) > 0$ (in 2D this is used in the proof of the four colour theorem).

For each grain i let $M(i)$ be the number of $j \neq i$ for which (i, j) is an edge.



A and B are interior grains but touch $\partial\Omega$.

Interior grains are ones for which $\partial\Omega_j \subset \bigcup_{k\neq j} \partial\Omega_k$, and the others are *boundary* grains.

The set of *triple points* is

$$T = \bigcup_{1\leq i_1<i_2<i_3\leq N} \partial\Omega_{i_1} \cap \partial\Omega_{i_2} \cap \partial\Omega_{i_3}.$$

Theorem Suppose each grain Ω_j is convex. Then every interior grain Ω_i is a convex polyhedron (i.e. an intersection of a finite number of open half-spaces) with at most $M(i)$ faces.

Theorem If each $\overline{\Omega}_j$ is a topological manifold with boundary then T is nowhere dense in $\bigcup_{j=1}^{N} \partial\Omega_j$.

Zero-energy microstructures for a polycrystal

For a polycrystal the total free energy is given by

$$I(\mathbf{y}) = \int_\Omega W(D\mathbf{y}(\mathbf{x}), \mathbf{x})\, d\mathbf{x},$$

where $W(\mathbf{A}, \mathbf{x}) = \psi(\mathbf{A}\mathbf{R}_i^T)$ for $\mathbf{x} \in \Omega_i$ and $\mathbf{R}_i \in SO(3)$.

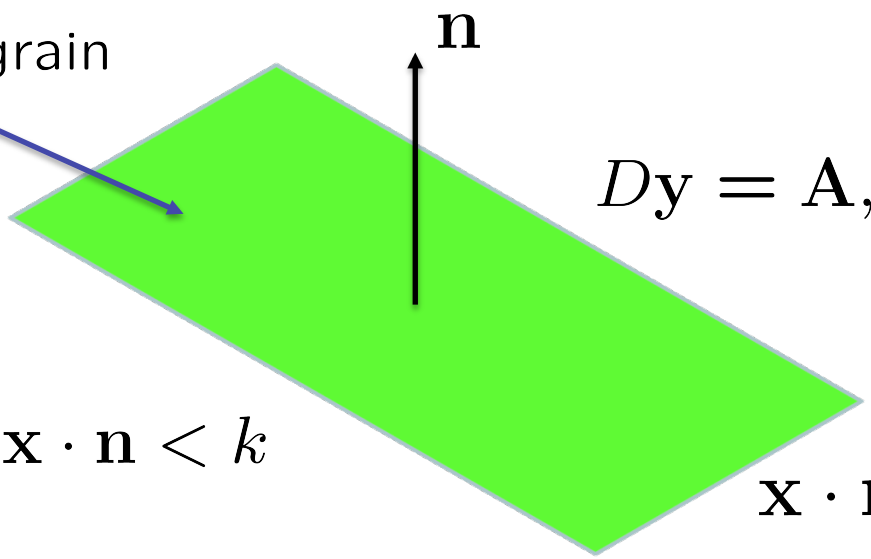
We fix $\theta < \theta_c$ and write $K = K(\theta)$, $\mathbf{U} = \mathbf{U}(\theta)$ etc.

Then a zero-energy microstructure corresponds to a gradient YM $(\nu_\mathbf{x})_{\mathbf{x}\in\Omega}$ with $\operatorname{supp} \nu_\mathbf{x} \subset K\mathbf{R}_i$ for a.e. $\mathbf{x} \in \Omega_i$, or equivalently to a macroscopic deformation gradient with

$$D\mathbf{y}(\mathbf{x}) \in (K\mathbf{R}_i)^{\mathrm{qc}} = K^{\mathrm{qc}}\mathbf{R}_i$$

for a.e. $\mathbf{x} \in \Omega_i$.

Constant deformation gradient in adjacent grains



We can assume that grain 1 has unrotated crystal axes. Hence for this to be a zero-energy deformation $\mathbf{A} = \mathbf{Q_1}\mathbf{U_i}$, $\mathbf{B} = \mathbf{Q_2}\mathbf{U_j}\tilde{\mathbf{R}}$, where $\mathbf{Q_1}, \mathbf{Q_2} \in SO(3)$ and $\tilde{\mathbf{R}} \in SO(3)$ is the rotation of grain 2.

For a rank-one connection we must have

$$\det(\mathbf{U_i^2} - \tilde{\mathbf{R}}^{\mathbf{T}}\mathbf{U_i^2}\tilde{\mathbf{R}}) = 0.$$

The function

$$\mathbf{R} \mapsto \det(\mathbf{U_i^2} - \mathbf{R}^{\mathbf{T}}\mathbf{U_i^2}\mathbf{R})$$

is real analytic on $SO(3)$ and for $\mathbf{U}_i$ not a multiple of $\mathbf{1}$ is not identically zero. Hence (c.f. Mityagin 2015) its zero set is of measure zero. Thus for generic grain rotations such a zero-energy deformation is impossible.

Zero-energy microstructures possible for any grain geometry and rotations

These correspond to gradient YMs $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ such that $\operatorname{supp}\nu_{\mathbf{x}} \subset \bigcap_{\mathbf{R}\in SO(3)} K\mathbf{R}$ a.e., or equivalently to macroscopic deformation gradients satisfying

$$D\mathbf{y}(\mathbf{x}) \in \mathcal{E} := \bigcap_{\mathbf{R}\in SO(3)} K^{\mathrm{qc}}\mathbf{R} \text{ for a.e. } \mathbf{x}\in\Omega.$$

The set $\mathcal{E}$ was essentially defined in Bhattacharya & Kohn (1996,1997) in connection with the 'Taylor bound'.

Note that $\mathcal{E}$ is *isotropic*, i.e.

$$\mathbf{Q}\mathcal{E}\mathbf{R} = \mathcal{E} \text{ for all } \mathbf{Q},\mathbf{R}\in SO(3).$$