Multiscale Analysis of Non-Linear Dislocation Models

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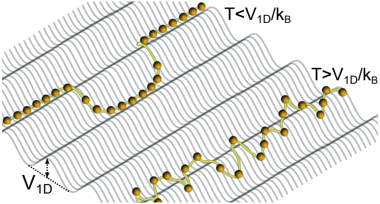
Motivation

- In many materials, dislocations move through a kink mechanism between periodic minima

- Many theories for an effective mobility law, but little rigorous analysis

- We want to understand the rôle of **Free Energy Barriers** and **kink-kink interactions**

A kink-bearing model



- For a line of nodes $\mathbf{x}=\{\mathrm{x}_i\}$

$$V(\mathbf{x}) - b\sigma\sum_i \mathrm{x_i} = \underbrace{\frac{\kappa}{2}\sum_{ij}\mathrm{x}_i\mathrm{K}_{ij}\mathrm{x}_j}_{\text{Node Interaction}} + \underbrace{\mathrm{V_{1D}}\sum_i \sin^2\left(\frac{\pi}{a}\mathrm{x}_i\right)}_{\text{Peierls Barrier}} \underbrace{-b\sigma\sum_i \mathrm{x_i}}_{\text{Applied Stress}}$$

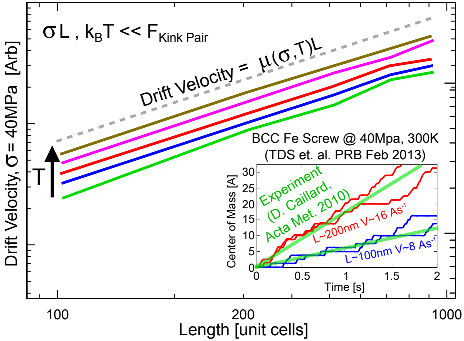
- Integrate with Langevin dynamics

$$\gamma\dot{\mathrm{x}}_i = -\nabla_i V(\mathbf{x}) + b\sigma + \sqrt{2\mathrm{k_B T}\gamma}\eta_i(t) \qquad (\eta = \text{White Noise})$$

- TDS *et al.* PRB Feb 2013, TDS PRE June 2013

Scaling and system size

- Natural quantity of interest: **center of mass** $\bar{\mathrm{x}} = \sum_i \mathrm{x}_i / N$
- $\kappa, \gamma, \mathrm{V}_{1\mathrm{D}}$ from MD $\Rightarrow$ **quantitative agreement** with experiment



- Drift velocity highly non-linear in $\sigma, \mathrm{k_B T}$ but linear in length L

Transport in periodic environments

- We want to understand the transport properties of $\bar{x}$, averaging out all other DOF.
- We have investigated the Fokker-Planck equation and renormalised to reach $t \to \infty$
- System periodic so $\rho(\bar{x})$ (n.b. $F(\bar{x}) = -\mathrm{k_B T} \ln \rho(\bar{x})$)

$$\rho(\bar{x}) = \rho(\bar{x}+a) = Z^{-1} \int \delta\left(\sum_i x_i/N - \bar{x}\right) e^{-\beta(V(\mathbf{x}) - bL\sigma\bar{x})} \mathrm{d}\mathbf{x}.$$

- This implies $\bar{x} \in [0,a]$ for $\int \rho < \infty$; but need $\bar{x} \in \mathbb{R}$ for drift / diffusion!

Multiscale Analysis

- To solve this we consider the Fokker-Planck equation of the original system with $\bar{x} \in [0, a]$ and **in addition** the coarse-grained coordinate

$$\chi \equiv \epsilon \bar{x} \qquad \epsilon \ll 1$$

whilst rescaling time as

$$t \to \frac{t}{\epsilon} \quad \text{(Drift)} \quad , \quad \frac{\mathrm{t}}{\epsilon^2} \quad \text{(Diffusion)}$$

- As $\epsilon \to 0$ we rigorously show the Fokker-Planck equation is solved by

$$\Phi_\epsilon(\chi, \mathbf{x}, t) = \Phi_0(\chi, t) + \epsilon \Phi_1(\mathbf{x}, t) + \epsilon^2 \Phi_2(\mathbf{x}, t) + \ldots$$

- We obtain a FP equation for Φ_0 which gives **analytical** bounds on the transport properties (TDS, PRE June 2013)

