Dislocation Climb Models: from atomistic scheme to dislocation dynamics

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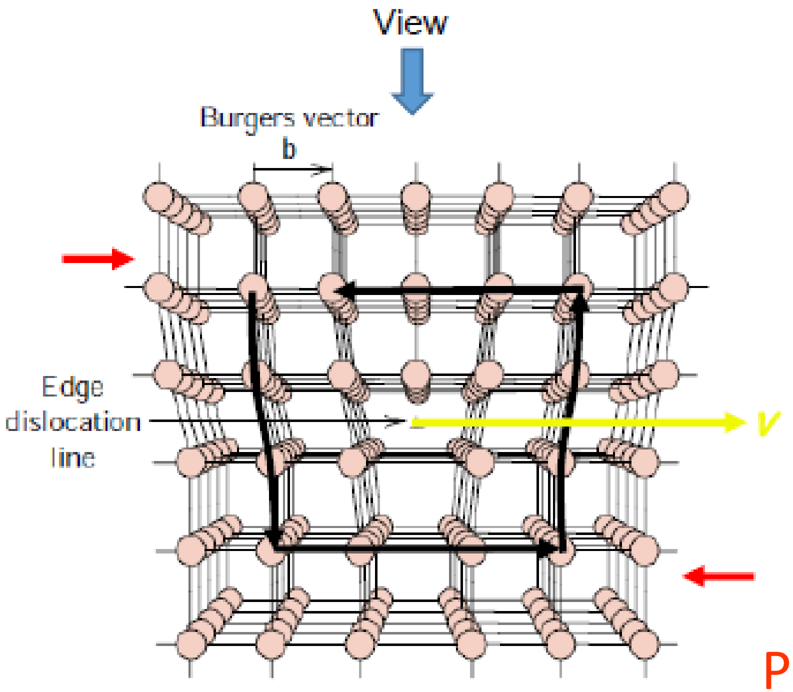
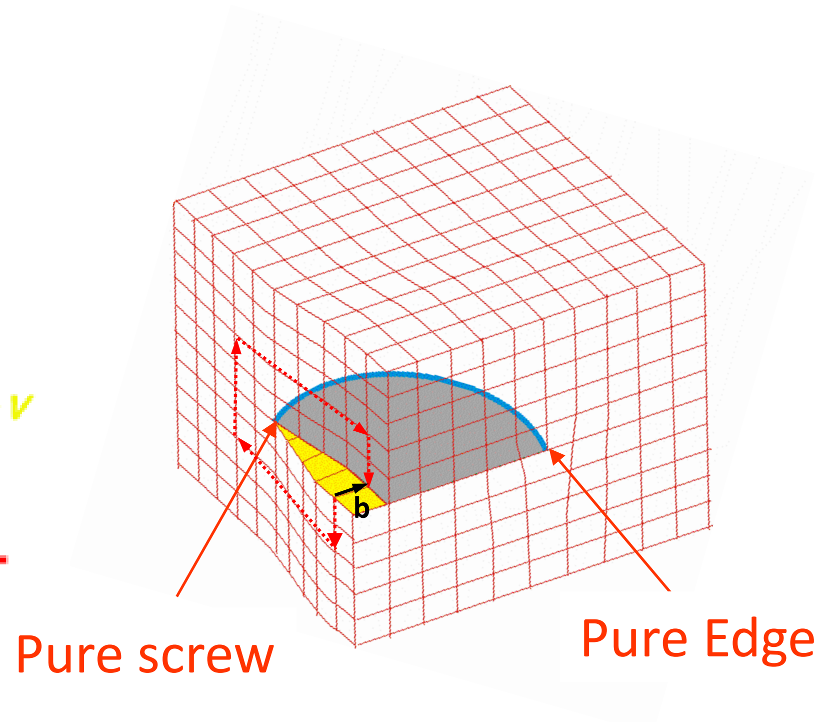
- Dislocations: line defects in crystals

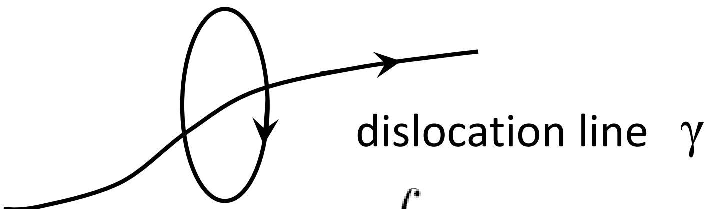
EDGE **MIXED** **SCREW**





- Atomic description

- Continuum description



$$\oint_L d\mathbf{u} = \mathbf{b}$$

u = (u_1,u_2,u_3) is the elastic displacement vector (multi-valued)

