Dislocation distributions at positive temperature

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Structure

1. Ariza-Ortiz model
2. Dislocations and grain boundaries
3. Read-Shockley law
4. Positive temperature and order

Motivation for the Ariza-Oritz model

- Simulation of large scale atomistic models is hard: Grains, plasticity, cracks, temperature etc
- Bottlenecks: Parametrisation and computation
- The Ariza-Ortiz model has a natural representation of grains and plastic slips and is computationally cheap.

The Ariza-Ortiz model

Reference configuration: Face-centered cubic lattice

$$\mathcal{L} = \{n_1 b_1 + n_2 b_2 + n_3 b_3 \ : \ n \in \mathbb{Z}^3\}$$

$$\text{where } b_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, b_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, b_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

Nearest neighbors: $x \sim y$ if $x, y \in \mathcal{L}$ and $|x - y| = 1$,

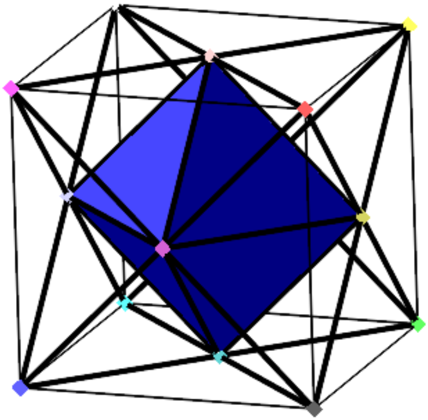
Displacement: $u(x) \in \mathbb{R}^3, \ x \in \mathcal{L}$,

Slip: $\sigma(x, y), \ x \sim y$,

Energy:

$$H_{\mathrm{AO}}(u, \sigma) = \frac{1}{2} \sum_{x \sim y} [(u(y) - u(x) - \sigma(x, y)) \cdot (y - x)]^2.$$

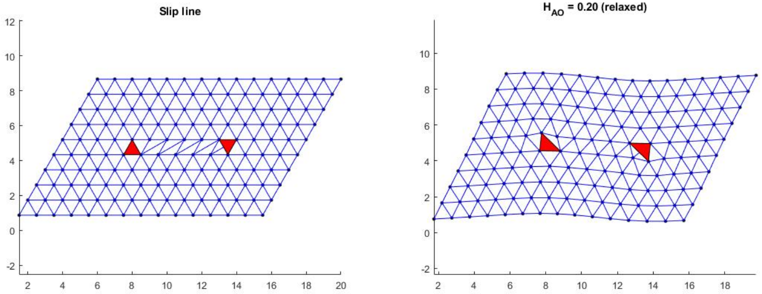
Cubic structure of fcc



Point particle configurations

$$\mathcal{C} = \{x + u(x) \ : \ x \in \mathcal{L}\}$$

Example: Dislocation dipole



Left: Unrelaxed dislocation dipole. Right: Relaxed dipole.
Warning: Picture misleading because bonds not determined by σ.

Continuum version

$$H_{\mathrm{cont}}(u,\sigma) = \frac{1}{2}\int_\Omega \mathbb{C}(\nabla u + \sigma) : (\nabla u + \sigma)\,\mathrm{d}x$$

with $\mathbb{C} \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ elastic tensor, $u \in H^1(\Omega, \mathbb{R}^d)$, $\sigma \in L^2(\Omega, \mathbb{R}^{d\times d})$.

Core radius approach: Cermelli-Leoni (2005), Garroni-Leoni-Ponsiglione (2010), DeLuca-Garroni-Ponsiglione (2012), ...

Continuum approach struggles with grains, grain boundary energy, Read-Shockley formula

Symmetries

Translation

$$H_{\mathrm{AO}}(u+s,\sigma) = H_{\mathrm{AO}}(u,\sigma)$$

if s is constant.

Linearised rotation

$$H_{\mathrm{AO}}(u+s,\sigma) = H_{\mathrm{AO}}(u,\sigma)$$

if $s(x) = S\,x$ for some skew-symmetric matrix $S \in \mathbb{R}^{3\times 3}$.

