Dislocation Climb in Discrete Dislocation Dynamics

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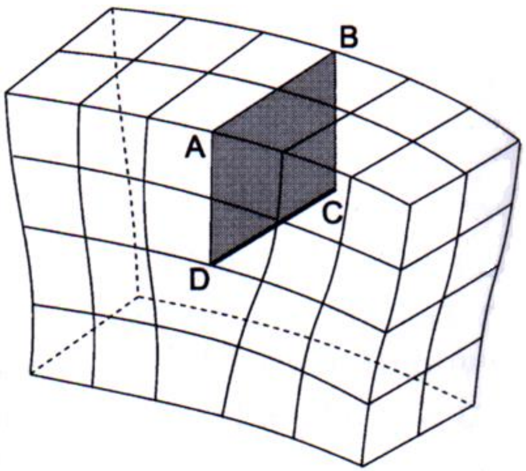
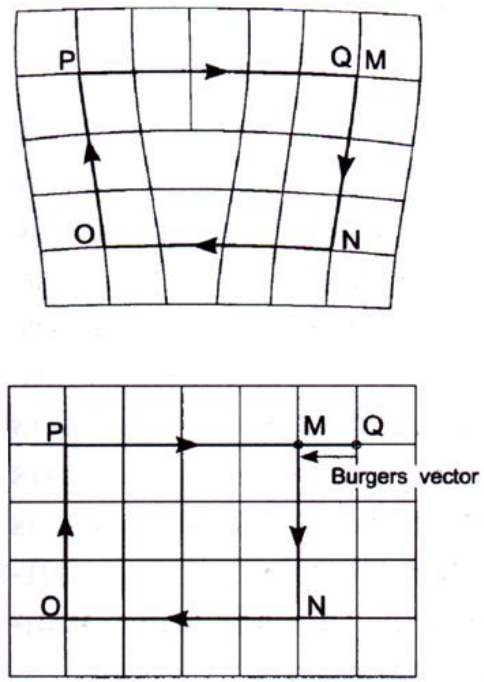
HKUST-ICERM Program on Integral Equation Methods, Fast Algorithms and Their Applications to Fluid Dynamics and Materials Science, HKUST, 3 -13 Jan 2017