L is any close contour enclosing dislocation line

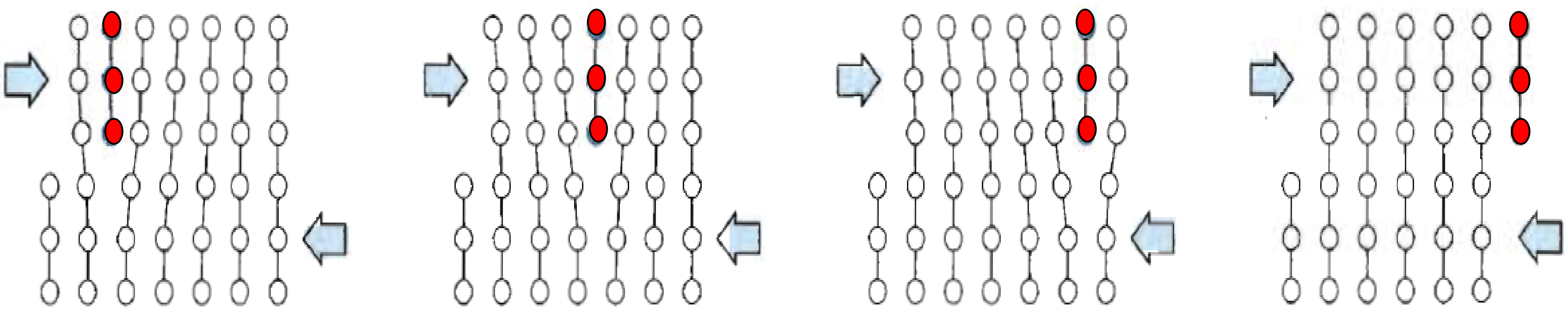
b is the Burgers vector

- Dislocations:Primary carriers of plastic deformation

- Motions of dislocations include glide and climb

Dislocation glide

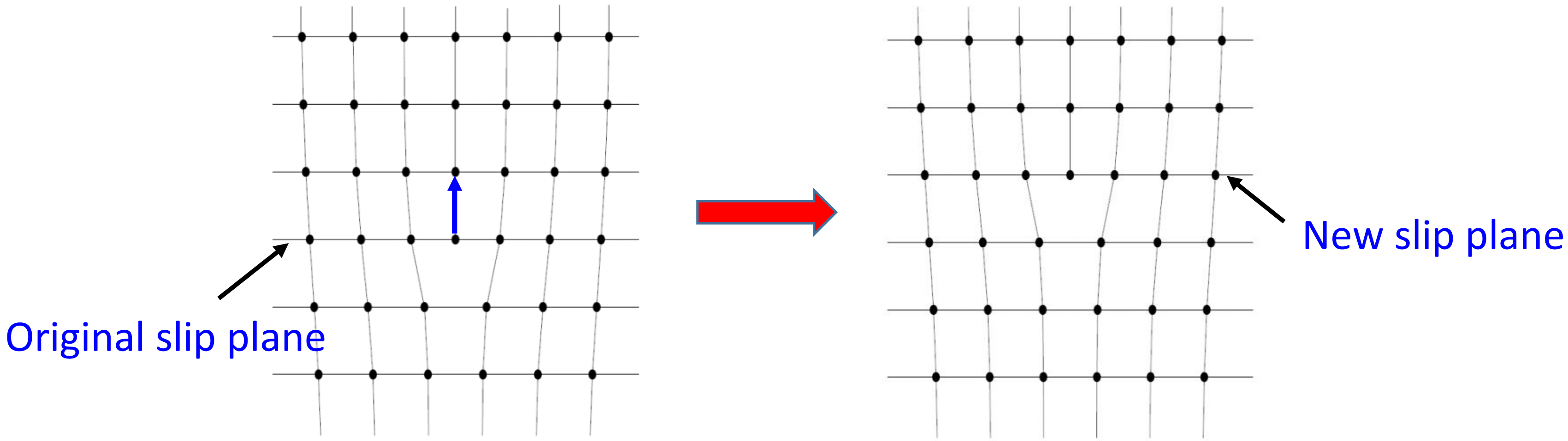
- Dislocations mainly move by glide at not very high temperatures.
- Motion within the slip plane (containing the dislocation and its Burgers vector).
- Conservative motion.



Dislocation climb

- Absorbing and emitting vacancies/interstitials.

- Non-conservative motion.



Dislocation climb plays important roles in the plastic deformation of crystalline materials at high temperature, e.g. in dislocation creep.

Peach-Koehler force

$$\boldsymbol{f} = (\boldsymbol{\sigma} \cdot \boldsymbol{b}) \times \boldsymbol{\xi}$$

$\boldsymbol{b}$: the Burger's vector,
$\boldsymbol{\xi}$: the dislocation line direction,
$\boldsymbol{\sigma}$: the stress tensor.

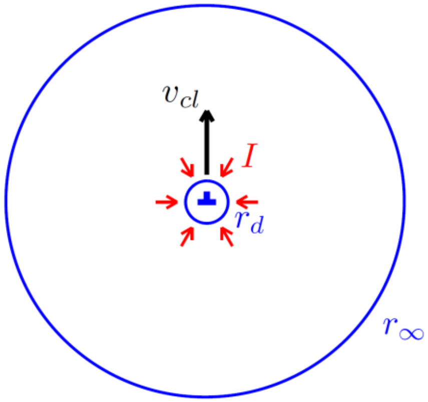
Glide velocity of dislocations

$$\boldsymbol{v} = \boldsymbol{M} \cdot \boldsymbol{f}$$

$\boldsymbol{M}$: mobility

- Vacancy diffusion assisted dislocation climb, follows vacancy diffusion equation (in equilibrium when climb is slow)