Gauge invariance

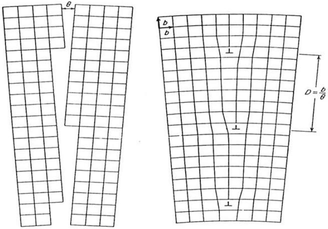
$$H_{\mathrm{AO}}(u+v,\sigma+\mathrm{d}v) = H_{\mathrm{AO}}(u,\sigma)$$

for all $v : \mathcal{L} \to \mathcal{L}$ where $\mathrm{d}v(x,y) = v(x) - v(y)$.

Linearised rotations account for Euclidean invariance.

Low energy structures: Grains (Materials Sciences perspective)

Grain boundaries can be seen as walls of edge dislocations with the same Burgers vector.



Low energy structures: Grains (Ariza-Ortiz perspective)

Definition

(u, σ) supports a 'perfect grain' $\mathcal{G} \subset \mathcal{L}$ with orientation $S \in \mathbb{R}^{3\times 3}_{\mathrm{skew}}$

$$u(x) - u(y) - \sigma(x, y) = \begin{cases} S(x-y) & \text{if } \{x, y\} \subset \mathcal{G}, \\ 0 & \text{if } \{x, y\} \subset \mathcal{G}^c, \end{cases}$$

$$\sigma(x, y) = 0 \text{ if } x \sim y \text{ and } \{x, y\} \subset \mathcal{G}^c.$$

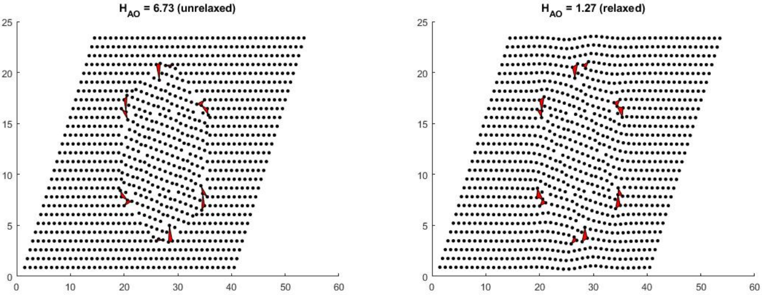
Energy cost of a grain is **not** automatically proportional to **volume** of grain thanks to the invariance under linearized rotations.

Theorem (Upper bound)

$$\min\{H(u, \sigma) \ : \ (u, \sigma) \textit{ support perfect grain } \mathcal{G} \textit{ with orientation } S\} \leq |\partial \mathcal{G}|.$$

The minimum energy is bounded by the size of the grain **boundary**.

Visualization

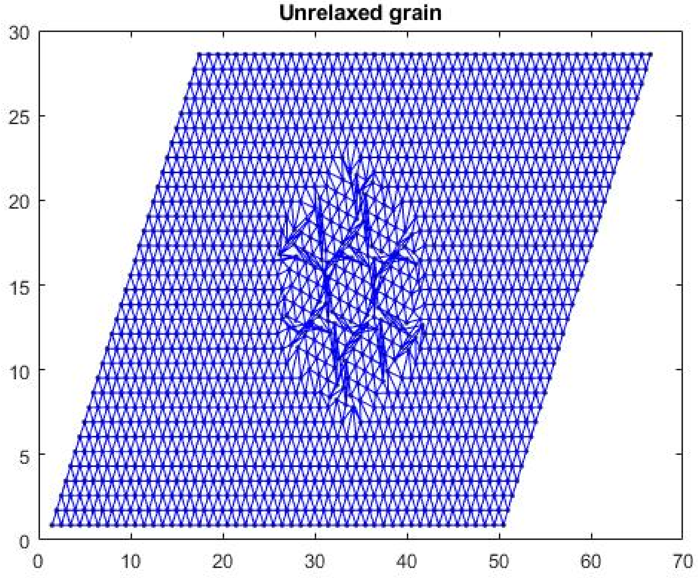


Left: Displacement u with $S = \frac{1}{5}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

Right: Relaxed displacement field u_σ which minimizes $H_{\mathrm{AO}}(\cdot, \sigma)$ subject to Neumann boundary conditions.

Colored triangles indicate the support of $\mathrm{d}\sigma$.

Visualisation of unrelaxed grain with slips



Construction of upper bound

Particularly simple examples of lattice invariance are shear bands:

$$u(x) = f(x \cdot m)\, b$$

with

- $b \in \mathcal{L}$ Burger's vector
- $m \in \mathbb{R}^3$ slip plane normal, satisfies $b \cdot m = 0$.