Dislocations: line defects in crystals

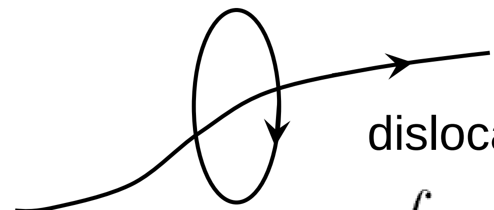
- Atomic description





edge dislocation

- 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

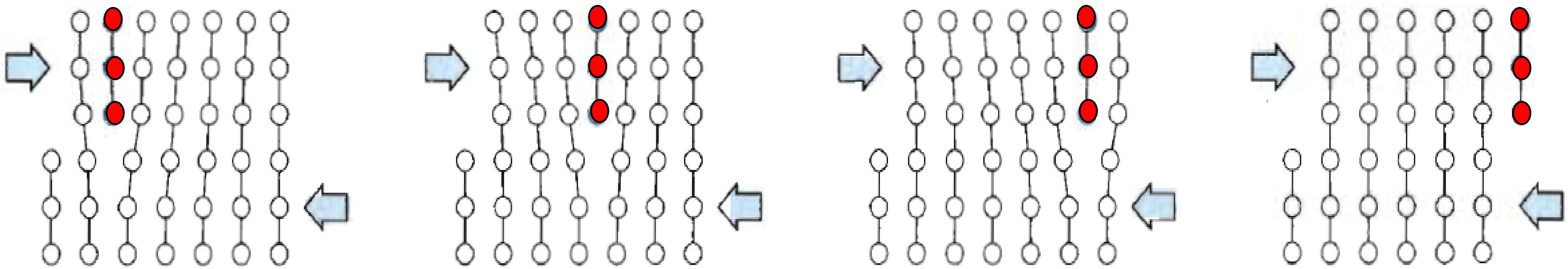
b is the Burgers vector

Dislocations and plastic deformation

Primary carriers of plastic deformation

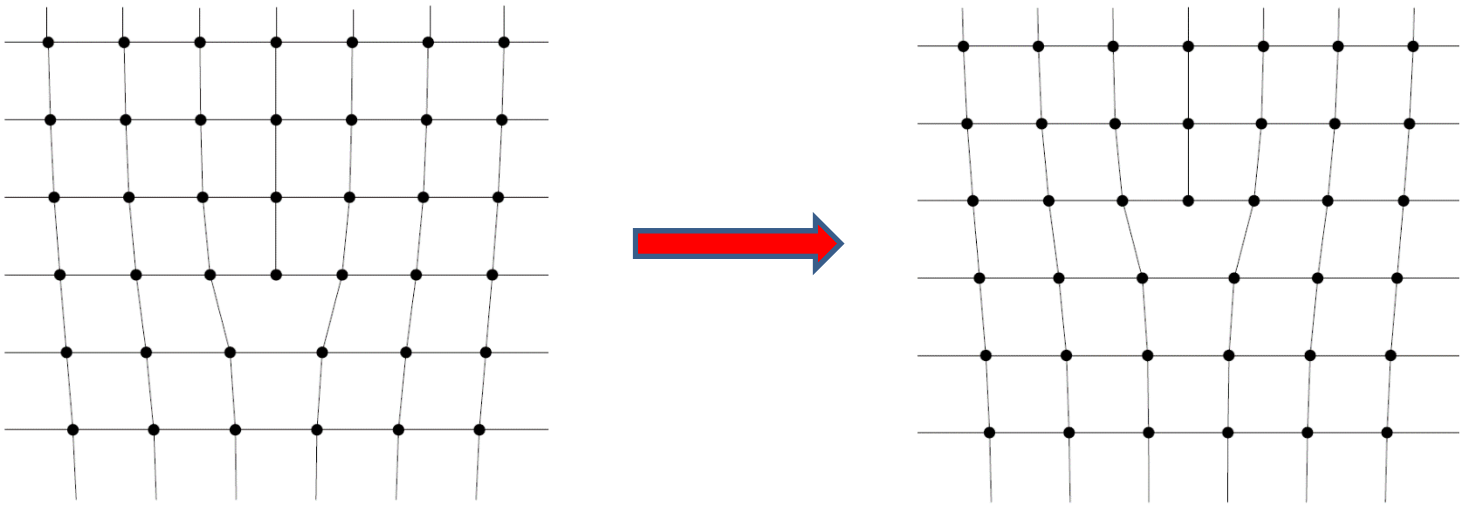
Dislocation Glide

- 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

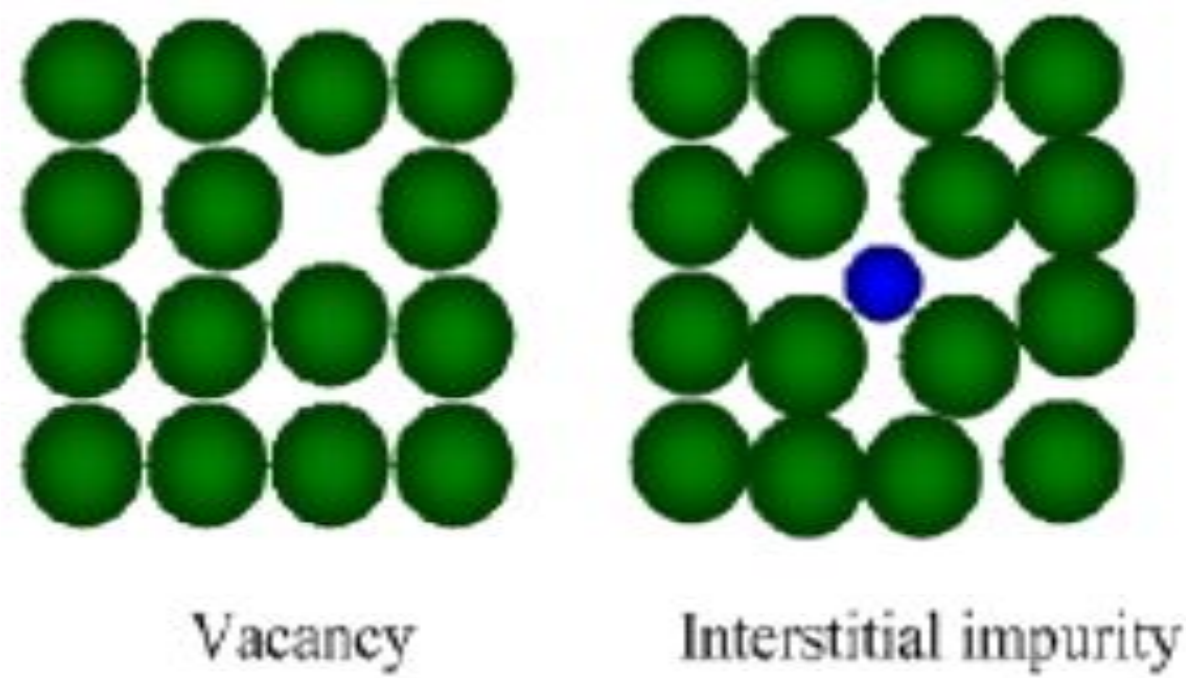
Non-conservative motion of dislocations



Absorbing vacancies/interstitials

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

Point Defects



Continuum Dislocation Theory

displacement vector $\mathbf{u}=(u_1,u_2,u_3)$

strain tensor $$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)$$

stress tensor $$\sigma_{ij} = \sum_{k,l} C_{ijkl}\varepsilon_{kl}$$

$$\nabla \cdot \boldsymbol{\sigma} = 0$$

with dislocation $$\oint_L d\mathbf{u} = \mathbf{b}$$ or $$\nabla \times \boldsymbol{w} = \boldsymbol{\xi}\delta(\boldsymbol{\gamma})\otimes \boldsymbol{b}$$

$$\boldsymbol{w_{ij}} = \partial u_j / \partial x_i$$