$$\frac{\partial c}{\partial t} = \nabla \cdot (D_v \nabla c) = 0$$



- Equilibrium condition near dislocation (boundary condition depending on the climb PK force)

$$c_d = c_0 e^{-\frac{f_{\mathrm{cl}}\Omega}{b_e k_B T}} \qquad f_{\mathrm{cl}} = \mathbf{f} \cdot (\boldsymbol{\xi} \times \mathbf{b}/b_e)$$

f_{cl}: climb PK force
$b_e = b \sin \beta$

- Climb velocity is associated with vacancy flux into the dislocation

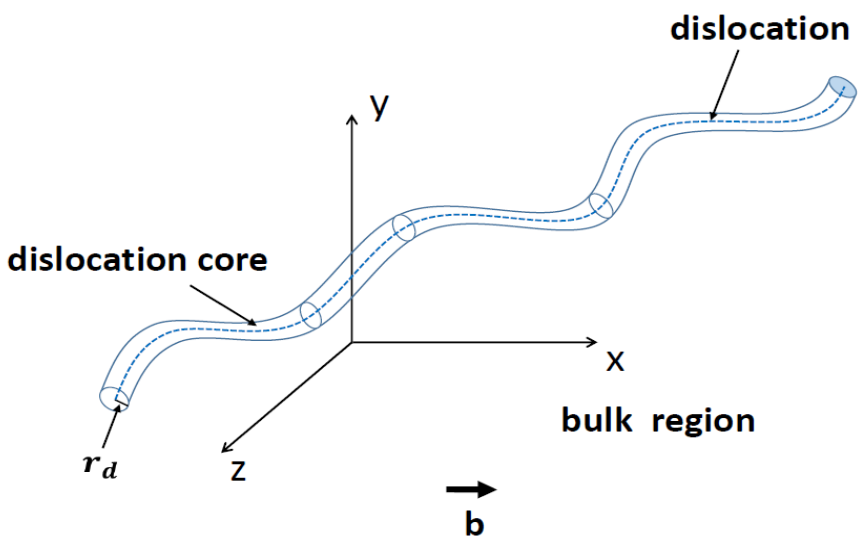
β: angle between dislocation line direction ***ξ*** and the Burgers vector ***b***

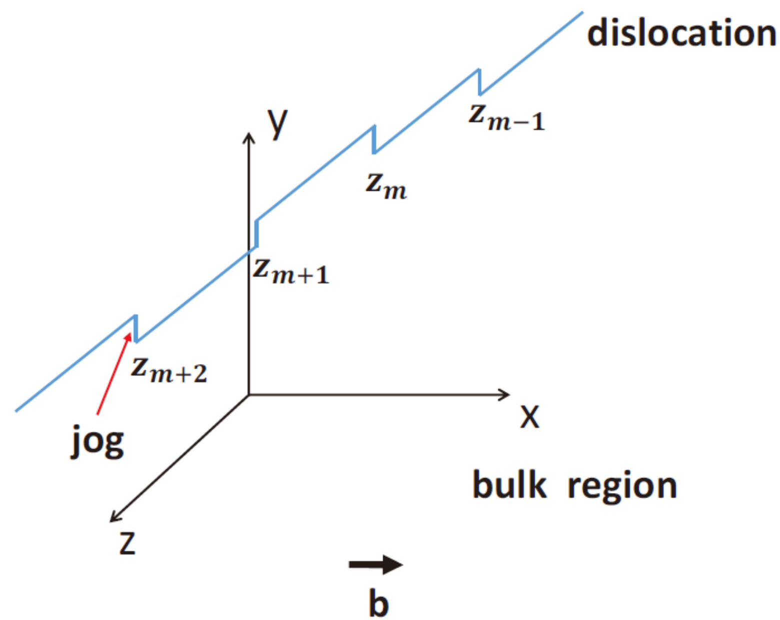
$$v_{\mathrm{cl}} = \frac{2\pi r_d D_v}{b_e} \frac{\partial c}{\partial n}\bigg|_{r_d}$$

Hirth & Lothe, *Theory of Dislocations*, 1982.

Pipe diffusion

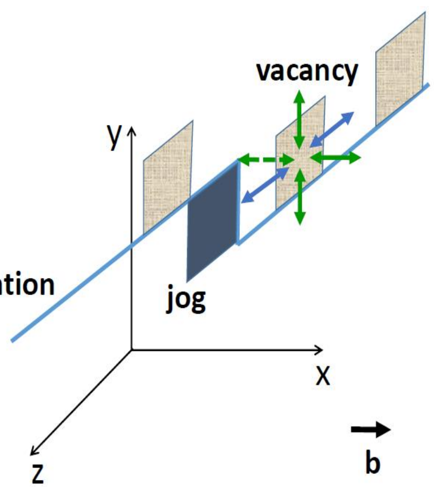
- Most earlier work focuses on vacancy diffusion in the bulk. The boundary condition is Dirichlet condition.
- Real dislocations may not be perfect sources or sinks, implying that both climb and pipe diffusion could cooperate with jog dynamics.

