Kink limited motion of line defects: multiscale simulation and analysis

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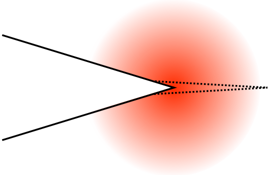
Outline

- Dislocations and Fracture
- The Frenkel-Kontorova Model
- Multiscale analysis of FK transport
- Atomistic calulation of free energies
- Kink-limited motion through obstacles
- Comparison to experiment

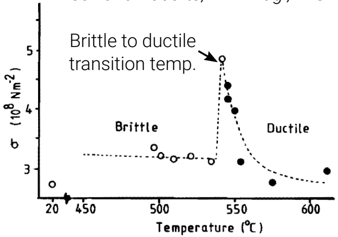
The brittle to ductile transition

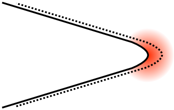
- The fracture toughness of many materials show a peak with temperature



Brittle cleavage

Fracture of silicon
Hirsch and Roberts, Phil. Mag., 1989



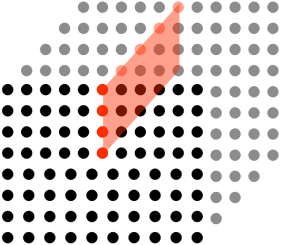


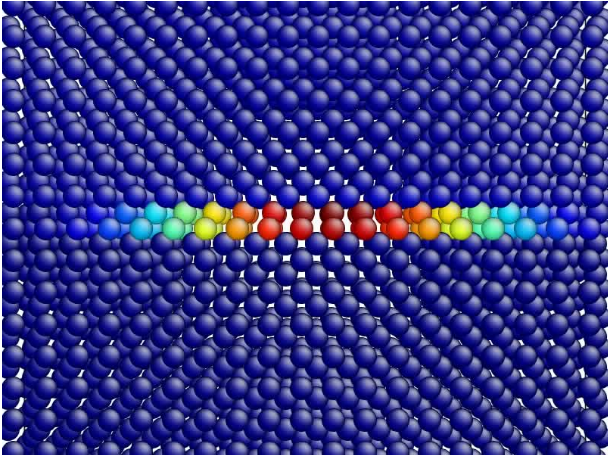
Ductile failure

- Microstructure dependent BDT temperature a critical materials parameter
- Structural nuclear applications must understand ΔBDTT under irradiation
- Crack blunting requires plastic deformation ⇒ **dislocations**

Dislocations

- Crystalline materials concentrate plastic deformation in dislocation lines of highly deformed “cores” with surrounding elastic fields





Dislocations

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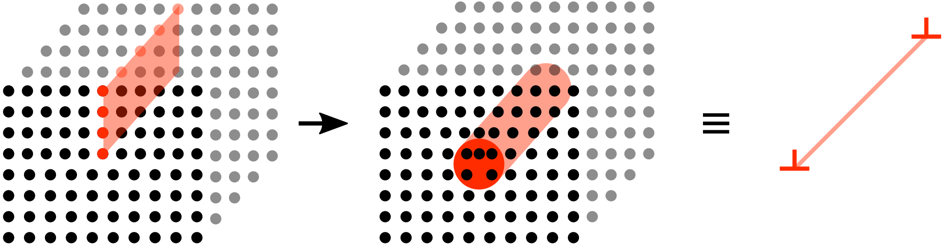
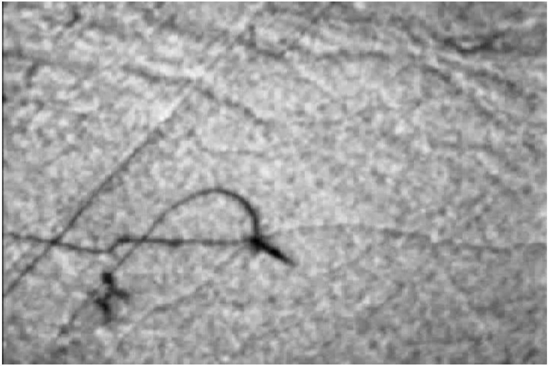


- The creation and migration of dislocations typically controls crystal plasticity

- Dislocations can carry away deformation, reducing the stress intensity

Dislocations

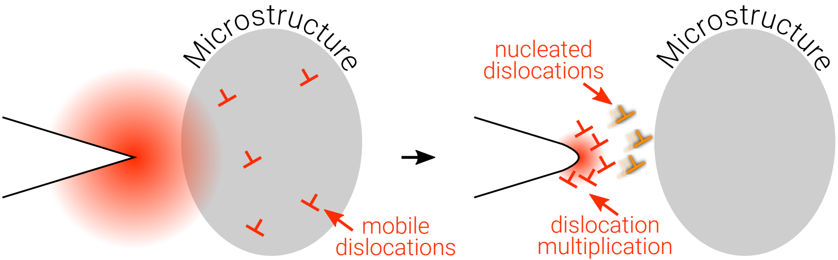
- Dislocations can be seen under the tunnelling electron microscope



- From Caillard, Acta Met. 2013. Note anisotropic shape...