w: distortion tensor, b: Burgers vector, ξ: dislocation line direction

Long-range interaction of dislocations

Peach-Koehler formula for the stress (isotropic linear elasticity, whole space):

$$\boldsymbol{\sigma} = \frac{\mu}{4\pi}\oint_C (\mathbf{b}\times\nabla')\frac{1}{R}\otimes d\mathbf{l}'$$

$$+\frac{\mu}{4\pi}\oint_C d\mathbf{l}'\otimes(\mathbf{b}\times\nabla')\frac{1}{R}$$

$$-\frac{\mu}{4\pi(1-\nu)}\oint_C \nabla'\cdot(\mathbf{b}\times d\mathbf{l}')(\nabla\otimes\nabla-\mathbf{I}\nabla^2)R$$

C is the dislocation line
x', y', z' are integral variables
$R=[(x-x')^2+(y-y')^2+(z-z')^2)]^{1/2}$
μ and ν are elastic constants

Peach-Koehler force $\boldsymbol{f} = (\boldsymbol{\sigma}\cdot\boldsymbol{b})\times\xi$

Discrete Dislocation Dynamics

Direct simulation of motion and interaction of dislocations

Three-dimensional DDD simulations:

Kubin et al, *Solid State Phenomena* 1992, …

Glide velocity of dislocations $\boldsymbol{v} = \boldsymbol{M} \cdot \boldsymbol{f}$ M: mobility

Dislocation climb by mobility law in DDD

Raabe, Phil Mag 1998 (Osmotic force)

Ghoniem, Tong, Sun, Phys. Rev. B 2000 (Osmotic force)