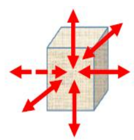




A mesoscopic dislocation dynamics model for vacancy-assisted dislocation climb from stochastic model on the atomistic scale

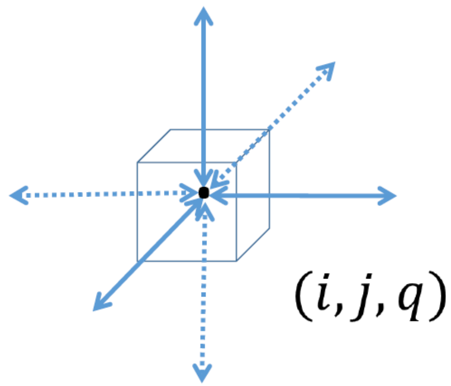
Incorporates the following microscopic mechanisms

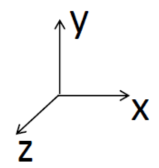




(i) Bulk vacancy diffusion;
(ii) Vacancy exchange dynamics across bulk and dislocation core;
(iii) Vacancy pipe diffusion along the dislocation line;
(iv) Vacancy attachment-detachment kinetics at jogs leading to dislocation climb.

Model assumptions

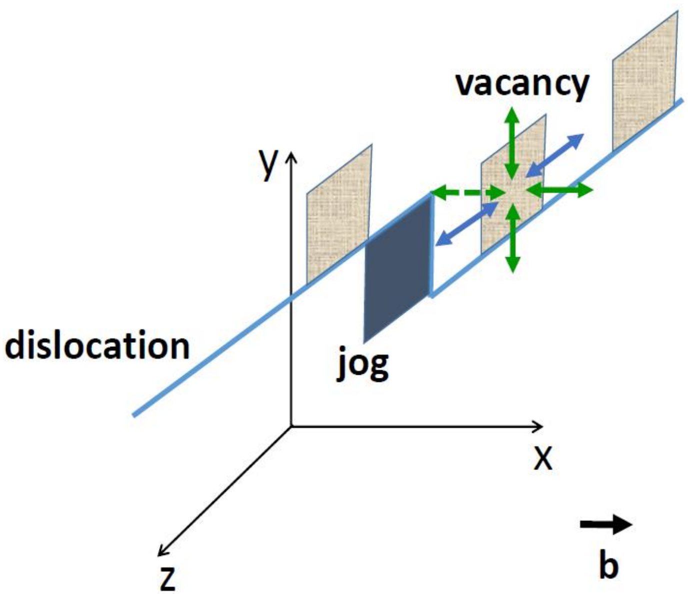


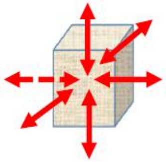


(1) A vacancy is only allowed to move along the x, y, z axes directions and inverse directions.

(2) The jogs are noninteracting and have low density, i.e. vacancy at most has one direction to jump into the jog .

Model assumptions: vacancy migration probabilities in different lattice sites





$$c_J = c_0^c e^{-\frac{f_{cl}\Omega}{bkT}}$$

Equilibrium vacancy concentration at a jog site

where $c_0^c = e^{-\frac{E_C^f}{kT}}$

reference equilibrium vacancy concentration in the dislocation core

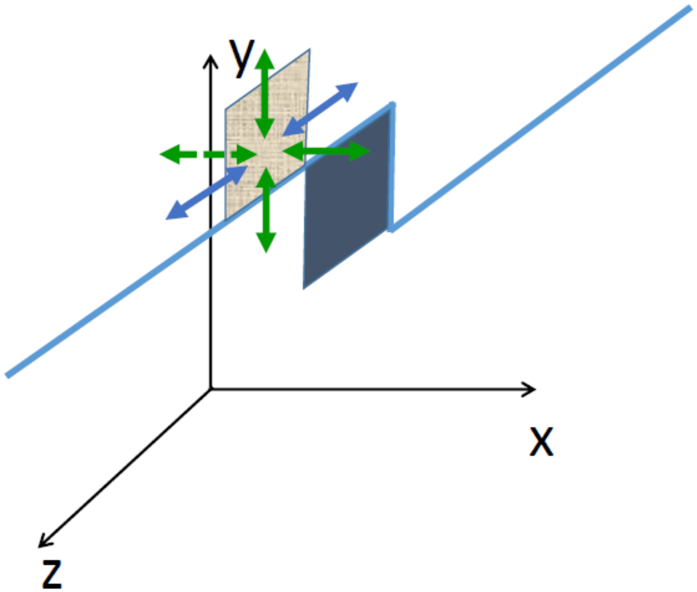
$$\Gamma_v = \Gamma_v^0 e^{-\frac{E^v}{kT}}$$ **Bulk diffusion**

$$\Gamma_c = \Gamma_c^0 e^{-\frac{E^c}{kT}}$$ **Pipe diffusion**

$$\Gamma_v \phi_v k_v = \Gamma_{c-v}^0 e^{-\frac{E^{c-v}}{kT}}$$ **Diffusion from core to bulk , the same in jog**

$$\Gamma_v \phi_v = \Gamma_{v-c}^0 e^{-\frac{E^{v-c}}{kT}}$$ **Diffusion from bulk to core, the same in jog**

