At high T / under irradiation, plasticity involves dislocation climb → motion out of the glide plane → non conservative: absorption / emission of point defects

**Goal:** DD simulations with a dislocation climb model based on the diffusion of point defects

**1st step:** climb due to vacancy diffusion
1) Properties of jogged dislocation:
   structure, glide mobility, interaction with a vacancy
   ➔ what can we learn from atomistic simulations (EAM) ?

2) Climb mobility law (bulk diffusion)

3) DD simulations with climb
   - test cases
   - coarsening of a vacancy loop population
   - climb and glide

4) Climb associated with pipe diffusion

Most of the work in fcc metals (Al, Au, Cu, Ni)
Jogged Dislocation: Atomic Structure

Dislocation climb  
→ creation of two jogs

Classical picture:
Jog line perpendicular to dislocation glide plane

But
• in fcc metals  
  dissociated dislocation crystallography  
• in DD simulations  
  discretization length ~10b  
  → super jogs

\[ z = [\bar{1}11] \]
\[ y = [\bar{1}12] \]
\[ x = [110] \]
Jogged Dislocation: Atomic Structure

Super-jog in FCC structure:

- Jog line in compact (111) plane (tetrahedron face)
  - obtuse & acute jogs

\[
\begin{align*}
  x &= [1\bar{1}0] \\
  y &= [\bar{1}12] \\
  z &= [\bar{1}11]
\end{align*}
\]
Jogged Dislocation: Atomic Structure

Super-jog: height = 5 (111) planes

Structure in agreement with “line tension” description

P.B. Hirsch, Phil. Mag. 7 (1962), 67.
Jogged Dislocation: Atomic Structure

Super-jog in FCC structure:
- Jog line in compact (111) plane
  - both jogs dissociated
  - glissile configuration

$z = [\bar{1}11]$
$y = [\bar{1}12]$
$x = [110]$
Jogged Dislocation: Atomic Structure

Super-jog in FCC structure:
- Jog line in compact (111) plane
  - both jogs dissociated
  - glissile configuration
- Jog line = compact [110] direction
  (tetrahedron edge)

\[ z = [\bar{1}11] \]
\[ y = [\bar{1}12] \]
\[ x = [110] \]
Structure in agreement with “line tension” description
P.B. Hirsch, Phil. Mag. 7 (1962), 67.
Super-jog in FCC structure:

- Jog line in compact (111) plane
  - both jogs dissociated
  - glissile configuration

- Jog line = compact [110] direction
  - one dissociated jog (sessile?)
  - less stable
**Cu: jog of height $2d_{111}$**

Energy of the double jog (eV)

Most stable configuration of the acute and obtuse jog = glissile
Cu: variation of the jog energy with its height

Energy of the double jog (eV)

Jog height ($d_{111}$ units)
Jogged Dislocation: Atomic Structure

Jog: height = 1 (111) planes

Cu simulation box

\[ z = [\bar{1}11] \]
\[ y = [\bar{1}12] \]
\[ x = [110] \]

hcp (stacking fault)  dislocation core
Jogged Dislocation: Atomic Structure

Jog: height = 1 (111) planes

\[ x = [110] \]
\[ z = [1\bar{1}1] \]
\[ y = [\bar{1}12] \]

- hcp (stacking fault)
- dislocation core
Jogged Dislocation: Atomic Structure

**Jog: height = 1 \( (111) \) planes**

Cu simulation box

![Diagram of Cu simulation box with jogged dislocations](image)

- **z = [\overline{1}11]**
- **y = [\overline{1}12]**
- **x = [110]**

- Orange: hcp (stacking fault)
- Blue: dislocation core
Jogged Dislocation: Atomic Structure

Jog: height = 1 (111) planes

- Obtuse jog (tight)
- Acute jog (dissociated)

- hcp (stacking fault)
- dislocation core
Jogged Dislocation: Mobility

MD simulations (Parrinello-Rahman + Nosé-Hoover)