Dislocations and the BDT

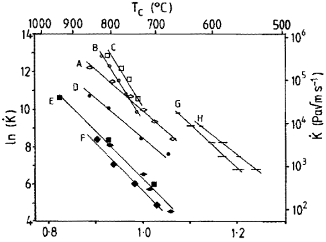
- Crack blunting requires the creation and motion of **dislocations**
- Hirsch and Roberts argued that existing dislocations migrate to a crack, where they emit dislocations that carry away deformation from the tip



- This picture strongly implies the **BDT is controlled by dislocation mobility**

Dislocations and the BDT

- The Hirsch Roberts model was dramatically validated in silicon



Brittle to ductile transition temperature of silicon
Hirsch and Roberts, Phil. Mag., 1989

Experiment	Activation energy Intrinsic Si (2×10^{13} Pcm^{-3})	*n*-type Si (2×10^{18} Pcm^{-3})
BDT (Samuels and Roberts 1989)	2·1 ± 0·1 eV	1·6 ± 0·1 eV
BDT (St John 1975)	1·9 eV	—
Dislocation velocity (George and Champier 1979)	2·2 eV	1·7 eV
Dislocation velocity (Imai and Sumino 1983)†	2·3 eV	1·7 eV

† Doping levels used were 2×10^{12} Bcm^{-3} and $6{\cdot}2\times10^{18}$ Pcm^{-3}

BDT activation energy: $\log_e \dot{\epsilon}_{\mathrm{ext.}}(T_{\mathrm{BDT}}) = A - U_{\mathrm{BDT}}/k_B T_{\mathrm{BDT}}$

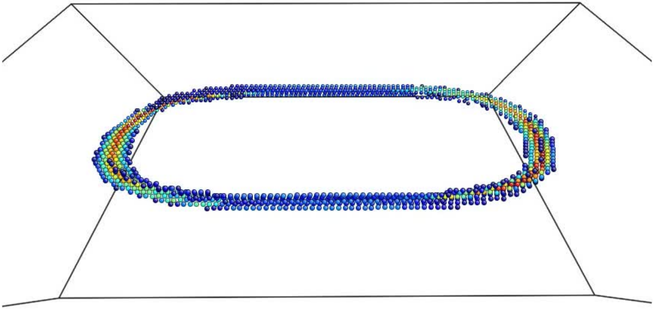
Dislocation velocity: $\log_e v_{\mathrm{dislo}} = B - U_{\mathrm{dislo}}/k_B T$

Orowan Law: $\dot{\epsilon} = b\rho_{\mathrm{dislo}} v_{\mathrm{dislo}}, \quad \Rightarrow \quad U_{\mathrm{dislo}} = U_{\mathrm{BDT}}$

- But what is the activation energy U_{dislo} for dislocation motion?

Dislocations in bcc metals

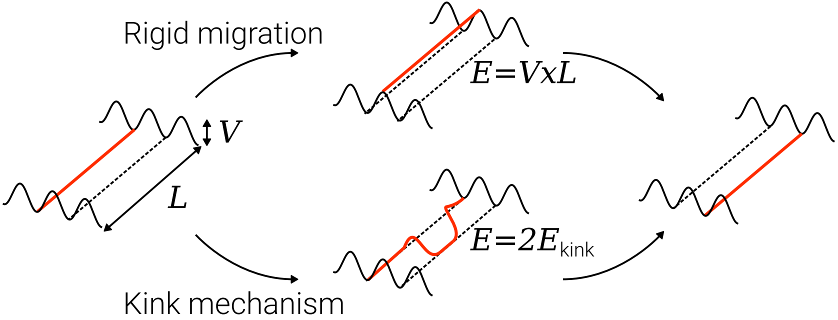
- The dominant $1/2\langle 111\rangle\{10\bar{1}\}$ dislocations are highly anisotropic



- Mobility controlled by rare kink nucleation on $1/2\langle 111\rangle$ screw dislocations

The kink mechanism

- The dislocation core energy varies periodically with the host lattice, resulting in a periodic 'Peierls' barrier to migration



- If $L > 2E_{\text{kink}}/V$, minimum energy path is **kink nucleation**

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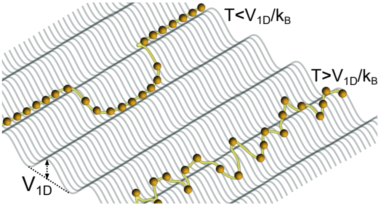
The Frenkel-Kontorova model

- Kink-limited dislocations well captured by the **FK model**

- Line of nodes $\mathbf{x}$=$[\mathrm{x}_1, \mathrm{x}_2 ... \mathrm{x}_N] \in \mathbb{R}^{\mathrm{N}}$ with fixed spacing b

$$U(\mathbf{x}) = \underbrace{\frac{\kappa}{2b^2}\sum_{ij} \mathrm{x}_i \mathrm{K}_{ij} \mathrm{x}_j}_{\text{Interaction}} + \underbrace{\sum_i \mathrm{V}_{1\mathrm{D}}(\mathrm{x}_i)}_{\text{Lattice Potential}}$$



- Integrate with Langevin dynamics

$$\gamma\dot{\mathrm{x}}_i = -\nabla_i U(\mathbf{x}) + b\sigma + \sqrt{2\gamma\beta^{-1}}\dot{W}_i \qquad (b\sigma = \text{Applied Stress})$$

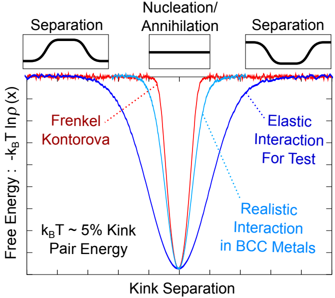
- Kink Energy $E_k \sim \sqrt{\kappa|V_{1\mathrm{D}}|}$, Width $w_k \sim \sqrt{\kappa/|V_{1\mathrm{D}}|}$, 'Discreteness' $\sim e^{-w_k/b}$

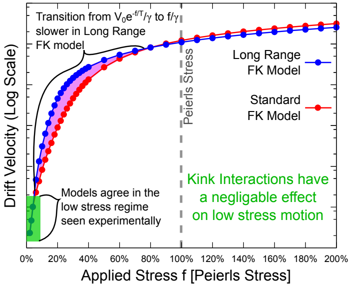
- Parametrize from MD/DFT (TDS *et al.* PRB 2013, Dezerald *et al.* PRB 2015)

The Frenkel-Kontorova model

- Classic FK couples neighbors; other options $K_{ij} = 1/N - \delta_{ij}$ (Curie-Weiss) or

$$\mathbf{x}\cdot\mathbf{K}\cdot\mathbf{x} = \underbrace{\sum_i (x_{i+1}-x_i)^2}_{\text{Classic FK } \to b^2|\nabla x(s)|^2} \to \underbrace{\sum_{ij} \frac{(x_{i+1}-x_i)(x_{j+1}-x_j)}{\sqrt{1+(i-j)^2/\alpha^2}}}_{\text{Elastic } 1/d \text{ Kink Interaction}} \qquad \underbrace{\omega(k) \to ck\sqrt{K_0(k/\alpha)}}_{\text{Dispersion (TDS Thesis 2015)}}$$





- $\Rightarrow$ kink interaction weakly perturbs low stress drift (more work needed!)