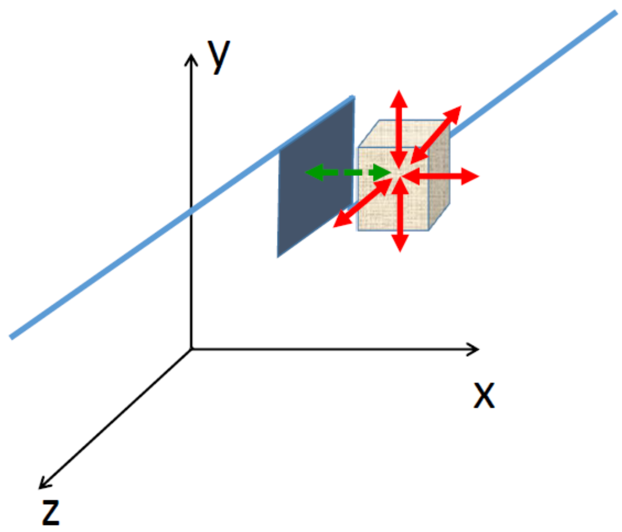
For vacancies along the dislocation line and near the jog:



$$c_{i,j,q}^{c,n+1} = (1 - 2\Gamma_c\tau)c_{i,j,q}^{c,n} + \Gamma_c\tau c_{i,j,q-1}^{c,n} + \Gamma_c\tau c_J$$

$$+\Gamma_v\phi_v\tau(c_{i-1,j,q}^{v,n} + c_{i+1,j,q}^{v,n} + c_{i,j-1,q}^{v,n} + c_{i,j+1,q}^{v,n}) - 4\Gamma_v\phi_v k_v\tau c_{i,j,q}^{c,n}.$$

For vacancies in the bulk and near the jog:



$$c_{i,j,q}^{v,n+1} = (1 - 5\Gamma_v \tau) c_{i,j,q}^{v,n} + \Gamma_v \phi_v k_v \tau c_J - \Gamma_v \phi_v \tau c_{i,j,q}^{v,n}$$

$$+ \Gamma_v \tau (c_{i+1,j,q}^{v,n} + c_{i,j-1,q}^{v,n} + c_{i,j+1,q}^{v,n} + c_{i,j,q-1}^{v,n} + c_{i,j,q+1}^{v,n}).$$

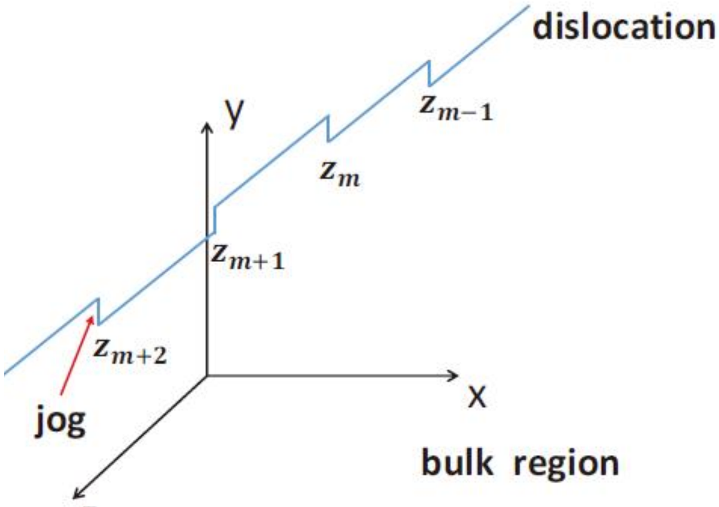
Stochastic motion of a jog depends on the stochastic migration behavior of vacancies nearest to it

Jog velocity:

$$V_{\text{jog}} = \Gamma_c b(c^{c,n}_{i,j,q+1} + c^{c,n}_{i,j,q-1}) + \Gamma_v b\phi_v(c^{v,n}_{i-1,j,q} + c^{v,n}_{i+1,j,q} + c^{v,n}_{i,j-1,q} + c^{v,n}_{i,j+1,q})$$
$$-(2\Gamma_c b + 4\Gamma_v b\phi_v k_v)c_J.$$

The jog dynamics model

$$
\begin{cases}
c_t^v = D_v\left(c_{xx}^v + c_{yy}^v + c_{zz}^v\right), & \text{in the bulk,} \\
-\dfrac{\partial c^v}{\partial n} = \dfrac{1}{l_\phi}\left(c^v - k_v c^c\right)\Big|_{r=r_d}, & \\
c^v = c_\infty\big|_{r=r_\infty}, &
\end{cases}
$$



$$
\begin{cases}
c_t^c = D_c c_{zz}^c + \dfrac{2\pi r_d D_v}{b^2 l_\phi}\left(\dfrac{1}{2\pi r_d}\displaystyle\int_{r=r_d} c^v \, dl - k_v c^c\right), & \text{on the dislocation,} \\
c^c = c_0^c e^{-\frac{f_{\mathrm{cl}}\Omega}{bkT}}\Big|_{z=z_m}, &
\end{cases}
$$

At a jog

How to Solve them together?