The pairs (b, m) are called slip systems. There are 12 slip systems and 4 slip planes in fcc:

$$m_1 = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix},\ m_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix},\ m_3 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, m_4 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Construct u and σ (I)

Decomposition of linearised rotation into shear bands.

$$S = \begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix} \quad = \quad b_1 \otimes m_2 - b_2 \otimes m_1 - b_6 \otimes m_4$$

with

$$b_1 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, b_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \; b_6 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

Construct u and σ (II)

$$\varphi(x) = \mathbf{1}_{\mathcal{G}}(x)\left(\lfloor x \cdot m_2 \rfloor b_1 - \lfloor x \cdot m_1 \rfloor b_2 - \lfloor x \cdot m_4 \rfloor b_6 - Sx\right)$$

Observe that $\|\varphi\|_\infty < C$ *independently* of grain size.

$$\sigma(x,y) = \begin{cases} \varphi(x) - \varphi(y) & \text{if } x, y \in \mathcal{G}, \\ 0 & \text{else.} \end{cases},$$

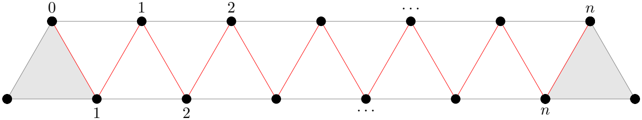
$$u(x) = \mathbf{1}_{\mathcal{G}}(x)\left[S(x - x_{\mathrm{center}}) + \varphi(x)\right]$$

Energy density of dislocation configurations (2 dim)

Dislocation dipole

$$q^n_{\mathrm{dip}} \quad = \quad (\mathbf{1}_{f_0} - \mathbf{1}_{f_n})\, b_1 \tag{1}$$

with $b_1 = \binom{1}{0}$, $b_3 = -\frac{1}{2}\binom{1}{\sqrt{3}}$ and $f_n = (0, b_1, -b_3) + nb_1$.



Shaded triangles, corresponding to faces f_0 and f_n, indicate the support of q^n_{dip}. In red: the support of a slip field σ^n_{dip} such that $\mathrm{d}\sigma^n_{\mathrm{dip}} = q^n_{\mathrm{dip}}$.

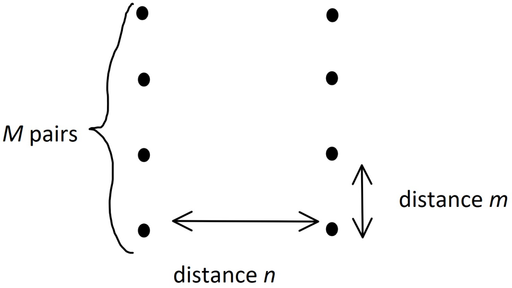
Exterior calculus notation:

$$\begin{aligned} \mathrm{d}u(x,y) &= u(x) - u(y), \\ \mathrm{d}\sigma(x,y,z) &= \sigma(x,y) + \sigma(y,z) + \sigma(z,x). \end{aligned}$$

Dislocation configurations cont'd

Dislocation wall

$$q_{\mathrm{grain}}^{M,n,m}(f) = \sum_{j=1}^{M} q_{\mathrm{dip}}^{n}(f - jm(b_2 - b_3)).$$



Number of dislocation pairs: M
Distance between dislocation cores with same (different) signs: m (n).

Energy of dipoles and walls

Theorem

$$
\begin{aligned}
E_{\rm dip}(n) &= \min\left\{H_{AO}(u,\sigma)\ :\ {\rm d}\sigma = q_{\rm dip}^{n}\right\} = \frac{\log n}{2\pi\sqrt{3}} + O(1), \quad n \gg 1,\\
E_{\rm grain}(n,m) &= \lim_{M\to\infty} \frac{1}{\sqrt{3}mM} \min\left\{H_{\rm AO}(u,\sigma)\ :\ {\rm d}\sigma = q_{\rm grain}^{M,n,m}\right\}\\
&= \frac{\log m}{6\pi m} + O(1/m), \quad m \gg 1.
\end{aligned}
$$

Energy of dipole grows **logarithmically** with distance. Energy of wall is **proportional** to length of wall and **independent** of distance.

