Screw dislocation mobility:
Monte Carlo models to Discrete Dislocation Dynamics

Tom Hudson
(Warwick Mathematics Institute)

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Many everyday solid materials are crystalline
Simplest structures are Bravais lattices (Iron, cubic structures)
More generally, multilattices (Graphite, hexagonal lattice structure)
Crystal Plasticity = ‘slip’ of crystallographic planes.

http://www.doitpoms.ac.uk/tlplib/miller_indices/uses.php
Crystal plasticity

Orowan (1934), Polanyi (1934), Taylor (1934):
Slip occurs via motion of dislocations.
Dislocations

- **Geometric** lattice defects
- Assigned a Burgers vector, $\mathbf{b}$, and line direction, $\mathbf{l}$.
- Simplest types: screw ($\mathbf{b} \parallel \mathbf{l}$) and edge ($\mathbf{b} \perp \mathbf{l}$).
Computational modelling of crystal plasticity

Hierarchy of crystal plasticity models:

Electronic structure: True chemistry, $\sim 10^3$ atoms

$\Downarrow$ Potentials for/coupling to: $\Downarrow$

Molecular Dynamics: Statistical mechanics. $\sim 10^6$ atoms, but longest feasible trajectory length $\sim 10^{-6}$s

$\Downarrow$ Mobility + topological laws for: $\Downarrow$

Discrete Dislocation Dynamics: Statistical mechanics: single crystal/multiple grains, trajectory length $\sim 10^{-1}$s.

$\Downarrow$ Numerical constitutive laws for: $\Downarrow$

Continuum crystal plasticity: human time– and length–scales.
Dislocation Dynamics

http://computation.llnl.gov/largevis/atoms/ductile-failure/
Dislocation Dynamics

http://paradis.stanford.edu/site/about
Dislocation Dynamics

Discrete Dislocation Dynamics (DDD) is the solution of the problem

$$\dot{\Gamma}(s) = M[f(s, \Gamma)],$$

where

- $\Gamma(s)$ is a parametrisation of time–dependent dislocation lines
- $f$ is the Peach–Köhler force, $f = (\sigma \cdot b) \wedge l$, with:
  - $\sigma$ the stress at $\Gamma(s)$,
  - $b$ the Burgers vector, and
  - $l = \frac{\Gamma'(s)}{|\Gamma'(s)|}$ the line direction.
- $M$ is a mobility function, usually $M[f] = \alpha f$, or $\alpha(l - n \otimes n)f$.

Note:

- $\sigma$ is a nonlocal function of the dislocation configuration.
- Dislocation junctions are more complicated.

Questions: When is DDD valid, and what should $M$ be?
Kinetic Monte Carlo models

- Hamiltonian \( H(p, q) = \frac{1}{2}|p|^2 + V(q) \).
- Temperature \( T, \beta := k_B^{-1} T^{-1} \).
- Equilibrium density = \textbf{Gibbs measure}
  \[ Z(\beta)^{-1} \exp (-\beta V(q)) dq. \]
- Sample via ergodic dynamics, e.g.
  \[
  \dot{q} = M^{-1} p \\
  \dot{p} = -\nabla V(q) - \gamma M^{-1} p + \sqrt{2\gamma \beta^{-1}} \dot{W}
  \]
- If \( \beta \gg 1 \), \( q \) ‘waits’ near local minima.

\textbf{Eyring–Kramers rule:}
Waiting times for transitions between minima are exponentially distributed.
Kinetic Monte Carlo models

1. Define states $\mu$, $\nu$.

2. Fix neighbouring states $N_\mu$.

3. **Eyring–Kramers rule**: jump time from $\mu$ to $\nu$ exponentially distributed [Hänggi–Talker–Borcovec ‘90, Berglund ‘13] with rate

   \[ R(\mu \rightarrow \nu) = A(\mu \rightarrow \nu) \exp \left[ -\beta B(\mu \rightarrow \nu) \right], \]

   where
   - $A(\mu \rightarrow \nu)$ is entropic prefactor $\approx$ ‘width’ of the minimal pathway
   - $B(\mu \rightarrow \nu)$ is energy barrier $= \text{‘height’ of saddle between states.}$
Kinetic Monte Carlo models

1. Define states $\mu$, $\nu$.

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3. **Eyring–Kramers rule**: jump time from $\mu$ to $\nu$ exponentially distributed [Hänggi–Talker–Borcovec ‘90, Berglund ‘13] with rate

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   where
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4. **KMC model**: Wait until first transition, move to new state, repeat. If transition times are independent:

   $$\tau \sim \min_{\nu \in \mathcal{N}_\mu} \exp[R(\mu \to \nu)] = \exp\left[ \sum_{\nu \in \mathcal{N}_\mu} R(\mu \to \nu) \right],$$

   and

   $$\mathbb{P}[\mu \to \nu'] = \frac{R(\mu \to \nu')}{\sum_{\nu \in \mathcal{N}_\mu} R(\mu \to \nu)}.$$
Toy model for screw dislocations

- Project along Burgers vector:
  \[ \sim \text{ lattice } L \text{ in–plane.} \]
- Cylinder, cross–section \( D_{n,0} = nD \cap L \).
- **Assume** vertical movement of ‘columns’ only.
- Anti–plane deformation:
  \[ y : nD_{n,0} \to \mathbb{R}. \]
- Finite diff, \( dy(b) := y(e) − y(e'). \)
- **Assume** NN interaction.