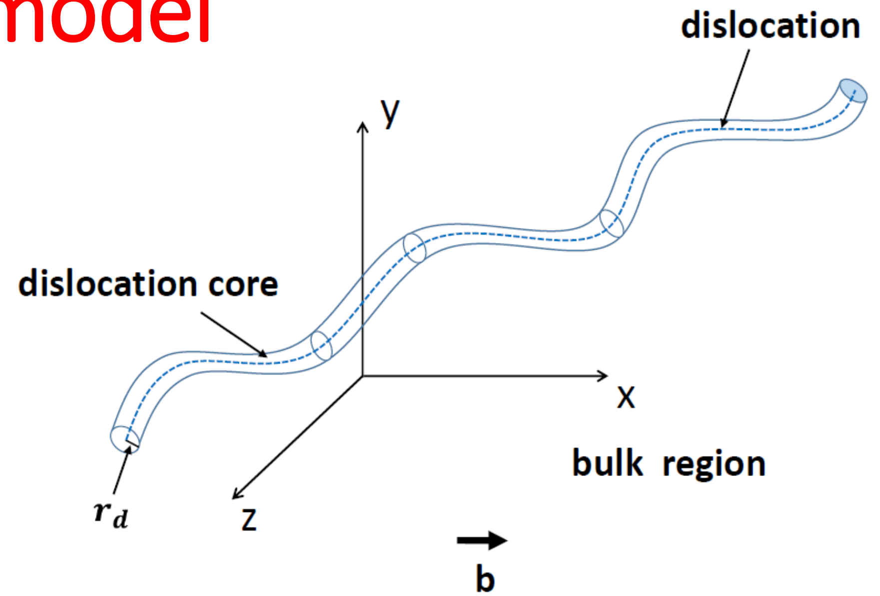
$$l_\phi = b/\phi_v$$

Adaption for general dislocation core radius

$$
\begin{aligned}
v_{\text{jog}}^{(m)} &= \sum_{s=+,-} \mathbf{j}^c \cdot \mathbf{n}^c\big|_{z=z_m^{(s)}} + \frac{1}{b}\int_{r=r_d} \mathbf{j}\cdot\mathbf{n}\, dl\Big|_{z=z_m} \\
&= D_c\left[c_z^c(z_m^+) - c_z^c(z_m^-)\right] + \frac{2\pi r_d D_v \phi_v}{b^2}\left(\frac{1}{2\pi r_d}\int_{r=r_d} c^v\, dl - k_v c_0 e^{-\frac{f_{\mathrm{cl}}\Omega}{bkT}}\right)\Big|_{z=z_m}
\end{aligned}
$$

The dislocation dynamics model

$$\begin{cases} c_t = D_v(c_{xx} + c_{yy} + c_{zz}), \quad \text{in the bulk,} \\ -\dfrac{\partial c}{\partial n} = \dfrac{1}{l_\phi}(c - c_d)\Big|_{r=r_d}, \\ c = c_\infty|_{r=r_\infty}, \end{cases}$$



$$v_{\text{cl}} = \frac{2\pi r_d D_v}{b l_\phi}\left(\frac{1}{2\pi r_d}\int_{r=r_d} c\ dl - c_d\right) + D_c b \frac{\mathrm{d}^2 c_d^c}{\mathrm{d}s^2}$$

$$= \frac{1}{b}\int_{r=r_d} \mathbf{j}\cdot\mathbf{n}\ dl + D_c b \frac{\mathrm{d}^2 c_d^c}{\mathrm{d}s^2}$$

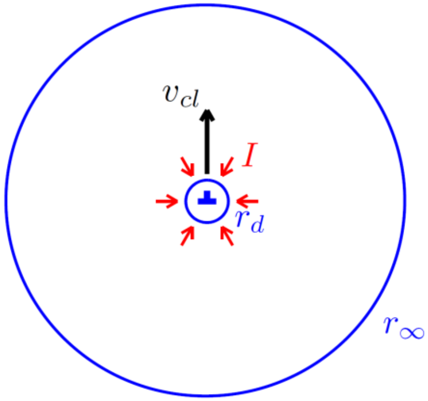
$$c_d(z) = c_0 e^{-\frac{f_{\text{cl}}(z)\Omega}{bkT}}$$

$$k_v c_0^c = c_0$$

$$c_d^c(z) = c_0^c e^{-\frac{f_{\text{cl}}(z)\Omega}{bkT}}$$

- Dislocation climb velocities of some special cases
- Climb velocity of a straight edge dislocation

$$v_{\rm cl} = \frac{2\pi D_v}{b\left(\ln\frac{r_\infty}{r_d} + \frac{l_\phi}{r_d}\right)}(c_\infty - c_d).$$



Comparing the classical climb velocity formula in *J.P. Hirth & J. Lothe, Theory of Dislocations, 1968*

$$v_{\rm cl} = \frac{2\pi D_v}{b\ln\frac{r_\infty}{r_c}}(c_\infty - c_d)$$

Difference:

