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
- Comparison to experiment
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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

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

Brittle cleavage

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*

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Intrinsic Si ($2 \times 10^{11}$ Pcm$^{-3}$)</th>
<th>n-type Si ($2 \times 10^{18}$ Pcm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BDT (Samuels and Roberts 1989)</td>
<td>$2.1 \pm 0.1$ eV</td>
<td>$1.6 \pm 0.1$ eV</td>
</tr>
<tr>
<td>BDT (St John 1975)</td>
<td>$1.9$ eV</td>
<td>—</td>
</tr>
<tr>
<td>Dislocation velocity (George and Champier 1979)</td>
<td>$2.2$ eV</td>
<td>$1.7$ eV</td>
</tr>
<tr>
<td>Dislocation velocity (Imai and Sumino 1983)$^\dagger$</td>
<td>$2.3$ eV</td>
<td>$1.7$ eV</td>
</tr>
</tbody>
</table>

$^\dagger$ Doping levels used were $2 \times 10^{12}$ Bcm$^{-3}$ and $6.2 \times 10^{18}$ Pcm$^{-3}$

**BDT activation energy:**

\[
\ln \dot{\epsilon}_{\text{ext}}(T_{\text{BDT}}) = A - U_{\text{BDT}}/k_B T_{\text{BDT}}
\]

**Dislocation velocity:**

\[
\ln \dot{v}_{\text{dislo}} = B - U_{\text{dislo}}/k_B T
\]

**Orowan Law:**

\[
\dot{\epsilon} = b \rho_{\text{dislo}} \dot{v}_{\text{dislo}}, \quad \Rightarrow \quad U_{\text{dislo}} = U_{\text{BDT}}
\]

- But what is the activation energy $U_{\text{dislo}}$ 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

\[ E = V \times L \]

\[ E = 2E_{kink} \]

• If \( L > \frac{2E_{kink}}{V} \), dislocations move by kink pair nucleation

• In some cases \( U_{\text{dislo}} = 2E_{kink} \) but we find in important limits \( U_{\text{dislo}} = E_{kink} \)
The kink mechanism

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

![Diagram showing the energy distribution of kink pairs](image)

- 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.

\[ \sigma_{xz} = \sigma, \quad b_x = b \]

Shear through / pinch off

- To pin, obstacle must balance the dislocation PK force \( \sim \mu b^2 \cos \Theta = Lb\sigma \)

- We pinch off at \( \Theta = \pi/2 \) ⇒ **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 $\Gamma = \omega \exp \left( -\frac{U_{\text{dislo}}}{k_B T} \right)$. 

\[
\begin{align*}
\sigma_{xz} &= \sigma \\
b_x &= b \\
n_k h_k &\uparrow
\end{align*}
\]
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Calculating the activation energy

• Atomistic calculations can (with effort) evaluate $U_{\text{dislo}}(\sigma, T)$ 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’ $F_k$

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

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

• $\Rightarrow$ velocity for short segments: $v_{\text{dislo}}(L, \sigma, T) = \omega L \exp(-2/\beta F_k(\sigma, T))$

• $v \propto L$ has been seen in TEM observations (Caillard, Acta Mat. 2010)

• However, still need to explore the full $(\sigma, T, L)$ parameter space
Length dependent mobility

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

![Diagram](image)

**A**
- Glide Direction
- Pinned Line
- Periodic Line

**B**
- Log|Velocity|
- 
- \( E = F_k \)
- \( E = 2F_k \)
- \( \sigma = 0.06\sigma_p \)
- \( \sigma = 0.12\sigma_p \)
- \( \sigma = 0.18\sigma_p \)
- \( L = 1000b \)
- \( 0.10 \quad 1 / k_B T \quad 0.17 \)

**C**
- Activation Energy
- \( E = F_k \)
- \( E = 2F_k \)
- \( \sigma = 0.06\sigma_p \)
- \( k_B T = 0.12F_k \)
- \( L = 1000b \)

**D**
- Velocity [Arb.]
- Vel. ~ const.
- \( \sigma = 0.06\sigma_p \)
- \( k_B T = 0.12F_k \)
- \( L = 1000b \)
Length dependent mobility

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

\[ L^*(\sigma, T) = b \exp (\beta F_k(\sigma, T)) \]

- Simulations and theory agree: \( U_{\text{dislo}} \) halves when dislocation is longer than

\[ L \leq L^*(\sigma, T) : \quad v_{\text{dislo}}(L, \sigma, T) = L\omega_0\exp [-2\beta F_k(\sigma, T)] \]

\[ L \geq L^*(\sigma, T) : \quad v_{\text{dislo}}(L, \sigma, T) = b\omega_0\exp [-\beta F_k(\sigma, T)] \]
Length dependent mobility

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

  \[ v \sim \exp[-\beta F_k] \quad \text{for} \quad L > L^* \]

  \[ L_{i-1} > L^* \]

  \[ v \sim \exp[-2\beta F_k] \quad \text{for} \quad L_i < L^* \]

  \[ L < L^* \]

  \[ \sigma_F \sim 1/L \]

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

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

![Graph showing the relationship between $-F/k_BT$ and $1/k_BT$ with different pressures and their corresponding slopes.](image)

![Graph showing the relationship between $L^*$ and $T$ for different pressures.](image)
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Modified Orowan flow law

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

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

- This evidenced the modified Orowan flow law
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Comparison to experiment

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

$$\log_e |\dot{\varepsilon}_{\text{unirr}}(T_{\text{BDT}})| = \ln |\rho b^2| - \beta_{\text{BDT}} F_k$$

$$\simeq A - \beta_{\text{BDT}} U_k \quad \Rightarrow \quad U_{\text{dislo}} = U_k$$

- We find striking agreement with BDT fracture data and DFT calculations
  
Comparison to experiment

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

\[
T_{\text{BDT}}^{\text{irr}} = \frac{2F_k}{F_k/T_{\text{BDT}}^{\text{unirr}} + \ln |\langle L \rangle / b|} \leq 2T_{\text{BDT}}^{\text{unirr}}
\]

• 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

\[ v \sim \exp[-\beta F_k] \quad \tilde{\ell}_{i-1} > L^* \]

\[ v \sim \exp[-2\beta F_k] \quad \tilde{\ell}_i < L^* \]

\[ \sigma_F \sim 1/L \]

• 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)

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