**Potential:** \( \psi(r) = \frac{1}{2} \lambda \text{dist}(r, \mathbb{Z})^2 \)

**Total energy:** \( E_n(y) = \sum_{b \in D_{n,1}} \psi(dy(b)) \)
Toy model for screw dislocations

Smallest ‘height’ difference:

\[ \alpha(b) = dy(b) \mod 1 = dy(b) - z(b),\]

\[ z(b) = \arg\min_{z \in \mathbb{Z}} |z - dy(b)| \]

Define Burgers vector of ‘cell’ \(C\):

\[ \sum_{b \in \partial C} \alpha(b) \in \{-1, 0, +1\}. \]

\(\rightsquigarrow\) Identification of dislocations.

**NB:** Ambiguous if \(dy(b) \in \mathbb{Z} + \frac{1}{2}\)

\(\leftrightarrow\) Change of dislocation position.

**Theorem** [H–Ortner ‘14, H–Ortner ‘15, H ‘16]

Under appropriate assumptions on the dislocation geometry, there exist local minima of the energy \(E_n\) containing dislocations.
Toy model for screw dislocations

Initial state $\mu$: 

[Diagram showing a circular and a more complex geometric structure with blue dots and red triangles.]
Toy model for screw dislocations

Transition $\mu \rightarrow \nu$: 

[Diagram showing a toy model with points and arrows indicating the transition process.]
Final state $\nu$: 

Toy model for screw dislocations
KMC model for screw dislocation motion

Recall: $R = Ae^{-\beta B}$. Can we say anything about the energy barriers?

**Theorem**

[H '16]

There is an explicit formula for the energy barrier in terms of finite differences of dual lattice Green’s functions. Moreover, asymptotically,

$$
B_n(\mu \to \nu) = \lambda c_0 + n^{-1} \frac{1}{2} \lambda f \cdot a + o(n^{-1})
$$

where:

- $c_0$ is constant and depends only on the lattice, and
- $f \cdot a$ is the component of the **Peach–Köhler force** on the dislocation moving in dual lattice direction $a$, where:

$$
f = (\sigma \cdot \mathbf{b}) \wedge \mathbf{l},
$$

$\sigma = \text{stress}, \quad \mathbf{b} = \text{Burgers vector}, \quad \mathbf{l} = \text{dislocation line direction}.$
KMC model for screw dislocation motion

Use explicit formula to prescribe rates

\[ \mathcal{R}(\mu \rightarrow \nu) = A_0 T \exp \left[ -\beta B(\mu \rightarrow \nu) \right], \]

\( A_0 = \text{fixed prefactor}, \quad T = \text{time scaling}, \quad \beta = \text{inverse temperature}. \)
Deterministic scaling regime

Consider regime where:

- Temperature is low, $\beta_n \gg 1$,
- Size of domain relative to lattice spacing is large $\sim n \gg 1$, and
- System is observed over a long timescale relative to microscopic times $\sim$ multiply rates uniformly by $T_n \gg 1$.

If $A(\mu \rightarrow \nu) = A_0 + o(1)$ as $\beta, n \rightarrow \infty$, a key quantity is

$$\frac{T_n R_n(\mu \rightarrow \nu)}{n} = \frac{T_n A_0 e^{-\beta_n \lambda c_0}}{n} \exp \left( - \frac{\beta_n \lambda}{2n} f \cdot a \right) + o(n^{-1}).$$

- ‘Macroscopic velocity’
- System behaviour governed by parameters $A$ and $B$. 
Deterministic scaling regime

\[ A = n^{-1} \mathcal{T}_n A_0 e^{-\beta_n \lambda c_0} \]

- \( A_0 e^{-\beta_n \lambda c_0} \) = hopping rate for 1 dislocation in full lattice (stress free).
- \( \mathcal{T}_n A_0 e^{-\beta_n \lambda c_0} \) = microscopic hops in unit observed time.
- \( n^{-1} \mathcal{T}_n A_0 e^{-\beta_n \lambda c_0} \) = proportion of macroscopic body covered in unit observed time.
Deterministic scaling regime

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\[ B = \frac{1}{2} n^{-1} \beta_n \lambda \]

- \( n^{-1} \lambda f \cdot a \) = work done against macroscopic stress in one hop.
- \( \beta_n \) = inverse of thermal energy available.
- \( \frac{1}{2} n^{-1} \beta_n \lambda \) = ratio of microscopic energy barrier to thermal energy.
Deterministic scaling regime

- $A = n^{-1} T_n A_0 e^{-\beta_n \lambda c_0}$
  - $A_0 e^{-\beta_n \lambda c_0} =$ hopping rate for 1 dislocation in full lattice (stress free).
  - $T_n A_0 e^{-\beta_n \lambda c_0} =$ microscopic hops in unit observed time.
  - $n^{-1} T_n A_0 e^{-\beta_n \lambda c_0} =$ proportion of macroscopic body covered in unit observed time.