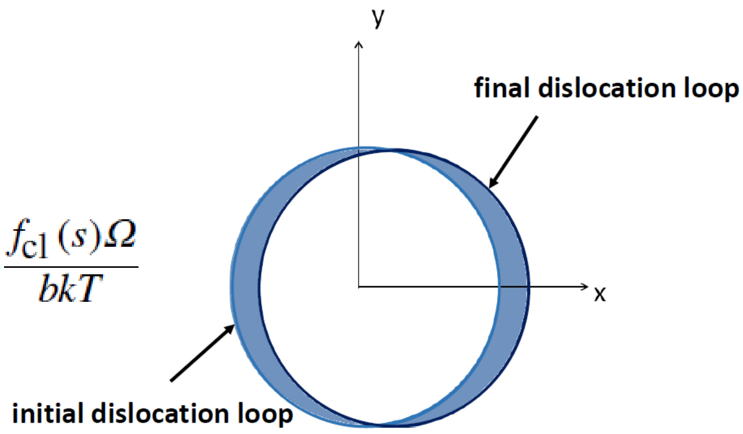
An extra term $\frac{b}{\phi_v r_d}$ is due to the imperfect sink/source, from jog structure and pipe diffusion.

Prismatic loop translation by pipe diffusion at low temperature

$$D_v \approx 0 \;\Rightarrow\; v_{\mathrm{cl}} = D_c b \frac{\mathrm{d}^2 c_d^c}{\mathrm{d}s^2}$$

$$c_d^c(s) = c_0^c e^{-\frac{f_{\mathrm{cl}}(s)\Omega}{bkT}}$$

$$\Rightarrow\; \frac{\mathrm{d}S}{\mathrm{d}t} = 0$$



Area of the loop S is unchanged by the translation due to the pipe diffusion [Kroupa & Price, Phil. Mag. 1961]

Gives a quantitative understanding of the translation of prismatic loops due to pipe diffusion

Climb velocity for prismatic loop translation

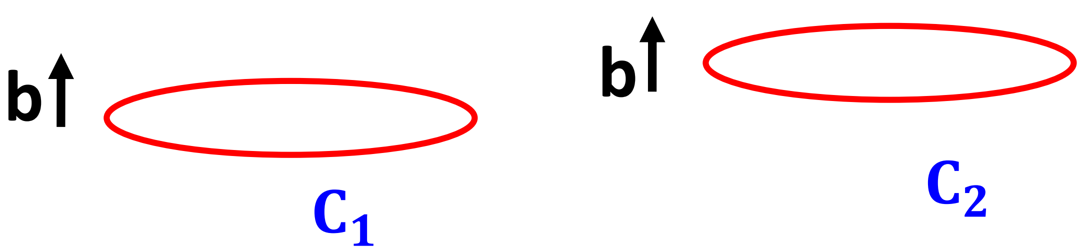
$$v_{\mathrm{cl}} = D_c b \frac{\mathrm{d}^2 c_d^c}{\mathrm{d}s^2} \quad \text{where} \quad c_d^c(s) = c_0^c e^{-\frac{f_{\mathrm{cl}}(s)\Omega}{bkT}}$$

$$\begin{aligned} f_{\mathrm{cl}} &= f_{\mathrm{loops}} + f_{\mathrm{ex}} \\ &= b\sigma_{33} + f_{\mathrm{ex}} \\ &= \frac{\mu b^2}{4\pi(1-\nu)} \oint_C \frac{x - x_1}{((x-x_1)^2 + (y-y_1)^2)^{\frac{3}{2}}} dy - \frac{y - y_1}{((x-x_1)^2 + (y-y_1)^2)^{\frac{3}{2}}} dx + f_{\mathrm{ex}} \end{aligned}$$

C for all dislocation loops

Self stress of the loop C_1: from (x, y) on C_1

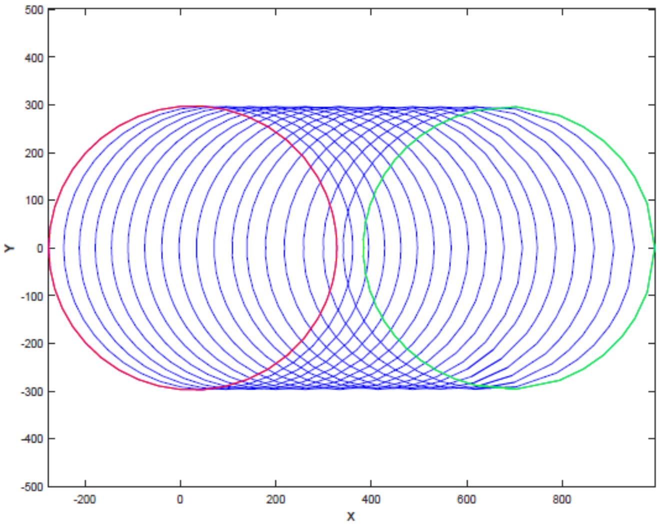
Stress from other loop C_2: from (x, y) on C_2