Multiscale Analysis

- In general, we find **free energy landscapes overestimate mobilities**

- Namely, with $F(\bar{x}) \equiv -\mathrm{k_B T} \ln \rho(\bar{x}, \sigma = 0)$ we find

$$D < \frac{\mathrm{k_B T}/N\gamma}{\int_0^a e^{\beta F(\bar{x})}\mathrm{d}\bar{x} \int_0^a e^{-\beta F(\bar{y})}\mathrm{d}\bar{y}} \quad \beta \to \infty \quad \underbrace{\frac{\omega_{\mathrm{MIN}}\omega_{\mathrm{DK}}}{\sqrt{\beta}\gamma} \prod_i \frac{\omega^i_{\mathrm{MIN}}}{\omega^i_{\mathrm{DK}}} e^{-\beta F_{\mathrm{DK}}}}_{\text{Kramers TST}}$$

- We also find for the drift velocity $\mu(\sigma, \beta)L$ that

$$\mu(\sigma, \mathrm{T}) < \frac{\mathrm{k_B T}(1 - e^{-\beta b L a \sigma})/N\gamma}{\int_0^a e^{\beta(F(\bar{x}) - bL\sigma\bar{x})}\mathrm{d}\bar{x} \int_{\bar{x}}^{\bar{x}+a} e^{-\beta(F(\bar{y}) - bL\sigma\bar{x})}\mathrm{d}\bar{y}}$$

- Non-linear but **not** phenomenological (c.f. Kocks-Argon)

Free energy barriers are under estimates

- Free energy assumes $0(\epsilon)$ dynamics are only in $\bar{x}$ $(\Phi_1(\mathbf{x}) = \Phi_1(\bar{x}))$
- Not surprising as entropic maximum pathway neglects correlations
- But as $\rho(\bar{x}) = Z^{-1}e^{-\beta F(\bar{x})}$ solves steady state must **at least** have

$$\frac{\partial}{\partial t}\rho(\bar{x},t) = \frac{\partial}{\partial \bar{x}}\left(\frac{1}{\gamma(\bar{x})}\left(\frac{\partial F(\bar{x})}{\partial \bar{x}}\rho(\bar{x},t) + \mathrm{k_B T}\frac{\partial}{\partial \bar{x}}\rho(\bar{x},t)\right)\right)$$

  or non-Markovian dynamics (ongoing work).

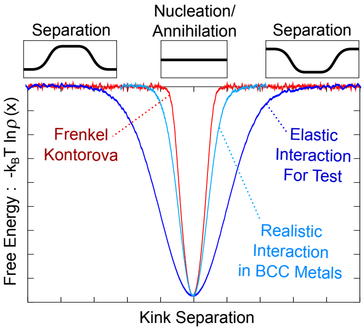
- But are these bounds useful?

Testing free energy barriers

- We have tested these bounds using FK chain and a chain with long range kink interactions

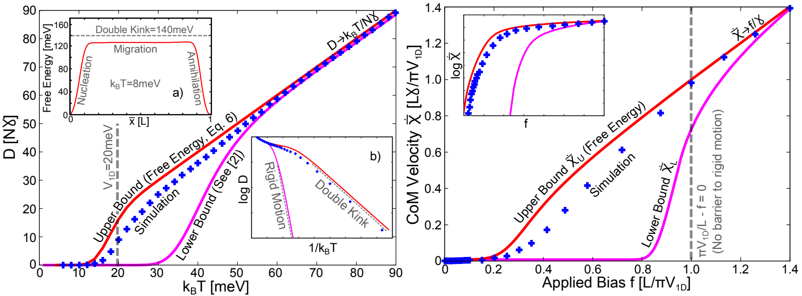
$$\sum_{ij} x_i K_{ij} x_j = \underbrace{\sum_i (x_{i+1} - x_i)^2}_{\text{Frenkel Kontorova}} \quad \rightarrow \quad \underbrace{\sum_{ij} \frac{(x_{i+1} - x_i)(x_{j+1} - x_j)}{\sqrt{1 + (i-j)^2/\alpha^2}}}_{\text{Elastic Interaction}}$$

Gives elastic kink-kink interaction of $1/d$.



Free energy barriers are good under estimates

- We have calculated $F(\bar{x})$ through a histogram method for both chains-



- Against standard assumptions, kink-kink interaction has negligable effect on critical stress.

Conclusions

- Multiscale analysis allows rigorous understanding of otherwise intractable problems
- Even under purely diffusive dynamics the free energy underestimates work (c.f. Crook's relation).
- However, the bounds are good estimates and offer non-linear mobility laws which are **not phenomenological**
- Please see T D Swinburne PRE June 2013 for more detail.
- Realistic kink-kink interactions do **not** affect the critical shear stress. Instead (in preparation)

Thank you for listening

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