Transport in the FK model

- Natural quantity of interest: transport of **center of mass** $\bar{\mathrm{x}} \equiv \sum_i \mathrm{x}_i/N$
- Transport: $\sigma = 0 \Rightarrow \langle(\Delta\bar{\mathrm{x}})^2\rangle \to 2\bar{D}\Delta t \qquad \sigma \neq 0 \Rightarrow \langle\Delta\bar{\mathrm{x}}\rangle \to \bar{\mu}\Delta t$
- $\bar{x}$ naturally isolated in **eigenbasis of K** as zero eigenmode:

$$\mathsf{K}\cdot\hat{\mathbf{v}}_k = \lambda_k\hat{\mathbf{v}}_k, \quad a_k = \hat{\mathbf{v}}_k\cdot\mathbf{x}, \quad \bar{x} = a_0/\sqrt{N}, \quad \lambda_0 \equiv 0$$

- System periodic so reduced density $\rho(\bar{x})$ (n.b. $F(\bar{x}) = -\beta^{-1}\ln\rho(\bar{x})$) periodic:

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

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

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Multiscale Analysis

- Consider the coarse-grained coordinate $\chi \equiv \epsilon \bar{x} \in \mathbb{R}$, $\epsilon \ll 1$ and rescaled time

$$t \rightarrow \frac{t}{\epsilon} \qquad (\text{Drift}: \quad \epsilon \partial_t \phi = \epsilon \mu \partial_\chi \phi),$$

$$t \rightarrow \frac{t}{\epsilon^2} \qquad (\text{Diffusion}: \quad \epsilon^2 \partial_t \phi = \epsilon^2 D \partial_\chi^2 \phi).$$

- As $t \rightarrow \infty$ ($\equiv \epsilon \rightarrow 0$), χ is independent from rapidly oscillating $\bar{x}$.
- The adjoint Fokker-Planck then admits the multiscale solution (as $\epsilon \rightarrow 0$)

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

as detailed in book by Pavliotis and Stuart (2008)

- We find **analytical** bounds on $\bar{D}$ and an accurate ansatz for $\bar{\mu}$
- TD Swinburne, Phys. Rev. E 88, 012135 (2013)

Multiscale Analysis

- We work in **eigenbasis**: $\hat{\mathsf{v}}_l \cdot \mathsf{K} \cdot \hat{\mathsf{v}}_k = \lambda_k \delta_{lk},\ a_k = \hat{\mathsf{v}}_k \cdot \mathsf{x},\ \bar{x} = a_0/\sqrt{N},\ \lambda_0 \equiv 0$
- Energy is then $U(\bar{x}, \{a_k\}) = \sum_k \frac{\lambda_k^2}{2} a_k^2 + \sum_i V_{1\mathrm{D}}\left(\bar{\mathsf{x}} + \sum_k a_k [\hat{\mathsf{v}}_k]_i\right)$ with aFP

$$N\beta\gamma \frac{\partial \Phi}{\partial t} \equiv \hat{L}_{\mathrm{aFP}} \Phi = -\beta \frac{\partial U}{\partial \bar{\mathsf{x}}} \frac{\partial \Phi}{\partial \bar{\mathsf{x}}} + \frac{\partial^2 \Phi}{\partial \bar{\mathsf{x}}^2} + N \sum_k -\beta \frac{\partial U}{\partial a_k} \frac{\partial \Phi}{\partial a_k} + \frac{\partial^2 \Phi}{\partial a_k^2}$$

- Fluctuations $\{a_k\} \in \mathbb{R}^{\mathrm{N}-1}$ have quadratic confinement but $\bar{\mathsf{x}}$ unbound
- With slow $\chi = \epsilon \bar{\mathsf{x}}$ and rescaling $t \to t/\epsilon^2$ we have multiscale aFP for Φ_ϵ

$$N\beta\gamma \frac{\partial \Phi_\epsilon}{\partial t} = \frac{\partial^2 \Phi_\epsilon}{\partial \chi^2} + \frac{2}{\epsilon} \frac{\partial^2 \Phi_\epsilon}{\partial \chi \partial \bar{\mathsf{x}}} - \frac{\beta}{\epsilon} \frac{\partial U}{\partial \bar{\mathsf{x}}} \frac{\partial \Phi_\epsilon}{\partial \chi} + \frac{1}{\epsilon^2} \hat{L}_{\mathrm{aFP}} \Phi_\epsilon$$

Multiscale Analysis

- With $\Phi_\epsilon = \Phi_0 + \epsilon\Phi_1 + \epsilon^2\Phi_2 + ...$ hierarchy of aFP equations as $\epsilon \to 0$:

$$O\left(\frac{1}{\epsilon^2}\right) : \hat{L}_{\mathrm{aFP}}\Phi_0 = 0 \quad \Rightarrow \Phi_0 = \Phi_0(t,\chi)$$

$$O\left(\frac{1}{\epsilon}\right) : \hat{L}_{\mathrm{aFP}}\Phi_1 - \beta\frac{\partial U}{\partial \bar{\mathrm{x}}}\frac{\partial \Phi_0}{\partial \chi} = 0 \ \Rightarrow \Phi_1 = \phi(\bar{\mathrm{x}}, \{a_k\})\Phi_0, \quad \hat{L}_{\mathrm{aFP}}\phi = \frac{\partial U}{\partial \bar{\mathrm{x}}}$$

$$O(1) : \hat{L}_{\mathrm{aFP}}\Phi_2 + \frac{\partial^2\Phi_0}{\partial\chi^2} + 2\frac{\partial^2\Phi_1}{\partial\chi\partial\bar{\mathrm{x}}} - \beta\frac{\partial U}{\partial \bar{\mathrm{x}}}\frac{\partial \Phi_1}{\partial \chi} = N\beta\gamma\frac{\partial\Phi_0}{\partial t}$$

$$\Rightarrow N\beta\gamma\frac{\partial\Phi_0}{\partial t} = \left[\int_{\mathrm{x},\{a_k\}}\rho_\infty\left(1+\frac{\partial\phi}{\partial\bar{\mathrm{x}}}\right)\right]\frac{\partial^2\Phi_0}{\partial\chi^2}, \quad \rho_\infty = e^{-\beta U}/Z.$$

