THE UNIVERSITY OF WARWICK

Discrete Dislocations and the Read-Shockley Law

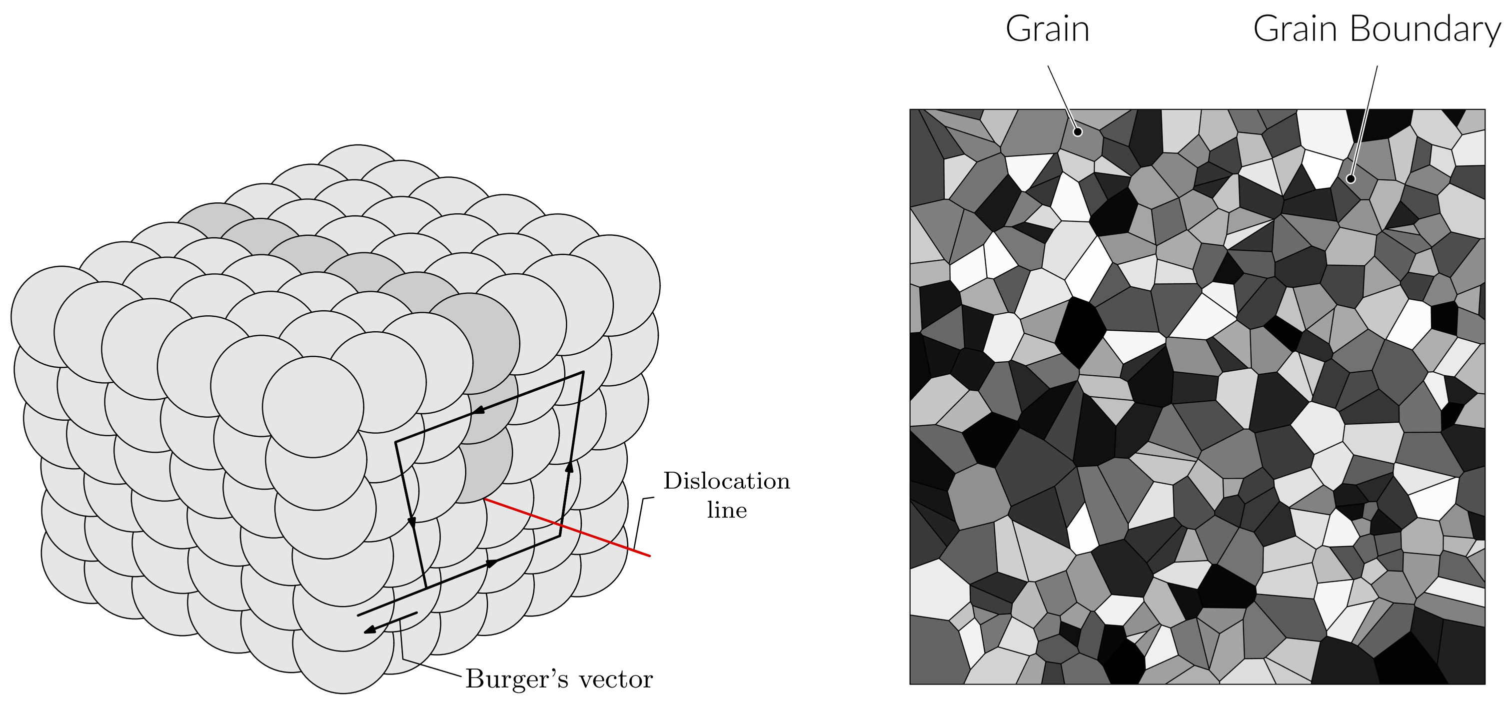
Anvarbek Atayev Dr. Florian Theil Dr. Thomas Hudson

Introduction

The study of material defects has been of much interest to the scientific community in recent years. This has been motivated by its direct application to engineering, where the presence of defects have a real and direct effect on material properties.

Grain Boundaries and Dislocations

Many solid materials exhibit a *polycrystalline form*, where their atomic structure is composed of a number of interacting, mutually rotated, sublattices known as grains, which are connected by *grain boundaries*.



Edge dislocation Polycrystal

Grain boundaries resulting from a **small** angular mismatch have been shown to be composed of line defects known as *edge dislocations*, which can be found in regions of lattice misalignment. Indeed, grain boundaries form as to minimise the stress due to the presence of defects.

Read-Shockley Law

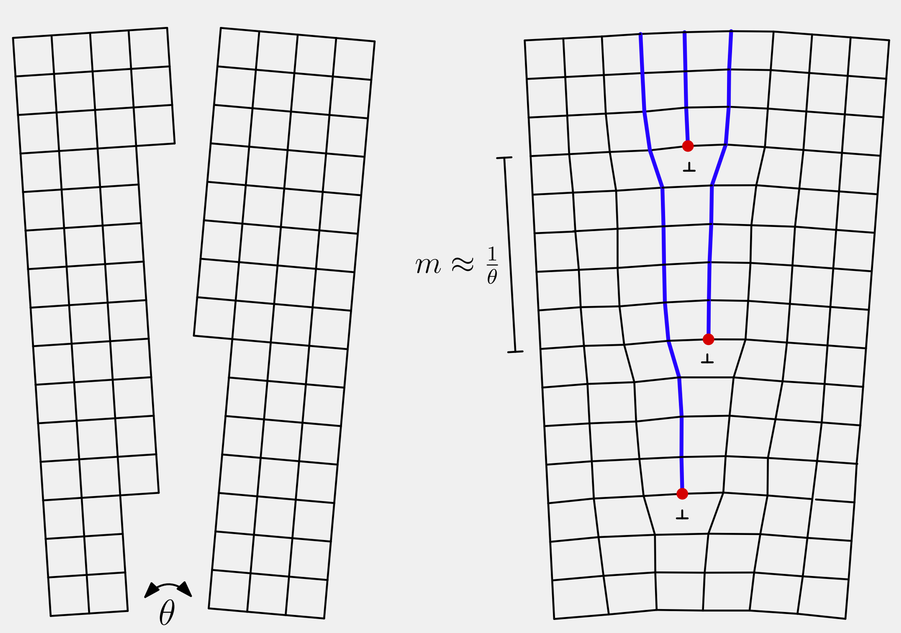
In classical linear elasticity theory, dislocations at positions x and y interact via $W(\mathsf{x}-\mathsf{y})$ where

$$W(x) := -\log|x| + \frac{x_1^2}{|x|^2} \qquad x \in \mathbb{R}^2, \tag{1}$$

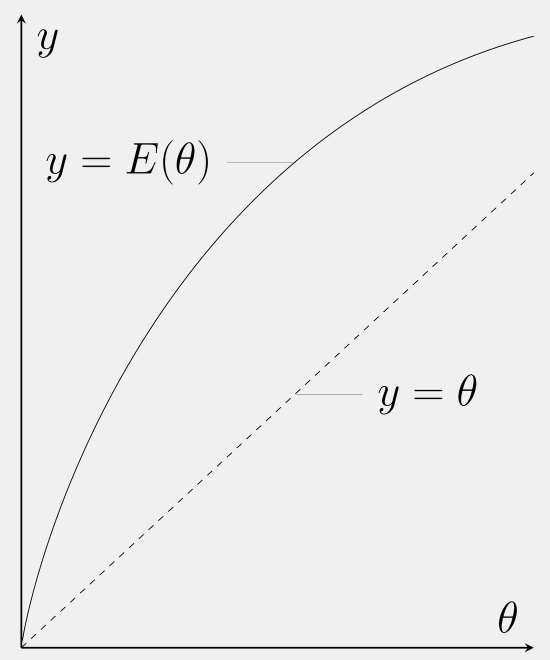
Under this model, in [RS50], Read and Shockley obtained the energy density of a wall of equispaced dislocations to be

$$E(\theta) = E_0\theta(A - \log\theta) \tag{2}$$

for a small angle $0 < \theta \ll 1$ and material constants E_0, A.



Small angle grain boundary



Energy Density

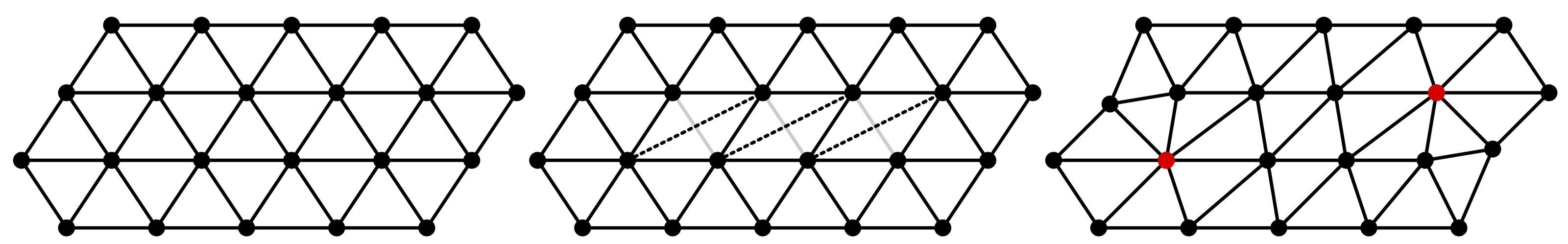
Flaw: Core radius approach used; *ignores* fine contributions from dislocation cores.

Question 1: Is the Read-Shockley law valid for a more refined dislocation model?

Ariza-Ortiz Dislocation Model, see [AO05]

Pros

- Removes need for dislocation core approximation as can treat dislocation directly
- Provides a more precise model of dislocations through an atomistic approach
- Simple enough to perform analysis



Undeformed Deformed

The energy of a lattice in the presence of a dislocation q can be defined as the optimal Ariza-Ortiz Hamiltonian under displacement and slip fields, u, σ, respectively

$$\text{Energy}(q) = \min_{\substack{(u,\sigma)\\ d\sigma = q}} \sum_{\substack{x,y\in\mathcal{L}\\ x\sim y}} \left[(u(x) - u(y) - \sigma(x,y)) \cdot (y-x)\right]^2, \tag{3}$$

In [GT21], the energy density of an infinite wall of equispaced dislocations, with spacing m, was found to follow the Read-Shockley law, i.e.

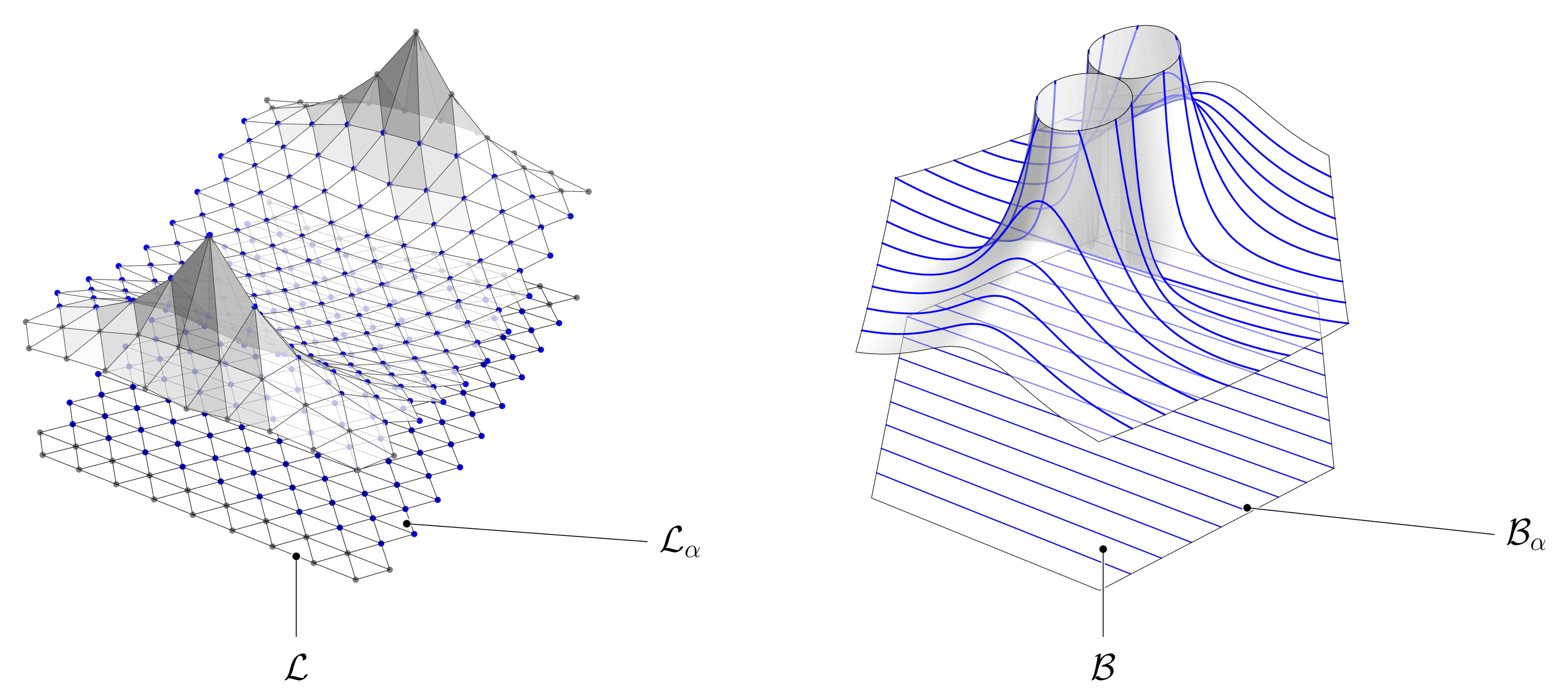
$$E^{\mathrm{AO}}(m) = -\frac{1}{m}\log\left(\frac{1}{m}\right) + \mathcal{O}\left(\frac{1}{m}\right) \quad \text{as } m \to \infty. \tag{4}$$

Question 2: Does a wall of equispaced dislocations define a grain boundary?