Cu, 300 K, 400 MPa

Simulation box
20x18x25 nm\(^3\)
~760 000 atoms

- 1 jog-free dislo
- 1 jogged dislo
  jog height = \(d_{111}\)

hcp (stacking fault)

dislocation core
Jogged Dislocation: Glide Properties

MD simulations (Parrinello-Rahman + Nosé-Hoover)

**Velocity (nm/ps)**

- Jog-free dislo
- Jog 1 $d_{111}$

**Stress (MPa)**

- Cu, 300 K
Jogged Dislocation: Glide Properties

MD simulations (Parrinello-Rahman + Nosé-Hoover)

Velocity (nm/ps)

Cu, 300 K

Stress (MPa)

Jog-free dislo
Jog 1 $d_{111}$
Jog 2 $d_{111}$
Jog 3 $d_{111}$
Jog 4 $d_{111}$
Jog 5 $d_{111}$
Jogged Dislocation – Vacancy Interaction

Jog: height = 1 (111) planes

- Obtuse jog (tight)
- Acute jog (dissociated)

hcp (stacking fault)  dislocation core
**Jogged Dislocation – Vacancy Interaction**

Cu simulation box

\[ x = [1\bar{1}0] \]
\[ z = [1\bar{1}1] \]
\[ y = [\bar{1}12] \]

\[ E_{V}^{\text{for}} = 1.272 \text{ eV} \]

\[ E_{V-D}^{\text{inter}} \] (eV)

\[ -1.274 \text{ eV} \]

\[ 0.114 \text{ eV} \]
Obtuse jog

$E_{jog} = 4.731 \text{ eV}$

- $x = [110]$
- $z = [\bar{1}11]$
- $y = [\bar{1}12]$

- $z = [\bar{1}11]$
- $y = [\bar{1}12]$
- $x = [110]$
Jogged Dislocation – Vacancy Interaction

Obtuse jog

Vacancy absorption

\[ E_{jog} = 4.731 \text{ eV} \]
\[ E_{jog} = 4.732 \text{ eV} \]
Obtuse jog

Vacancy absorption

\[ E_{\text{jog}} = 4.731 \text{ eV} \]

\[ E_{\text{jog}} = 4.732 \text{ eV} \]

\[ E_{\text{jog}} = 4.732 \text{ eV} \]
Jogged Dislocation – Vacancy Interaction

Acute jog

Vacancy absorption

$E_{\text{jog}} = 4.731 \text{ eV}$

Vacancy absorption

$E_{\text{jog}} = 4.733 \text{ eV}$

$E_{\text{jog}} = 4.732 \text{ eV}$
Dislocation Climb Rate: Vacancy Bulk Diffusion

Assumptions

- **segment** = infinite isolated straight dislocation
  - no interaction between the diffusion fields of different segments
- vacancy-dislocation elastic interaction neglected
- **jogs** and **pipe diffusion** not considered
  - dislocation = perfect sink for vacancies

Vacancy concentration

- far from the dislocation: $C_V^\infty$
- near the dislocation: $C_V^d = C_V^0 \exp \left( \frac{F_{cl} \Omega}{kT \sin(\theta)} \right)$

  $C_V^0$: vacancy equilibrium concentration
  $\Omega$: atomic volume
  $F_{cl} = \bar{F}_{PK} \cdot \bar{n}$: climb force (stress field)
  $\theta$: dislocation character

Climbing velocity

$$v_{cl} = M_{cl} \left( F_{cl} + F_{os} \right)$$

with  
$$F_{os} = \frac{kT}{\Omega} \left( 1 - \frac{C_V^\infty}{C_V^0} \right) b \sin \theta$$: osmotic force

$$M_{cl} = \frac{2\pi \Omega D_V C_V^0}{kT b^2 \sin^2 \theta \ln(R_\infty / r_c)}$$: climbing mobility