- We find (with an additional integration by parts) two expressions for $\bar{D}$:

$$(N\beta\gamma)\bar{D} = \int_{\mathrm{x},\{a_k\}}\rho_\infty\left(1+\frac{\partial\phi}{\partial\bar{\mathrm{x}}}\right) = \int_{\mathrm{x},\{a_k\}}\rho_\infty\left[\left(1+\frac{\partial\phi}{\partial\bar{\mathrm{x}}}\right)^2 + \sum_k\left(\frac{\partial\phi}{\partial a_k}\right)^2\right]$$

Multiscale Analysis - bounds for $\tilde{D}$

- Bounds from *two* Cauchy-Schwartz inequalities for $f(\bar{\mathrm{x}},\{a_k\}), g(\bar{\mathrm{x}},\{a_k\})$

$$\left(\int_{\bar{\mathrm{x}},\{a_k\}}\rho_\infty fg\right)^2 \leq \left(\int_{\bar{\mathrm{x}},\{a_k\}}\rho_\infty f^2\right)\left(\int_{\bar{\mathrm{x}},\{a_k\}}\rho_\infty g^2\right)$$

as f, g admit a Fourier expansion in $\bar{\mathrm{x}}$ one can also show

$$\left(\int_{\{a_k\}}\rho_\infty fg\right)^2 \leq \left(\int_{\{a_k\}}\rho_\infty f^2\right)\left(\int_{\{a_k\}}\rho_\infty g^2\right) \quad \forall\,\bar{\mathrm{x}} \in [0,a]$$

- Also define 'vibrational averages' of $V(\bar{\mathrm{x}},\{a_k\}) = \sum_i V_{1\mathrm{D}}\left(\bar{\mathrm{x}} + \sum_k a_k[\hat{\mathbf{v}}_k]_i\right)$

$$\langle e^{\pm\beta V};\bar{\mathrm{x}}\rangle_\lambda \equiv Z_\lambda^{-1}\int_{\{a_k\}} e^{\pm\beta V(\bar{\mathrm{x}},\{a_k\})-\beta\sum_k\lambda_k a_k^2/2} \quad \Rightarrow Z \equiv Z_\lambda \oint_{\bar{\mathrm{x}}}\langle e^{-\beta V};\bar{\mathrm{x}}\rangle_\lambda$$

Multiscale Analysis - bounds for $\tilde{D}$

- We first note that as $\phi \in \mathbb{R}$

$$\tilde{D} = \int_{x,\{a_k\}} \rho_\infty \left[\left(1+\frac{\partial\phi}{\partial\bar{x}}\right)^2 + \sum_k \left(\frac{\partial\phi}{\partial a_k}\right)^2\right] \geq \int_{x,\{a_k\}} \rho_\infty \left(1+\frac{\partial\phi}{\partial\bar{x}}\right)^2$$

- Applying the first CSI to $\int_{x,\{a_k\}} \rho_\infty \left(1+\frac{\partial\phi}{\partial\bar{x}}\right) e^{+\beta V} = a \left(\oint_{\bar{x}} \langle e^{-\beta V};\bar{x}\rangle\right)^{-1}$ gives

$$\tilde{D} \geq \tilde{D}_L = a^2 \left(\oint_{\bar{x}} \langle e^{-\beta V};\bar{x}\rangle \oint_{\bar{x}} \langle e^{+\beta V};\bar{x}\rangle\right)^{-1}$$

- Applying the second CSI to $\int_{\{a_k\}} \rho_\infty \left(1+\frac{\partial\phi}{\partial\bar{x}}\right) = \tilde{D}/a$ (from $\rho\hat{L}\phi = \rho\frac{\partial U}{\partial\bar{x}}$)

$$\tilde{D} \leq \tilde{D}_U = a^2 \left(\oint_{\bar{x}} \langle e^{-\beta V};\bar{x}\rangle \oint_{\bar{x}} \langle e^{-\beta V};\bar{x}\rangle^{-1}\right)^{-1}$$

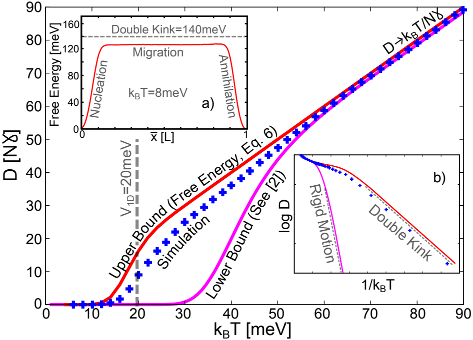
Multiscale Analysis - bounds for $\tilde{D}$

- Defining the **free energy profile** $F(\bar{x}) = -\beta^{-1} \ln |Z_\lambda \langle e^{-\beta V}; \bar{x} \rangle|$ we have

$$\frac{a^2}{\oint_{\bar{x}} e^{-\beta F} \oint_{\bar{x}} \langle e^{+\beta V}; \bar{x} \rangle} \leq \tilde{D} \leq \frac{a^2}{\oint_{\bar{x}} e^{-\beta F} \oint_{\bar{x}} e^{+\beta F}}$$

- C.f. 1D result $\tilde{D}_{1D} = a^2 \left(\oint e^{-\beta V} \oint e^{+\beta V} \right)^{-1}$ $\Rightarrow$ **$\tilde{D}_U$ is 1D diffusion in F(x)**

- We find $\tilde{D}_U$ a tight upper bound for **short lines** ($n_{kinks} \in [0, 2]$ when $\beta E_k \ll 1$)

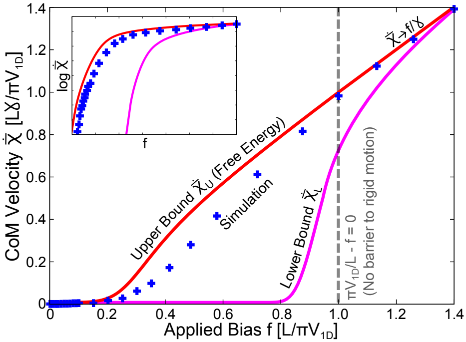


Multiscale Analysis - suggestion for $\tilde{\mu}$

- $\tilde{D}_U$ is 1D diffusion in $F(x)$. 1D drift (Stratonovich 1967) **suggests**

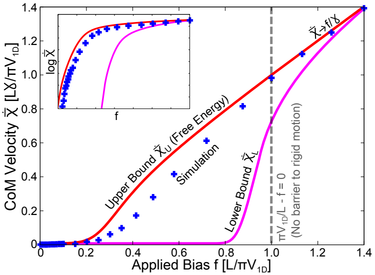
$$\tilde{\mu} = \beta\gamma\mu \leq \tilde{\mu}_U = \frac{a(1 - e^{-\beta Nab\sigma})}{\oint_{\bar{x}} e^{-\beta F(\bar{x}) + \beta Nab\sigma\bar{x}} \int_{\bar{x}}^{\bar{x}+a} e^{\beta F(\bar{y}) - \beta Nab\sigma\bar{y}}}$$

- Again, $\tilde{\mu}_U$ a tight upper bound for **short lines** ($n_{kinks} \in [0, 2]$ when $\beta E_k \ll 1$)

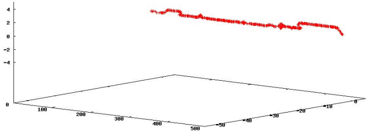


Multiscale Analysis - open questions

- Only rigorous transport result are overdamped bounds on *D*



- Proof of suggested drift bounds?
- Better coordinate than $\bar{x}$ for longer lines? (see later)
- Applications with exotic K_{ij}?
- Underdamped dynamics?
- Higher dimensional dislocation motion (cross slip)?
- Obstacles (see later)?



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Atomistic calulation of free energies

- $F(\bar{x})$ can represent FK dynamics **when $\bar{x}$ is a good reaction coordinate** (r)
- For kink nucleation, this means if $\bar{x} \leftrightarrow$ kink separation, $r = \bar{x}$ is OK
- With 'good' r and free energy profile $F(r)$ we recover TST rate $k(\beta)$:

$$\Delta F \equiv \max_r [F(r) - F(0)], \quad k(\beta) = \omega e^{-\beta \Delta F(\beta)}$$

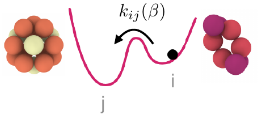
- *Harmonic* TST takes real modes $\{\omega_i(r)\}$ along minimum energy path:

$$k(\beta) \to \frac{\prod_{\omega \in \mathbb{R}} \omega_i(0)}{\prod_{\omega \in \mathbb{R}} \omega_i(r_{max})} e^{-\beta \Delta U}$$

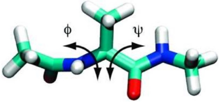
- Given start/end states, NEB method (Henkelman *et al.* JCP 2000) can find MEP $\mathbf{X}_0(r) \in \mathbb{R}^{3N}$, where affine parameter r is a good reaction coordinate
- HTST can be very useful but validity is hard to predict. **Calculate true ΔF**?

Atomistic calulation of free energies

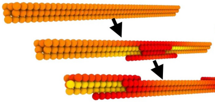
- Rare events are ubiquitous in materials science

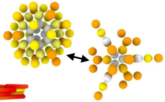


- Transition state theory rates require ΔF : $k_{ij}(\beta) = \omega_{ij} \exp\left[-\beta \Delta F(\mathrm{T})\right]$
- Harmonic approx. $\Delta F_{\mathrm{harm}}(\mathrm{T}) = \Delta U + \mathrm{k_B T} \Delta \ln \Pi_i \omega_i$ **often inaccurate**
- Anharmonic calculations (FT string, metadynamics, ABF) typically need one/many **collective variables** that capture the transition in question
- CV approach best for bio/chem
(small number of large fluctuations)



- But often impossible for crystal defects
(large number of small fluctuations)





Atomistic calulation of ΔF (with M-C Marinica, CEA Saclay)

- At 0K we calculate the **MEP** $\mathbf{X}_0(r) \in \mathbb{R}^{3N}$ between $\mathbf{X}_0(0), \mathbf{X}_0(1)$ with e.g. NEB

- Virtual work along MEP tangent : $U(r) - U(0) = \int_0^r \boldsymbol{\nabla} V(\mathbf{X}_0(r')) \cdot \partial_{r'} \mathbf{X}_0(r') \mathrm{d}r'$

- Can we do the same at finite T for **free energy barrier** ΔF?
  Yes, with key result from **ABF method** Darve *et al.* JCP 2008

- If one has a function $\xi(\mathbf{X}) = r$, can show for *any* $\mathbf{w} \in \mathbb{R}^{3N}$ s.t. $\mathbf{w} \cdot \boldsymbol{\nabla}\xi > 0$

$$\partial_r F(r) = \left\langle \frac{\mathbf{w} \cdot \boldsymbol{\nabla} V}{\mathbf{w} \cdot \boldsymbol{\nabla}\xi} + \beta^{-1} \boldsymbol{\nabla} \cdot \frac{\mathbf{w}}{\mathbf{w} \cdot \boldsymbol{\nabla}\xi} \right\rangle_{\xi(\mathbf{X})=r}, \quad \Delta F \equiv \max_{r\in[0,1]} \int_0^r \partial_{r'} F(r') \mathrm{d}r'$$

- But need $\boldsymbol{\nabla}\xi$ and 2nd term is $O(N^2)$- a big problem in high dimension

- However, for crystal defects, the MFEP at T>0K is often 'close' to the MEP

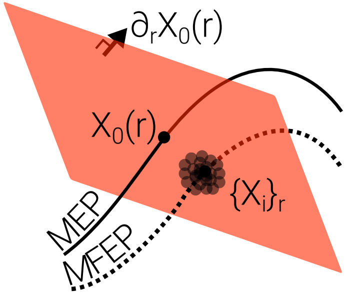
Atomistic calulation of ΔF (with M-C Marinica, CEA Saclay)

- New reformulation with $\mathbf{w} = \partial_r \mathbf{X}_0$ and $\xi(\mathbf{X}) \equiv \min_r |\partial_r \mathbf{X}_0 \cdot [\mathbf{X} - \mathbf{X}_0(r)]|^2$

$$\partial_r F(r) = \left\langle \psi(\mathbf{X}, r)\partial_r \mathbf{X}_0 \cdot \nabla U + \beta^{-1}\partial_r \ln \frac{|\psi(\mathbf{X}, r)|}{|\partial_r \mathbf{X}_0|} \right\rangle_r, \quad \Delta F \equiv \max_{r\in[0,1]} \int_0^r \partial_{r'} F(r')\mathrm{d}r'$$

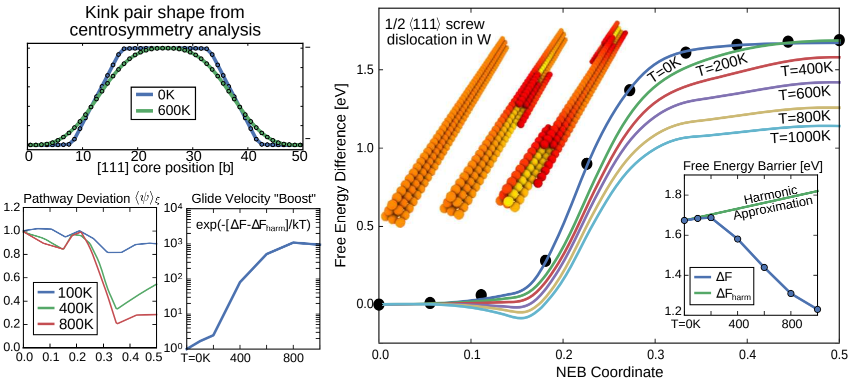
where $\langle \psi(\mathbf{X}, r)\rangle_r = \dfrac{\partial_r \mathbf{X}_0 \cdot \partial_r \langle \mathbf{X}\rangle_r}{|\partial_r \mathbf{X}_0|^2}$ i.e. projection of MFEP and MEP tangents

- We require $\Psi > 0$ (i.e. MFEP $\not\perp$ MEP)
- In general, *any* $\Psi > 0$ path is fine, permitting iterative scheme for high T
- TDS and Marinica PRL 2018



Atomistic calulation of ΔF (with M-C Marinica, CEA Saclay)

- Method permits large calculations (>10^5 atoms), for e.g. dislocation motion

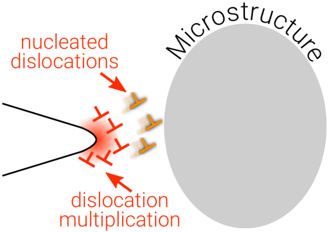


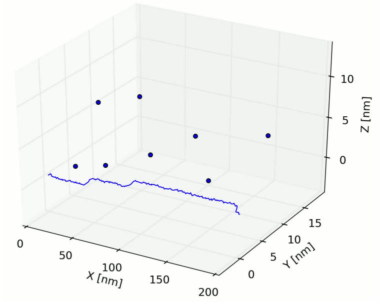
TDS and M-C Marinica, PRL 2018

- Constrained overdamped Langevin dynamics performed on parallelized ensemble with `PAFI-LAMMPS` code: email me if interested!

Free energy barriers → brittle to ductile transition

- $\Delta F = 2F_k$ has large σ, β dependence
- Poisson models $v \sim e^{-\beta\Delta F}$ able to capture dislocation motion ($\beta F_k \ll 1$)
- Validation of empirical relations for ΔF (e.g. Po *et al.* IJP 2016)
- But how do we connect these calculations to the BDT?
- We need the effect of **obstacles** on kink limited dislocation motion





Outline

- Dislocations and Fracture
- The Frenkel-Kontorova Model
- Multiscale analysis of FK transport
- Atomistic calulation of free energies
- Kink-limited motion through obstacles
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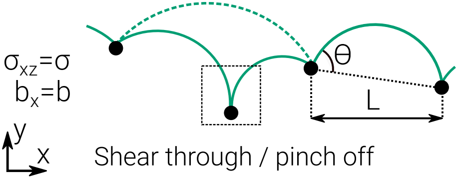
Orowan strengthening (with SL Dudarev, CCFE)

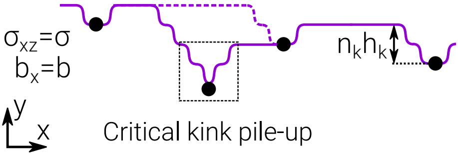
- The classic model of obstacle hardening treats dislocations as elastic lines which pin and **bow out** under stress (e.g. Nogaret and Rodney PRB 2006)



- To pin, obstacle must balance the dislocation PK force $\sim \mu b^2 \cos\Theta = Lb\sigma$
- We pinch off at $\Theta = \pi/2 \Rightarrow$ **flow stress** $\sigma_f = \alpha\mu b/L$, where $\alpha \in [0, 1]$
- **For $\sigma < \sigma_f$, dislocations do not move at any temperature**

Kink-limited Orowan strengthening (with SL Dudarev, CCFE)

- With a kink mechanism, dislocations no longer bow out (due to the Peierls potential) but still nucleate kinks, forming **kink pileups** at pinning points



- A pileup of n_k kinks induces a force of $n_k h_k \sigma b$ on an obstacle
- Bypass condition is therefore a threshold kink pile up size
- Pileup growth controlled by **dislocation velocity**, given in Poisson limit by

$$\langle \mathrm{v}_{\mathrm{dislo}}(\sigma, T, L)\rangle = \lim_{t\to\infty} \frac{v_k h_k}{tL} \int n_k(t)\mathrm{d}t = \frac{v_k h_k}{L} \langle n_k(\sigma, T, L)\rangle = h_k \Gamma_k(\sigma, T, L)$$

Generalized nucleation rate Γ_k or expected kink population $\langle n_k \rangle$

Kinks on a line (with SL Dudarev, CCFE)

- To find $\langle n_k(\sigma, T, L)\rangle$ we consider the partition function (with $\tilde{N} = L/b$ sites)

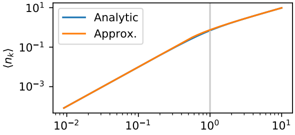
$$Z = \sum_{r=0}^{\tilde{N}/2} \frac{\tilde{N}!}{(\tilde{N}-2r)!(2r)!} e^{-2r\beta F_k} = \frac{1}{2}\left[1+e^{-\beta F_k}\right]^{\tilde{N}} + \frac{1}{2}\left[1-e^{-\beta F_k}\right]^{\tilde{N}}$$

- Distinguishable kinks $(2r)! \to (r!)^2$: $Z = \oint (1 + 2e^{-\beta F_k}\cos\Theta)^{\tilde{N}} \to I_0(2\tilde{N}e^{-\beta F_k})$

- Analytical velocity is *extremely* well approximated by stitching limiting cases

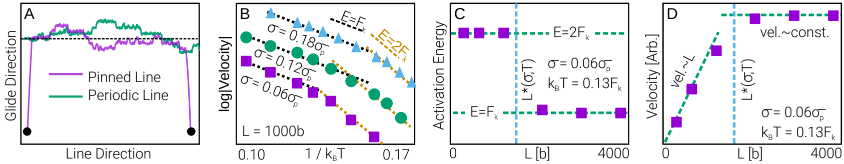
$$\langle v_k(\sigma, T, L)\rangle = \frac{v_k h_k}{L}\frac{\partial \ln Z}{\partial(-\beta F_k)} \simeq \begin{cases} h_k \omega \tilde{N} e^{-2\beta F_k(\sigma,\beta)} & L \leq L^*(\sigma,\beta) \\ h_k \omega e^{-\beta F_k(\sigma,\beta)} & L \geq L^*(\sigma,\beta)\end{cases}$$

- Critical quantity: **crossover** $L^*(\sigma, \beta) = b e^{\beta F_k(\sigma,\beta)}$



Length dependent mobility (with SL Dudarev, CCFE)

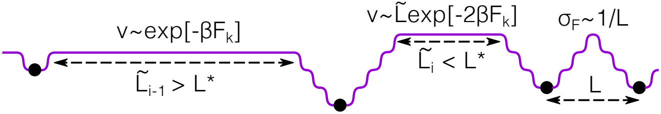
- We also used the Frenkel-Kontorova model to study longer lines numerically



- Simulations and theory agree: U_{dislo} **halves when dislocation is longer than**

$$L^*(\sigma, T) = b \exp\left(\beta F_k(\sigma, T)\right)$$

- Thus an additional spacing-dependent regime of kink-limited obstacle bypass at $L > L^*$ to the two seen in DD (Monnet *et al.* Acta Mat. 2010)



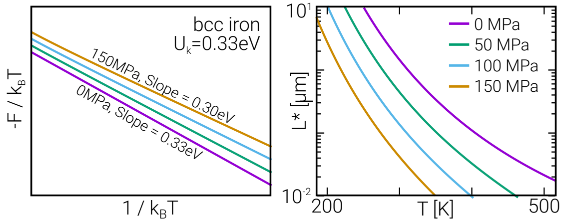
Length dependent mobility (with SL Dudarev, CCFE)

- Simulations and theory agree: **U_{dislo} : $2F_k \rightarrow F_k$ when length exceeds**

$$L^*(\sigma, T) = b \exp\left(\beta F_k(\sigma, T)\right)$$

- This is where our calculations of the σ, T dependence of F_k are useful..

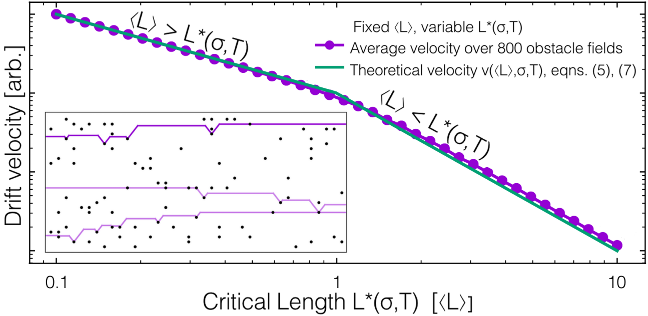
- We find the crossover **L^* can be $\ll$ μm under realistic σ, T regimes whilst leaving Arrhenius measurements almost unchanged at $U_k(\sigma = 0)$**



- Existence of L^* previously recognized (e.g. Hirth&Lothe, Dorn&Rajnak) but we find relevance in detailed, quantitative analysis of crossover length

Modified Orowan flow law (with SL Dudarev, CCFE)

- We used the $v_{\mathrm{dislo}}(L, \sigma, \mathrm{T})$ in kink-limited dislocation-obstacle simulations