Xiang et al, Acta Mater 2003; Xiang & Srolovitz, Phil Mag 2006

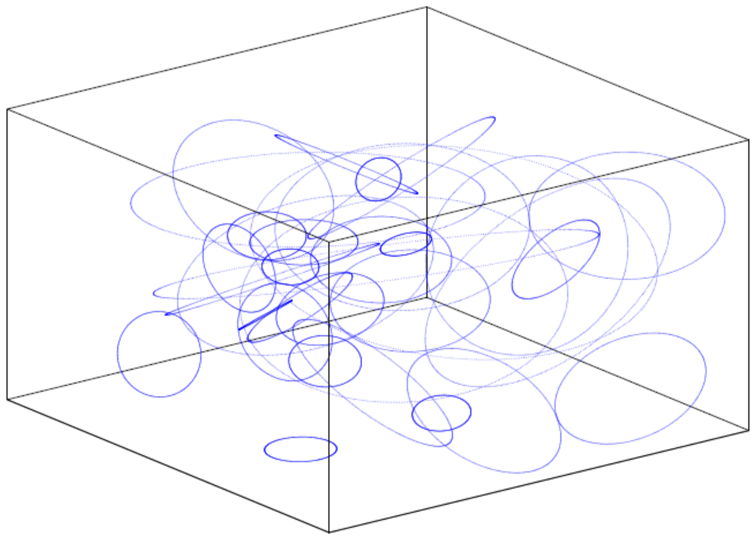
Arsenlis et al, Modelling Simul Mater Sci Eng 2007

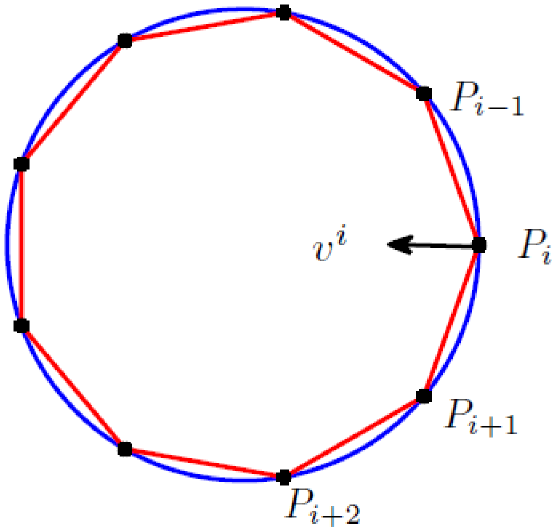
…

Discrete Dislocation Dynamics

Front tracking discretization

---- straight or curved dislocation segments





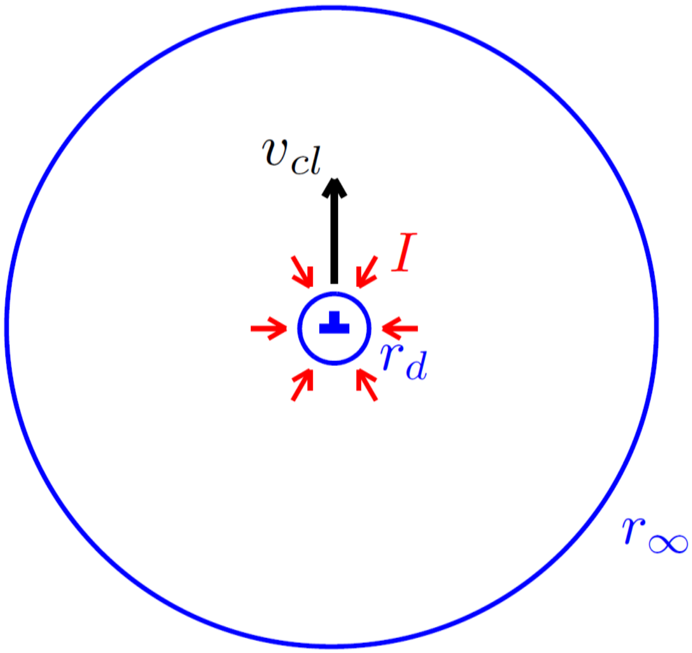
Level set dislocation dynamics method

Xiang, Cheng, Srolovitz, E, Acta Mater 2003.

Vacancy Diffusion Assisted Dislocation Climb

- 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)