$D_V$: vacancy diffusion coef.
Comparison with Atomic Simulations

M. Kabir, T. T. Lau, D. Rodney, S. Yip, K. J. Van Vliet

Use atomic simulations (relaxed KMC with empirical potential) to measure climbing velocity of a jogged dislocation in a vacancy supersaturation
Mixed [111] dislocation in bcc iron
**Analytical model** predicts:

\[
v_{cl} = \eta \frac{D_V}{b |\sin(\theta)| \ln(R_\infty / r_c)} \left| C_V^d - C_V^\infty \right|
\]

\[
C_V^d \ll C_V^\infty \quad \text{and} \quad R_\infty = \frac{1}{2 \sqrt{\rho_d}}
\]

\[
v_{cl} = -\eta \frac{D_V}{b |\sin(\theta)| \ln(2r_c \sqrt{\rho_d})} C_V^\infty
\]

\[
\frac{v_{cl}}{D_V C_V^\infty} = f(\rho_d) = \frac{-\eta}{b |\sin(\theta)| \ln(2r_c \sqrt{\rho_d})}
\]

Atomic simulations are well reproduced for

- all temperatures
- all dislocation densities
- all vacancy supersaturations

with \( \eta = 4\pi \) and \( r_c = 4.3 \, b \)
Comparison with Atomic Simulations

Atomic simulations\(^1\) vs analytical model\(^2\) (\(\eta = 4\pi\) and \(r_c = 4.3\) b)

Climbing velocity of a jogged dislocation in a vacancy supersaturation
Mixed [111] dislocation in bcc iron

3D Dislocation Dynamics Simulations

TriDis¹
- dislocations are discretized into pure edge and screw segments
- discretization length ~ 10b

aNuMoDis²
- Nodal code


- Fcc metals (Al)
- Climb only simulations
- Glide and climb simulations
• Pinned edge dislocation
• **Climb** activated by a **stress** (tensile stress parallel to the Burgers vector)
• No vacancy supersaturation $\frac{c_\infty}{c_0} = 1$

**Below threshold stress**

- Dislocation bows out
equilibrium shape defined by $d_{\text{bow}}/\lambda$

**Above threshold stress** ($\sigma = 5$ MPa)

- Source activated
- Rounded loops
Bardeen-Herring Source

- Pinned edge dislocation
- **Climb** activated by a **stress** (tensile stress parallel to the Burgers vector)
- No vacancy supersaturation \( \frac{c_\infty}{c_0} = 1 \)

Comparison with a line tension model

\[ \frac{d_{\text{bow}}}{\lambda} \text{ (below threshold stress)} \]

**Threshold stress**

\[ \lambda \text{ distance between anchoring points} \]

\[ \sigma_c (\text{MPa}) \]

\[ \frac{b}{\lambda} \]

\[ 4.0 \times 10^{-5} \text{ to } 1.4 \times 10^{-4} \]

\[ f_c \]

\[ 0 \text{ to } 0.5 \]

\[ \sigma/\sigma_{ib} \]

\[ 0 \text{ to } 0.6 \]

\[ 0 \text{ to } 0.7 \]

\[ 0 \text{ to } 0.8 \]

\[ 0 \text{ to } 0.9 \]

\[ 0 \text{ to } 1.0 \]

\[ 0 \text{ to } 1.1 \]

\[ 0 \text{ to } 1.2 \]

\[ 0 \text{ to } 1.3 \]

\[ 0 \text{ to } 1.4 \]

\[ 0 \text{ to } 1.5 \]

\[ 0 \text{ to } 2.0 \]

\[ 0 \text{ to } 2.5 \]

\[ 0 \text{ to } 3.0 \]

\[ 0 \text{ to } 3.5 \]

\[ 0 \text{ to } 4.0 \]

\[ \text{DDD} \]

\[ \text{Knight and Burton, 1989} \]

\( \Rightarrow \text{no artifact due to dislocation discretization} \)
- Pinned edge dislocation
- **Climb** activated by a **vacancy supersaturation**
- No applied stress