Energy Density of Dislocation Configurations

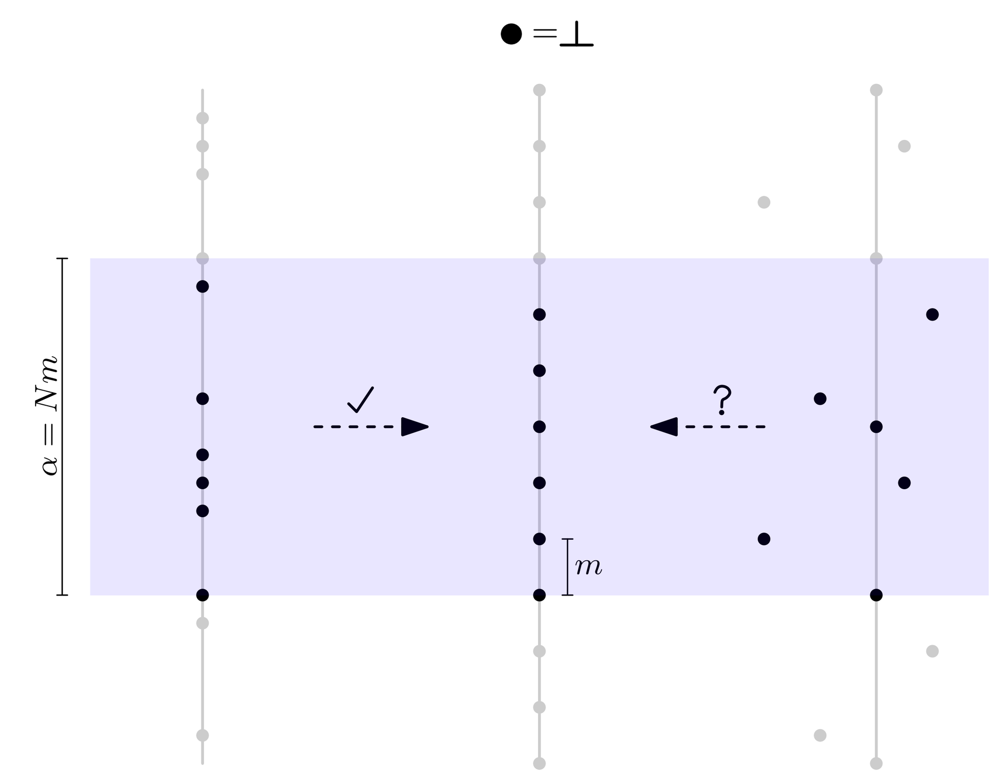
Under the Ariza-Ortiz model, the energy density of a periodic wall of dislocations of density m and positions $X = (\mathsf{x}_i)_{i=1}^N \subset \mathcal{L}_\alpha$ (with periodicity $\alpha = Nm$) can be found to be

$$E^{\mathrm{AO}}_\alpha(X) = \frac{1}{\alpha}\sum_{i=1}^N\sum_{j=1}^N \mathcal{W}_\alpha(\mathsf{x}_i - \mathsf{x}_j), \qquad \mathcal{W}_\alpha(\mathsf{x}) = \frac{1}{|\mathcal{B}_\alpha|}\int_{\mathcal{B}_\alpha} \psi(k)e^{ik\cdot\mathsf{x}}d\nu_\alpha(k). \tag{5}$$



$\mathcal{W}_\alpha$ in real space $\mathcal{W}_\alpha$ in Fourier space

Equilibirum Configurations of Dislocations



In-boundary modulations Equispaced Out-of-boundary modulations

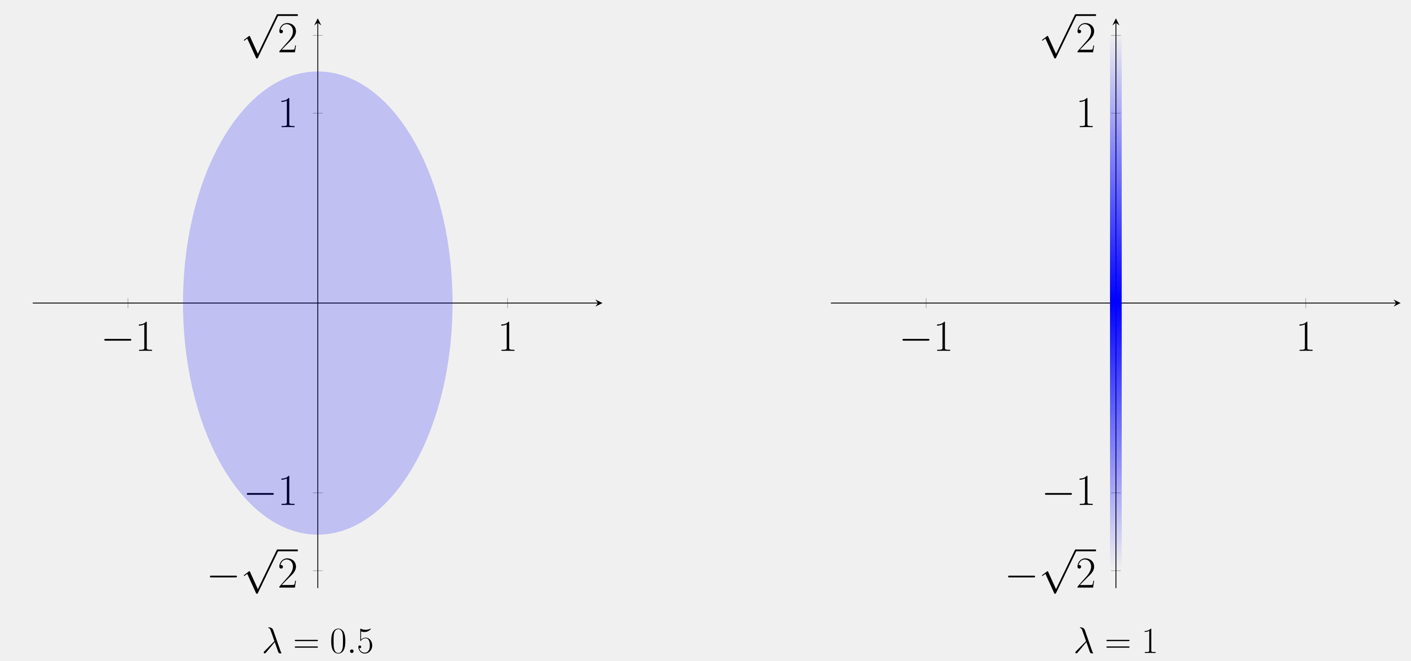
✓ Follows by convexity of $y \mapsto \mathcal{W}_\alpha(0,y)$ over *lattice points* and methods of [Ven78].

? Work in progress; progressing via comparison to continuum model.

Related Work: Equilibrium via Probability Distributions

Equilibrium *distributions* of dislocations in the sense of measures was determined for an interaction potential W and confinement potential V in [CMM⁺19], with

$$W(x;\lambda) = -\log|x| + \lambda\frac{x_1^2}{|x|^2} \qquad V(x) := \frac{|x|^2}{2} \qquad \lambda \in [-1,1], x \in \mathbb{R}^2. \tag{6}$$



$\lambda = 0.5$ $\lambda = 1$

Adherence to wall like structures determined in limit $|\lambda| \to 1^-$, representing grain boundaries.

References

[AO05] M. P. Ariza and M. Ortiz. Discrete crystal elasticity and discrete dislocations in crystals. *Archive for Rational Mechanics and Analysis*, 178(2):149–226, November 2005.

[CMM⁺19] J. A. Carrillo, J. Mateu, M. G. Mora, L. Rondi, L. Scardia, and J. Verdera. The equilibrium measure for an anisotropic nonlocal energy. June 2019.

[GT21] Alessandro Giuliani and Florian Theil. Long range order in atomistic models for solids. *Journal of the European Mathematical Society*, November 2021.

[RS50] W. T. Read and W. Shockley. Dislocation models of crystal grain boundaries. *Physical Review*, 78(3):275–289, May 1950.

[Ven78] W. J. Ventevogel. On the configuration of a one-dimensional system of interacting particles with minimum potential energy per particle. *Physica A: Statistical Mechanics and its Applications*, 92(3):343–361, July 1978.

anvar.atayev@warwick.ac.uk