Read-Shockley law: $\gamma(\theta) = (c_0 - c_1 \log\theta)\theta + o(\theta), \quad 0 < \theta <\ll 1,$
γ_s is the grain boundary energy density θ is the orientation difference.

Capacitor law

Compare with version of energy **not** invariant under linearized rotations.

$$\mathcal{E}[q] = \frac{1}{2}\min_{(u,\sigma)}\left\{|\mathrm{d}u-\sigma|^2 \;:\; \mathrm{d}\sigma = q\right\} = \frac{1}{2}\min_{v}\left\{|v|^2 \;:\; \mathrm{d}v = q\right\},$$

Theorem

$$\begin{aligned} \mathcal{E}[q^n_{\mathrm{dip}}] &= \frac{\sqrt{3}}{2\pi}\log n + O(1), && n \gg 1, \\ \lim_{M\to\infty}\frac{1}{M}\mathcal{E}[q^{M,n,m}_{\mathrm{grain}}] &= \frac{n}{2m} + O(1), && n \gg 1. \end{aligned}$$

- Recall from Physics: Energy of two capacitor plates is **proportional** to the distance.
- Invariance under linearized rotations affects scaling of energy minima significantly.

Random dislocation configurations

- Recall gauge invariance

$$H_{\mathrm{AO}}(u+v,\sigma+\mathrm{d}v) = H_{\mathrm{AO}}(u,\sigma) \text{ for all } v:\mathcal{L}\to\mathcal{L}.$$

- Slips σ and σ' are gauge equivalent if $\sigma-\sigma' = \mathrm{d}v$ for some v.
- $\mathcal{S}$ are representatives of non-equivalent slip fields.
- Boltzmann-Gibbs distribution

$$\mathbb{P}_\beta(u,\sigma) = \frac{1}{Z(\beta)}\exp(-\beta\,(H_{\mathrm{AO}}(u,\sigma)+w(\mathrm{d}\sigma)))$$

- Partition sum

$$Z(\beta) = \sum_{\sigma\in\mathcal{S}} \exp(-\beta\, w(\mathrm{d}\sigma)) \int \exp(-\beta\, H_{\mathrm{AO}}(u,\sigma))\,\mathrm{d}u.$$

- Exterior derivative

$$\mathrm{d}\sigma(x,y,z) = \sigma(x,y)+\sigma(y,z)+\sigma(z,x).$$

Existence of order at low temperatures

Quantify long-range order by observable

$$c_\beta(v_0; x, y) := \mathbb{E}_\beta(\cos([u(y) - u(x)] \cdot v_0)).$$

Theorem

There are positive constants C, β_0 such that

$$c_\beta(x, y; v_0) \geq e^{-C/\beta}\Big(1 + O\big(\tfrac{\log|x-y|}{|x-y|}\big)\Big), \qquad |x-y| \gg 1$$

if $v_0 \in \mathcal{L}^*$ and $\beta > \beta_0$.

Weaker notion of order: Orientational order (relevant in 2 dimensions)

$$c_\beta(v_0, h; x, y) := \mathbb{E}_\beta(\cos([u(x+h) - u(x) - u(y+h) + u(y)] \cdot v_0)).$$

Previous work

- Fröhlich and Spencer (CMP 1982) obtained similar results for the rotator models in three dimensions.
- In the two dimensional case (Fröhlich-Spencer 1981) only orientational order is present. The proof is harder (renormalisation group).
- Orientational order has been established in a mesoscopic version of the Ariza-Ortiz model by Bauerschmidt, Conache, Heydenreich, Merkl and Rolles (AHP 2019)

The key difference between earlier results by Fröhlich and Spencer and the current results is the invariance with respect to linearized rotations.