- $B = \frac{1}{2} n^{-1} \beta_n \lambda$
  - $n^{-1} \lambda f \cdot a =$ work done against macroscopic stress in one hop.
  - $\beta_n =$ inverse of thermal energy available.
  - $\frac{1}{2} n^{-1} \beta_n \lambda =$ ratio of microscopic energy barrier to thermal energy.

- Taking $n, \beta, T_n \to \infty$ with $A$ and $B$ fixed, the random process satisfies a Large Deviations Principle, i.e. trajectories concentrate around a deterministic limit.
Deterministic scaling regime

Theorem [H ’16]

If $A$ and $B$ are fixed as $n \to \infty$, the Markov processes $X^n_t$ with rates $T_n R_n(\mu \to \nu)$ the most probable trajectory of the system solves

$$\dot{x}_i = \mathcal{M}[-\partial x_i \mathcal{E}(x_1, \ldots, x_m)],$$

where $\mathcal{M}$ is the nonlinear mobility function

$$\mathcal{M}[\xi] = \left\{ \begin{array}{ll}
A \sum_{i=1}^{4} \sinh(B \xi \cdot e_i) e_i & \text{for the hexagonal lattice,} \\
A \sum_{i=1}^{6} \sinh(B \xi \cdot a_i) a_i & \text{for the square lattice} \\
\frac{A \sum_{i=1}^{6} \sinh(B \xi \cdot a_i) a_i}{2 \sum_{i=1}^{3} \cosh\left(\frac{1}{3} B \xi \cdot [a_{2i-1} + a_{2i}]\right)} & \text{for the triangular lattice,}
\end{array} \right.$$

and $e_i$ and $a_i$ are nearest neighbour directions in the square and triangular lattices respectively.

NB: $-\partial x_i \mathcal{E}(x_1, \ldots, x_m)$ is the Peach–Köhler force on the dislocation at $x_i$. 
Deterministic scaling regime

Recall: DDD usually uses a \textit{linear} mobility.

- Derived mobility is nonlinear, lattice–dependent:
  \( \rightsquigarrow \) \textit{New model with accompanying parameter regime}

- New justification for DDD from microscopic model

Is linearisation ever justified?

- \( B \to 0 \) and \( A \to \infty \) with \( AB = \omega \) constant recovers isotropic linear mobility (\( \Gamma \)-convergence: [Bonaschi-Peletier ‘14]).

- Corresponds to \( \beta \ll n \):
  \( \rightsquigarrow \) \textbf{LDP invalid}: temperature ‘too high’ (but see later)

- What about in practice?
Deterministic scaling regime

\[ \beta = 1000, \ n = 200. \ Dots = 200 \ KMC \ trials. \]

Dashed line = linear dynamics, Solid line = nonlinear dynamics.
Other regimes

- Suppose probability density $\rho$, then Fokker–Planck equation is

$$
\dot{\rho}(\mu) = - \sum_{\nu \in \mathcal{N}_{\mu}} d\rho(\mu, \nu) \mathcal{T}_n \mathcal{R}_n(\mu \to \nu)
= \sum_a \left( - n^{-1} \nabla \rho \cdot a + n^{-2} D^2 \rho : [a, a] + o(n^{-2}) \right) \mathcal{T}_n \mathcal{R}_n(\mu \to \nu).
$$

- Expand $\mathcal{T}_n \mathcal{R}_n(\mu \to \nu)$:

$$
\mathcal{T}_n \mathcal{R}_n(\mu \to \nu) = \mathcal{T}_n A_0 e^{-\beta \lambda c_0} \left[ 1 - \frac{\beta \lambda}{2n} f \cdot a + o(n^{-1}) \right].
$$

- Collecting terms, write $f = -\nabla \mathcal{E}$ and use symmetry,

$$
\dot{\rho} = \frac{\mathcal{T}_n}{n^2} A_0 e^{-\beta \lambda c_0} \left[ - \frac{1}{2} \beta \lambda c_1 \nabla \mathcal{E} \cdot \nabla \rho + c_2 \Delta \rho \right] + o(n^{-2}).
$$

- When $\mathcal{T}_n \sim n^2$ as $n \to \infty \leadsto \text{Brownian motion with drift } \nabla \mathcal{E}$.

- Q: Should DDD be random in even moderate temperature regimes?
Conclusion

Summary:

▶ Statistical mechanical treatment of simple anti–plane model for studying screw dislocations
▶ Markovian model proposed for thermally–driven dislocation motion
▶ Large Deviations Principle in low temperature, large body regime ⇾ explicit regime of validity and lattice–dependent mobility for Discrete Dislocation Dynamics

Outlook:

▶ Moderate temperature regime, convergence of DDD schemes

References: