Kink-limited Orowan strengthening and the brittle to ductile transition of irradiated & unirradiated bcc metals

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Helping to explain, not solve, the brittle to ductile transition of irradiated & unirradiated bcc metals

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Outline

- The brittle to ductile transition
- The kink mechanism
- Kink-limited Orowan strengthening
- Calculating the activation energy
- Modified Orowan flow law
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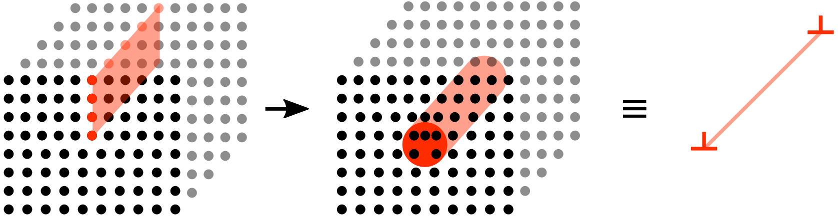
Dislocations

- Crystalline materials prefer to concentrate deformation in highly deformed "cores" with a **surrounding elastic field**

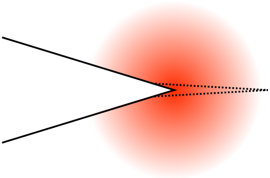


- The creation and migration of dislocations typically controls crystal plasticity

- Dislocations can carry away deformation, reducing the stress intensity

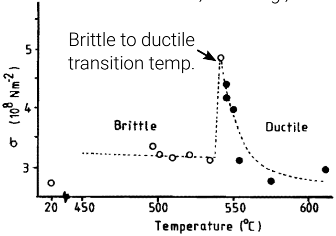
The brittle to ductile transition

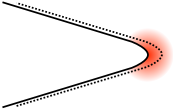
- The fracture toughness of many materials show a peak with temperature



Brittle cleavage

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

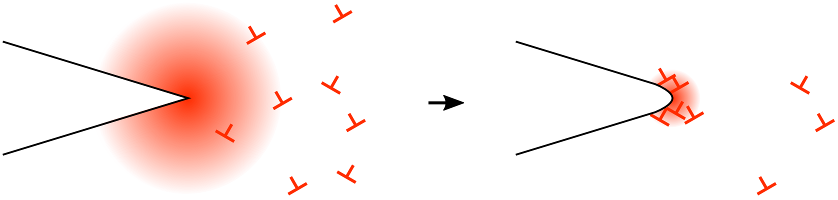




Ductile failure

The brittle to ductile transition

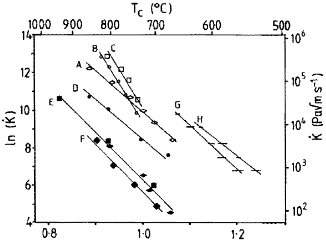
- Crack blunting requires the creation and motion of dislocations
- Hirsch and Roberts argued that existing dislocations migrate to a crack, where they emit dislocations that carry away deformation from the tip



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

The brittle to ductile transition

- 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})	Activation energy: 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: $\log_e \dot{\epsilon}_{\mathrm{ext.}}(\mathrm{T}_{\mathrm{BDT}}) = A - \mathrm{U}_{\mathrm{BDT}}/\mathrm{k}_{\mathrm{B}}\mathrm{T}_{\mathrm{BDT}}$

Dislocation velocity: $\log_e \mathrm{v}_{\mathrm{dislo}} = B - \mathrm{U}_{\mathrm{dislo}}/\mathrm{k}_{\mathrm{B}}\mathrm{T}$

Orowan Law: $\dot{\epsilon} = \mathrm{b}\rho_{\mathrm{dislo}}\mathrm{v}_{\mathrm{dislo}}, \quad \Rightarrow \quad \mathrm{U}_{\mathrm{dislo}} = \mathrm{U}_{\mathrm{BDT}}$

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

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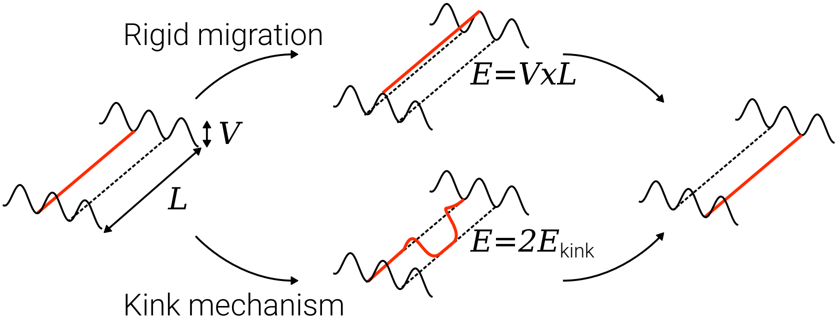
The kink mechanism

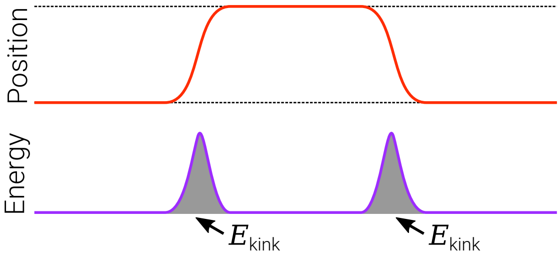
- The dislocation core energy varies periodically with the host lattice, resulting in a periodic 'Peierls' barrier to migration



- If $L > 2E_{\text{kink}}/V$, dislocations move by kink pair nucleation
- **In some cases** $U_{dislo} = 2E_{kink}$ **but we find in important limits** $U_{dislo} = E_{kink}$

The kink mechanism

- The energy of a separated kink pair is localized at the two kink sites



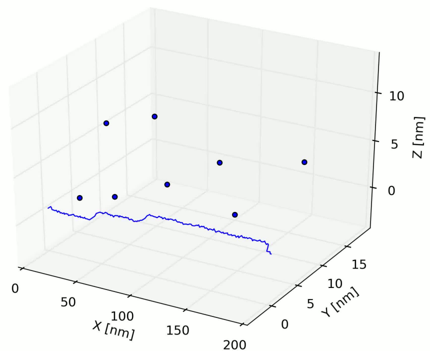
- As typically $E_{\text{kink}} \gg k_B T$, the kink nucleation rate is **thermally activated**

$$\Gamma(\sigma, T) = \omega \exp(-U_{\text{dislo}}(\sigma, T)/k_B T)$$
$$v_{\text{dislo}}(\sigma, T) = b\,(\Gamma(\sigma, T) - \Gamma(-\sigma, T)) \simeq b\Gamma(\sigma, T)$$

The kink mechanism

- The Hirsch Roberts model shows the BDT is controlled by dislocation mobility **through existing microstructure** (towards/away from cracks)

- We thus need to understand **kink-limited** motion through a field of obstacles



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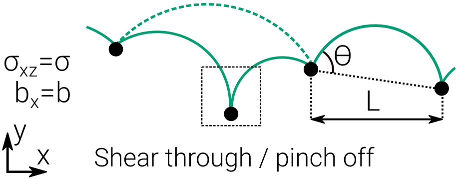
Orowan strengthening

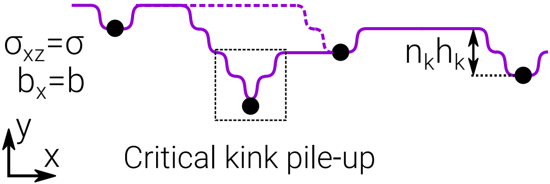
- The classic model of obstacle hardening ignores kinks, treating dislocations as elastic lines which glide, pin and **bow out** under an applied stress



- 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 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
- Flow condition is therefore a threshold kink pile up size
- **If kinks can nucleate, depinning is controlled by $\Gamma = \omega \exp\left(-U_{dislo}/k_B T\right)$**

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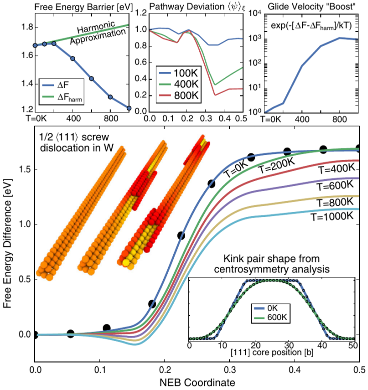
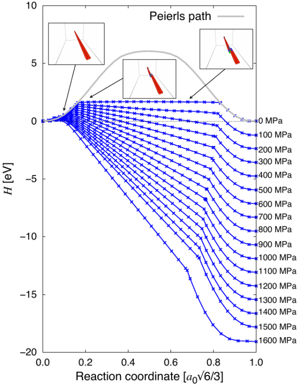
Calculating the activation energy

- Atomistic calculations can (with effort) evaluate $U_{\mathrm{dislo}}(\sigma, \mathrm{T})$ for **short lines**



TDS and M-C Marinica, PRL 2018



Stukowski *et al.* IJP 2016

- A significant dependence on applied stress and temperature is seen

Calculating the activation energy

- Atomistic calculations can be well modeled with a 'kink free energy' F_k

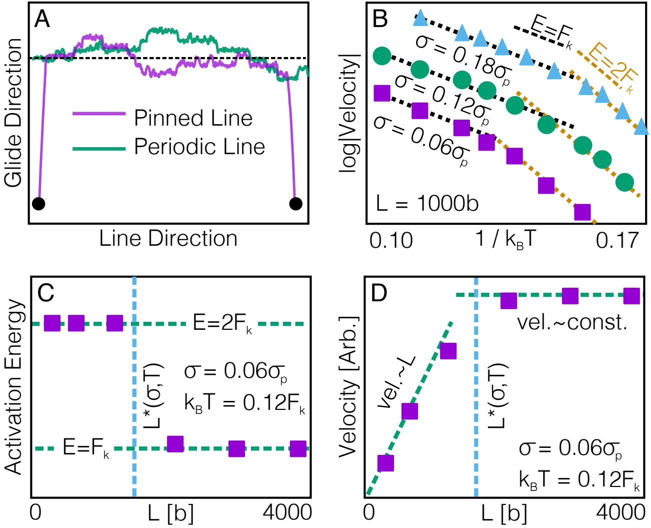
$$F_k(\sigma, \mathrm{T}) = U_k \left(1 - \frac{\mathrm{T}}{\mathrm{T}_{\mathrm{ath}}} - \frac{\sigma/\sigma_p}{1 - \mathrm{T}/\mathrm{T}_{\mathrm{ath}}}\right)$$

bcc Fe: $U_k = 0.33eV$, $\sigma_p \simeq 900$MPa and $T_{\mathrm{ath}} = 700K$

- $\Rightarrow$ **velocity for short segments**: $\mathrm{v}_{\mathrm{dislo}}(\mathrm{L}, \boldsymbol{\sigma}, \mathrm{T}) = \boldsymbol{\omega}\mathrm{L}\exp\left(-2\beta\mathrm{F}_{\mathrm{k}}(\boldsymbol{\sigma}, \mathrm{T})\right)$
- $\mathrm{v} \propto \mathrm{L}$ has been seen in TEM observations (Caillard, Acta Mat. 2010)
- However, still need to explore the full (σ, T, L) parameter space

Length dependent mobility

- We used the **Frenkel-Kontorova model** to study longer lines



Length dependent mobility

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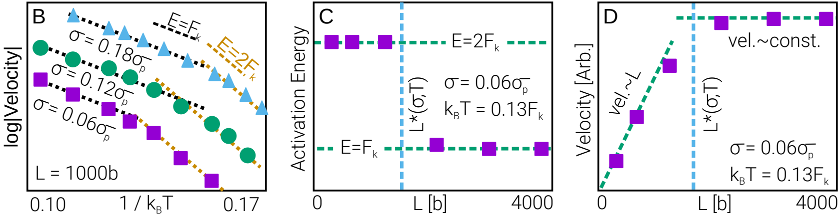


- Simulations and theory agree: **U_{dislo} halves when dislocation is longer than**

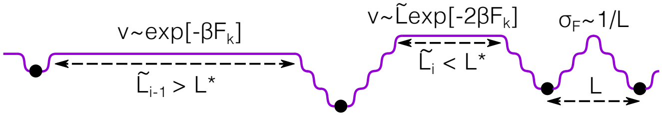
$$L^*(\sigma, \mathrm{T}) = b\exp\left(\beta F_k(\sigma, \mathrm{T})\right)$$

- **From atomistic/FK dislocation simulations we find a mobility law**

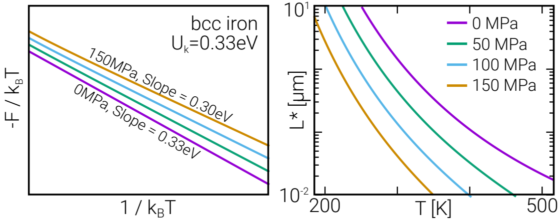
$$\mathrm{L} \leq \mathrm{L}^*(\boldsymbol{\sigma}, \mathrm{T}): \quad \mathrm{v_{dislo}}(\mathrm{L}, \boldsymbol{\sigma}, \mathrm{T}) = \mathrm{L}\omega_0 \mathrm{exp}\left[-2\beta \mathrm{F_k}(\boldsymbol{\sigma}, \mathrm{T})\right]$$
$$\mathrm{L} \geq \mathrm{L}^*(\boldsymbol{\sigma}, \mathrm{T}): \quad \mathrm{v_{dislo}}(\mathrm{L}, \boldsymbol{\sigma}, \mathrm{T}) = \mathrm{b}\omega_0 \mathrm{exp}\left[-\beta \mathrm{F_k}(\boldsymbol{\sigma}, \mathrm{T})\right]$$

Length dependent mobility

- As U_{dislo} halves when $L > \mathrm{L}^* = \mathrm{b}\exp\left(\beta \mathrm{F_k}(\sigma, \mathrm{T})\right)$, we find three regimes



- Importantly, the crossover L^* **can be $\ll \mu$m under realistic σ, T regimes whilst leaving Arrhenius measurements almost unchanged at $\mathrm{U_k}$**



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

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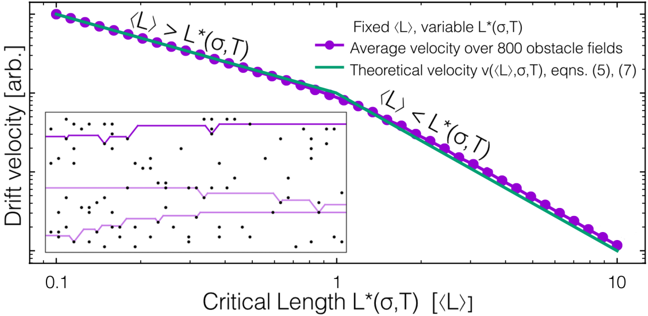
Modified Orowan flow law

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



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

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

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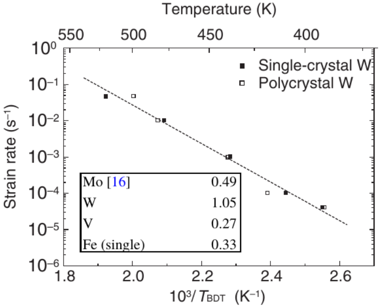
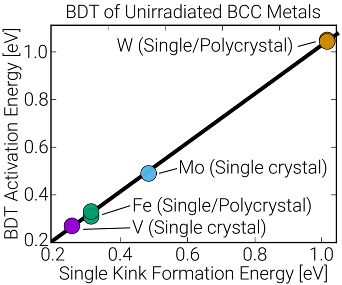
Comparison to experiment

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

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

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



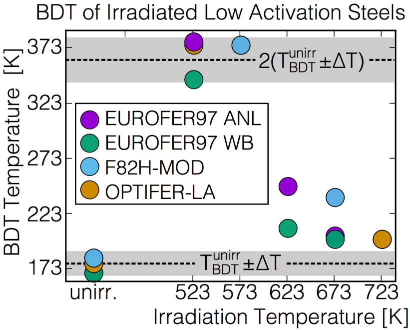


Comparison to experiment

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

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

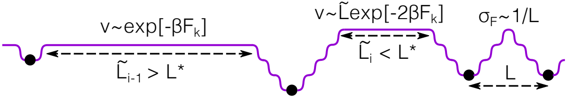
- We find qualitative agreement with BDT data on RAFM steels Gaganidze *et al.* 2006
- Lack of detailed microstructural analysis / well defined loading makes comparison harder



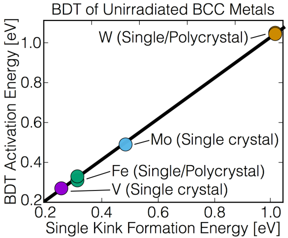
- Agreement across many steels $\Rightarrow$ **geometry influences BDT $\gtrsim$ chemistry?**

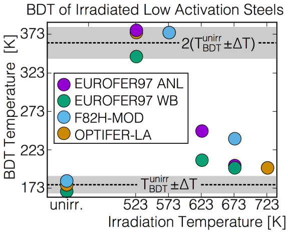
Thank you for listening

- Length dependent mobility law essential for kink-limited obstacle hardening



- *Existence* of L^* known but we find **L^* is routinely submicron $\Rightarrow$ influential**
- Modified Orowan law consistent with diverse BDT fracture experiments





- **Details: TDS and SLD, Physical Review Materials 2, 073608 (2018)**

`tiny.cc/tds110 tomswinburne@gmail.com`