- This evidenced the **modified Orowan flow law**

$$\dot{\epsilon} = \begin{cases} \rho_{\mathrm{dislo}} \mathrm{b} \langle \mathrm{L} \rangle \omega_0 \exp\left[-2\beta \mathrm{F_k}(\boldsymbol{\sigma}, \mathrm{T})\right] & \langle \mathrm{L} \rangle \leq \mathrm{L}^*(\boldsymbol{\sigma}, \mathrm{T}) \\ \rho_{\mathrm{dislo}} \mathrm{b}^2 \omega_0 \exp\left[-\beta \mathrm{F_k}(\boldsymbol{\sigma}, \mathrm{T})\right] & \langle \mathrm{L} \rangle \geq \mathrm{L}^*(\boldsymbol{\sigma}, \mathrm{T}) \end{cases}$$

Modified Orowan flow law (with SL Dudarev, CCFE)

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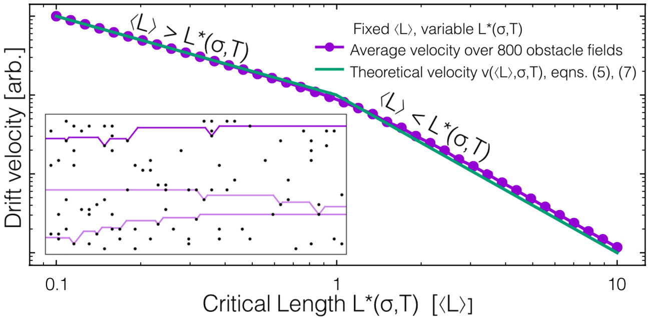

- N.B. analytical expression for $\langle L \rangle$ is obstacle strength (n_{th}) dependent

$$\langle L \rangle = \frac{\mathrm{n}_{\text{th}} w_k}{2} \left[\frac{\mathrm{erf}(\sqrt{\phi})}{2\sqrt{\phi/\pi}} + \frac{2+\phi}{\phi} \mathrm{e}^{-\phi} \right], \; \phi = \mathrm{c}\mathrm{n}_{\text{th}}^2 w_k h_k$$

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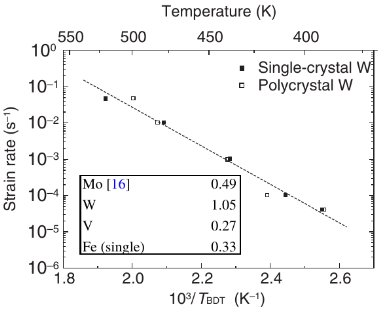
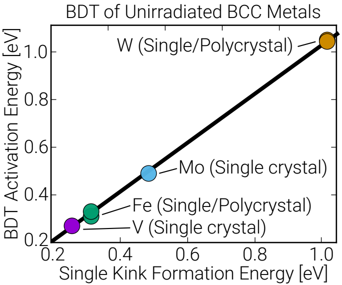
Comparison to experiment (with SL Dudarev, CCFE)

- For unirradiated, unworked materials, we expect $\langle L \rangle \geq L^*$ and therefore

$$\log_e |\dot{\epsilon}_{\mathrm{unirr}}(\mathrm{T}_{\mathrm{BDT}})| = \ln |\rho b^2| - \beta_{\mathrm{BDT}} F_k$$
$$\simeq A - \beta_{\mathrm{BDT}} U_k \quad \Rightarrow \quad \mathrm{U}_{\mathrm{dislo}} = \mathrm{U}_{\mathrm{k}}$$

- We find **striking agreement** with BDT fracture data and DFT calulations
  Giannattasio *et al.* Phys. Scr. 2007, Dezerald *et al.* PRB 2015





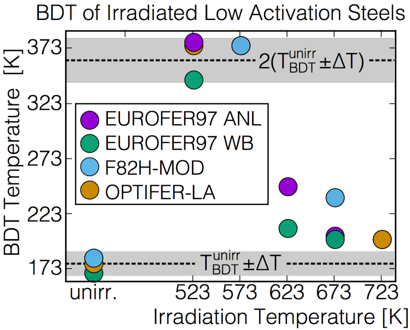
Comparison to experiment (with SL Dudarev, CCFE)

- For irradiated materials, where $\langle L \rangle$ is reduced, equating dislocation velocities at the BDT before and after irradiation yeilds

$$\mathrm{T}^{\mathrm{irr}}_{\mathrm{BDT}} = \frac{2F_k}{F_k/\mathrm{T}^{\mathrm{unirr}}_{\mathrm{BDT}} + \ln|\langle L \rangle / b|} \lesssim 2\mathrm{T}^{\mathrm{unirr}}_{\mathrm{BDT}}$$

- We find qualitative agreement with BDT data on RAFM steels Gaganidze *et al.* 2006

- Lack of detailed microstructural analysis / well defined loading makes comparison harder



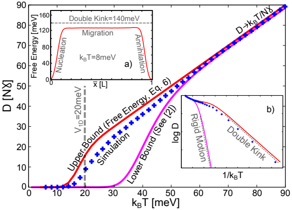
- Agreement across many steels $\Rightarrow$ **geometry influences BDT $\gtrsim$ chemistry?**

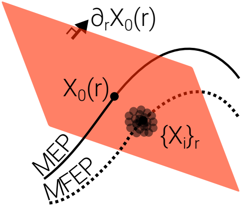
Thank you for listening

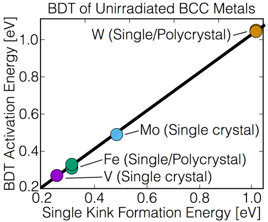
- **Multiscale analysis for the FK chain**
- Homogenized aFP for $\bar{x}$
- Exact bounds for FK $\tilde{D}$
- Many open problems
- TDS PRE 2013

- **Free energy barriers**
- ΔF from simple NEB
- Non-trivial pathways
- `LAMMPS-PAFI` code
- TDS and M-C Marinica, PRL 2018

- **Modelling the BDT**
- Kink-limited obstacle hardening model
- FK + stat. mech. explains diverse BDT experiments
- TDS and SL Dudarev, PRMaterials 2018







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