Decompose energy into elastic and dislocation energy

Recall

$$H_{\mathrm{AO}}(u,\sigma) = \frac{1}{2}\langle \mathrm{d}u - \sigma, B(\mathrm{d}u - \sigma)\rangle.$$

Let $q \in \Omega_2^*$ be the Burgers field such that $\mathrm{d}q = 0$ and

$$\sigma_q = \mathrm{argmin}\{H(0,\sigma) \ : \ \mathrm{d}\sigma = q\}, \quad u_q = \mathrm{argmin}_u H(u,\sigma_q),$$

then

$$H_{\mathrm{AO}}(u,\sigma) = H_{\mathrm{AO}}(u-u_q,0) + H_{\mathrm{AO}}(0,\sigma_q).$$

Hence $\mathbb{P}_\beta$ is a product distribution:

$$\mathbb{P}_\beta(u,\sigma) = \frac{\exp(-\beta\, H(u-u_q,0))}{Z_{\mathrm{el}}(\beta)} \times \frac{\exp(-\beta\,(H(0,\sigma_q) + w(\mathrm{d}\sigma)))}{Z_{\mathrm{disl}}(\beta)}.$$

Elastic fluctuations (spin waves)

Recall

$$c = \mathbb{E}_\beta(\exp(i\langle u, g\rangle))$$

for some $g \in \Omega_0$.
Choose $\mathrm{d}^* h = g$, then

$$\begin{aligned}
\mathbb{E}_\beta(\exp(i\langle u, g\rangle)) &= \mathbb{E}_\beta(\exp(i\langle u, \mathrm{d}^* h\rangle)) = \mathbb{E}_\beta(\exp(i\langle \mathrm{d}u, h\rangle)) \\
&= \mathbb{E}_\beta(\exp(i\langle u - u_q, g\rangle)) \times \mathbb{E}_\beta(\exp(-i\langle \sigma_q, h\rangle)
\end{aligned}$$

Fourier coefficient of a continuous and a discrete Gaussian measure.
Recall:

$$\int \exp(-\langle x, Ax\rangle) \cos(\langle k, x\rangle) \,\mathrm{d}x = \left(\frac{\pi}{|A|}\right)^{\frac{1}{2}} \exp(-\pi^2\langle k, A^{-1}k\rangle).$$

In our setting: A^{-1} is the Green's function. In three dimensions $A^{-1}(x, y) = O(|x - y|^{-1})$.

Dislocation fluctuations (vortex waves)

Cut a a long story short

The field σ_q satisfies

$$\begin{aligned} \mathrm{d}^* B\sigma_q &= 0, \\ \mathrm{d}\sigma_q &= q \end{aligned}$$

Continuum analogue:

$$\begin{aligned} \nabla \cdot (\sigma + \sigma^T) &= 0, \\ \mathrm{curl}\,\sigma &= q \end{aligned}$$

- Hodge decomposition: $\sigma = \mathrm{d}u + \mathrm{d}^* V, \quad (\sigma = \nabla u + \mathrm{curl}\ V)$.
- $V = \mathrm{d}\Delta^{-1} q$
- $H_{\mathrm{AO}}(0, \sigma_q) = \frac{1}{2}\langle Gq, BGq\rangle$ with $G = (1 - \mathrm{d}A^{-1}\mathrm{d}^* B)\mathrm{d}^*\Delta^{-1}$.

Need that

$$A^{-1}\mathrm{d}^* B^2 \mathrm{d}A^{-1}(x, x') = o(1), \quad |x - x'| \gg 1,$$

this holds if $A^{-1} = O(|x|^{-1})$

Cluster expansion

We are interested in $\frac{Z_\beta(h)}{Z_\beta(0)}$ with

$$Z_\beta(h) = \sum_{\mathrm{d}_2 q = 0} \exp(i\langle \sigma_q, h\rangle) \exp(-\beta(w(q) + H_{\mathrm{AO}}(0, \sigma_q))) = \sum_{\mathrm{d}_2 q = 0} K(q, h).$$

The dislocation configuration q can be decomposed into disjoint loops:

$$K(q, h) = \prod_{j=1}^{n} K(q_j, h).$$

Thus

$$Z_\beta(h) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{q_1, \ldots, q_n} \prod_{j=1}^{n} K(q_j, h).$$

Now estimate the individual terms!

Conclusions and Outlook

- First results on formation of crystals in three dimensions
- First rigorous, quantitative result on equilibrium dislocation configurations
- Results due to a complete decoupling between dislocations and elastic field

Outlook

- Two dimensions (orientational order, hexatic phases)
- Nonlinear versions, e.g. hard disks or hard balls at finite density.
- Quantitative discrete dislocation dynamics