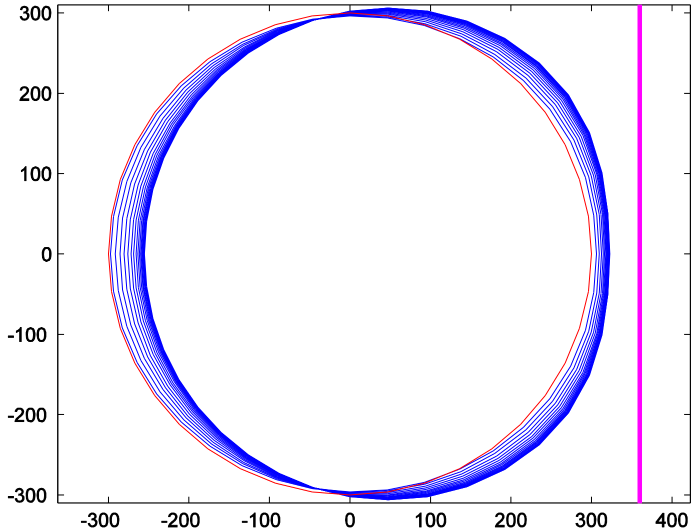
Simulation results for prismatic loop translation at not very low temperature (800K).

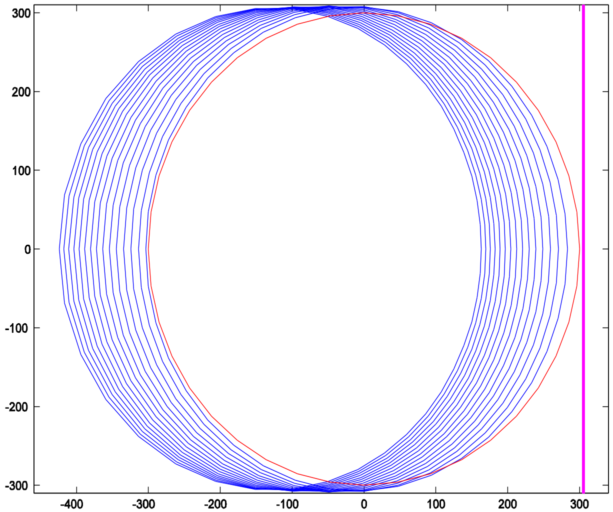
1. under the stress field

$$\sigma_{33} = a_0 x + b_0$$



2. under the stress field from an fixed infinite straight edge dislocation ($x_0 = 360b$, $z_0 = 50b$ for left fig; $x_0 = 305b$; $z_0 = 305b$ for right fig)



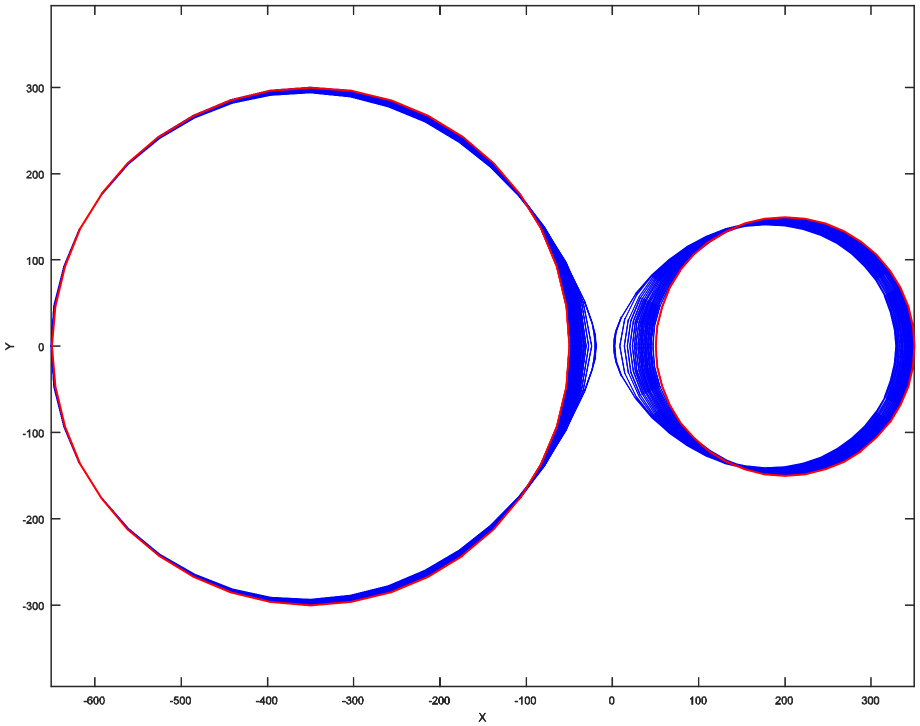


$3.\ self\ climb\ of\ two\ prismatic\ loops\ in\ the\ same\ habit\ plane$
$driven\ by\ loop - loop\ interaction$

$$R_1 = 300b$$

$$R_2 = 150b$$

d= $100b$(the distance between the closest points of two loops)



Summary

- An atomistic model on the microscopic scale for dislocation climb is developed.
- Model incorporates the pipe diffusion and bulk diffusion.
- Jog dynamics model is derived from the atomistic model, which consists of pipe diffusion equation and bulk diffusion equation.
- Dislocation dynamics model for dislocation climb is obtained by further upscaling in space and time from the jog dynamics model in the fast pipe diffusion limit.
- When the bulk diffusion is not very significant, the effect of pipe diffusion can be captured quantitatively, e.g. for the translation of a

Thank you