Osmotic force $\gg$ line tension

$\Rightarrow$ Equal force on each segment

$\Rightarrow$ **Diamond shape**

\[ \begin{align*}
\text{pinning points} \\
[1\ 0\ 1] \\
[1\ 2\ 1] \\
[1\ -2\ 1] \\
\end{align*} \]

Quenched Al-7%Mg alloy

Quenched Al

Experimental observations in Al

P.S. Dobson, P.J. Goodhew and R.E. Smallman, Phil. Mag. 16, 9 (1967)

J. Silcox and M. J. Whelan, Phil. Mag. 5, 1 (1960)

$r = r_0 \sqrt{1 - t / \tau}$ where $\tau = \tau_0 e^{E/k_B T}$

$E$: activation energy for vacancy diffusion.

Loop rounding during annihilation
Vacancy Loop Annihilation

Prismatic vacancy loop
- no applied stress
- no vacancy supersaturation (thin foils)

Line tension $\rightarrow$ **annihilation**
Heterogeneous climb force $\rightarrow$ loop **rounding**

\[
\begin{align*}
\text{[1 2 1]} & \quad \text{[1 -2 1]} \\
\mathbf{b} & = [-1 0 1]
\end{align*}
\]
Vacancy Loop Annihilation / Growth

Time evolution of the radius: \[ \dot{R} = \frac{\eta D_v c_0 F_{cl} \Omega}{b^2 kT} \left[ \frac{c_\infty}{c_0} - \exp \left( \frac{F_{cl} \Omega}{b kT} \right) \right] \]

No vacancy supersaturation
\[ \dot{R} = -\frac{\eta D_v c_0 F_{cl} \Omega}{b^2 kT} \]

Line tension
\[ F_{cl} = \frac{Gb^2}{R} \]

Surface decrease at a constant rate
\[ \dot{S} = 2\pi R \dot{R} = \text{cste} \]

With vacancy supersaturation
\[ \dot{R} = \frac{\eta D_v c_0 c_\infty}{b c_0} \]

Radius growth at a constant rate
\[ \dot{R} = \text{cste} \]
Annihilation

Depending on vacancy supersaturation kinetics is controlled by

- line tension \( \dot{S} = \text{cste} \)
- osmotic force \( \dot{R} = \text{cste} \)

\[

c_\infty / c_0 = 1.00 \\
c_\infty / c_0 = 1.05 \\
c_\infty / c_0 = 1.10 \\
c_\infty / c_0 = 1.50 \\
c_\infty / c_0 = 2.00 
\]

\( T = 500 \text{K} \)
Dislocation Loop Coarsening: Climb Only

- Distribution of vacancy prismatic dislocation loops
- The only sources and sinks for vacancies are the dislocation loops
- The loops cannot glide (*faulted loops*)

Parameters for Al
\[ T = 600K \]
\{110\} loops
Dislocation Loop Coarsening: Climb Only

Comparison with the theory\textsuperscript{1,2}

Mean radius

\[
R_{av}(t) = R_{av}^0 \left[1 + \alpha t\right]^{1/2}
\]

with \( \alpha = \frac{\eta C_v^0 D_v \mu \Omega}{2 \left(R_{av}^0\right)^2 kT} \)

Loop density

\[
N_{loops}(t) = N_{loops}^0 \frac{1}{1 + \alpha t}
\]

Vacancy supersaturation

\[
\frac{C_v(t)}{C_v^0} - 1 = \frac{\mu b \Omega}{kT R_{av}^0 \left[1 + \alpha t\right]^{1/2}}
\]

Dislocation Loop Coarsening: Climb Only

Comparison with the theory\textsuperscript{1,2}

Steady-state normalized size distribution

\begin{equation}
\begin{split}
g(z) &= \frac{1}{8e^2} \frac{z}{(z-2)^4} \exp\left(\frac{4}{z-2}\right) \\
\text{where} \quad z &= \frac{R}{R_{av}(t)}
\end{split}
\end{equation}

\textbf{Perfect agreement between DD simulations and theory}\textsuperscript{1,2}

Loops can glide and climb (*unfaulted loops*)

At $T = 600K$ (Al), $M_{gl} \sim 3.3 \times 10^5 \text{ (Pa s)}^{-1}$ \quad $M_{cl} \sim 1.75 \times 10^{-5} \text{ (Pa s)}^{-1}$

- climb motion only when glide is not effective (*adiabatic approximation*)

Parameters for Al

$T = 600K$

{110} loops
Dislocation Loop Coarsening: Glide and Climb

Acceleration of the coarsening kinetics because of loop coalescence induced by glide
Screw dislocation with kinks (edge segments)
Vacancy supersaturation
No applied stress
Climb and glide steps
→ helix formation

\[
\frac{c_\infty}{c_0} = 1.1 \quad T = 550K
\]
Pipe diffusion: accelerated diffusion of vacancies along dislocations

Vacancy flux between dislocation segments n-1 and n:

\[ J_{n-1 \rightarrow n} = -\frac{D_p C_V^n - C_V^{n-1}}{\Omega \left\| \vec{r}_n - \vec{r}_{n-1} \right\|} \]

Climbing velocity of segment n:

\[ v_{cl}^n = \frac{\pi r_c^2 D_p}{b l_n \sin(\theta_n)} \sum_i \frac{C_V^n - C_V^i}{\left\| \vec{r}_n - \vec{r}_i \right\|} \]

**Equilibrium vacancy concentration on segment n:**

\[ C_V^n = C_V^0 \exp\left(\frac{F_{cl}^n \Omega}{kT b \sin(\theta_n)}\right) \]

For small PK forces,

\[ v_{cl} \propto \frac{\partial^2 F_{cl}}{\partial s^2} \]
Pipe Diffusion: New Mechanisms

DD simulations with only pipe diffusion

Rounding of a prismatic loop (at constant surface)

Motion of prismatic loops perpendicular to their Burgers vector (at constant surface) ➔ coalescence

pipe diffusion and glide ➔ 3D motion of prismatic loops
bulk diffusion ➔ change of loop sizes

Mechanisms with different time scales: adiabatic approximation may be needed
Conclusions

**Atomistic simulations**
- Most stable configuration of a super-jog = dissociated jog in (111) plane
- A jogged dislocation is glissile
- Jog = perfect sink / source for vacancies
- Kinetics of vacancy diffusion towards dislocation core
  ➔ well described by “classical approach”¹

**Climb introduced in discrete dislocation dynamics simulations**
- climb velocity controlled by vacancy diffusion in the bulk²,⁴
- and pipe diffusion along dislocation lines

**Validation for pure climb cases**
- Bardeen-Herring sources²
- annihilation and growth of vacancy and interstitial loops²
- coarsening of vacancy prismatic loops³,⁴

**Climb and glide**
- coalescence due to glide⁴ ➔ acceleration of loop coarsening
- screw dislocation ➔ helix formation

Next possible developments in DD

- **elastic** interaction between vacancies and dislocations
- **interstitial** diffusion: I-V recombination
  - irradiation creep

- **inhomogeneous concentration** field for vacancy:
  - treat both evolution of vacancy concentration and dislocation movement
  - creep controlled by dislocations / grain boundaries
    - *cf* work of Amine Benzerga and S. M. Keralavarma (Texas A&M)

- **jogs**: vacancy concentration fixed by their equilibrium with jogs
  - climbing velocity: *cf* book* of Caillard and Martin
  - **evolution law** for the jog concentration on each segment

... and at the atomic scale

- **jog nucleation** from vacancy segregation on dislocations

---

* D. Caillard and J. L. Martin, *Thermally activated mechanisms in crystal plasticity* (Pergamon 2003)