$$c_d = c_0 e^{-\frac{f_{\mathrm{cl}}\Omega}{b_e k_B T}}$$

f_{cl}: climb PK force

$b_e = b \sin \beta$

- Climb velocity is associated with vacancy flux into the dislocation

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

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

$$f_{\mathrm{cl}} = \mathbf{f} \cdot (\boldsymbol{\xi} \times \mathbf{b}/b_e)$$

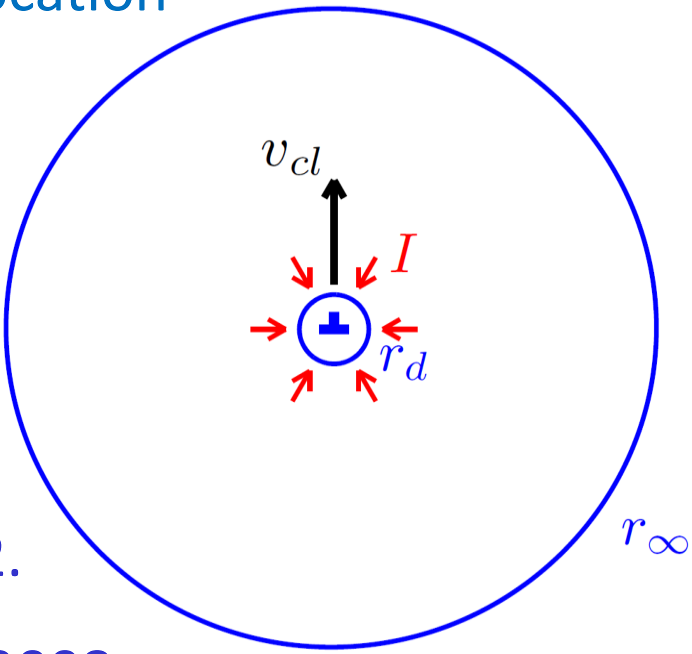
Hirth & Lothe, *Theory of Dislocations*, 1982.

Climb of a single straight edge dislocation

- Climb velocity of a single straight edge dislocation

$$c(r) = c_\infty + \frac{c_\infty - c_d}{\ln(r_\infty / r_d)} \ln \frac{r}{r_\infty}$$

$$v_{\rm cl} = \frac{2\pi D_v}{b \ln(r_\infty / r_d)} \left(c_\infty - c_0 e^{-\frac{f_{\rm cl}\Omega}{b k_B T}} \right)$$



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

Mordehai, Clouet, Fivel, Verdier, *Phil Mag* 2008.

- Reduce to the mobility law when $c_\infty = c_0$ and f_{cl} is small

$$v_{\rm cl} = m_c f_{\rm cl}, \qquad m_c = \frac{2\pi D_v c_0 \Omega}{b^2 k_B T \ln(r_\infty / r_d)}$$

Dislocation Climb with Vacancy Diffusion in DDD

- This climb velocity formula for straight edge dislocation was widely used in DDD (with modifications).

  Mordehai, Clouet, Fivel, Verdier, *Phil Mag* 2008.

  Bako et al, *Phil Mag* 2011.

  Morderhai & Martin, *Phys Rev B* 2011.

  Keralavarma et al, *Phys Rev Lett* 2012.

  Quek et al, *Modelling Simul Mater Sci Eng* 2013.

  …

- None of the existing methods solve vacancy diffusion (equilibrium) accurately for climb of general dislocation systems (multiple, arbitrary shape) in DDD.

Green's function formulation for Dislocation Climb

Yejun Gu, Xiang, Quek, Srolovitz, J Mech Phys Solids 2015

Vacancy diffusion (equilibrium) equation

$$\frac{\partial c}{\partial t} = D_v \Delta c - h\delta(\Gamma) = 0$$

$$h = b_e v_{\text{cl}}$$

Γ: dislocations

Solution using Green's function

$$c(x,y,z) = -\frac{1}{4\pi D_v}\int_\Gamma \frac{h(x_1,y_1,z_1)}{\sqrt{(x-x_1)^2+(y-y_1)^2+(z-z_1)^2}}dl + c_\infty$$

$$\text{Green's function } G(x,y,z) = -\frac{1}{4\pi D_v\sqrt{x^2+y^2+z^2}}$$

Equilibrium condition near a dislocation

$$-\frac{1}{4\pi D_v}\int_\Gamma \frac{h(x_1,y_1,z_1)}{\sqrt{(x-x_1)^2+(y-y_1)^2+(z-z_1)^2+r_d^2}}dl + c_\infty = c_0 e^{-\frac{f_{\text{cl}}\Omega}{b_e k_B T}}\Bigg|_{(x,y,z)}$$

for any point (x,y,z) on the dislocations.

Algorithm for Calculating Climb Velocity

1. Solve the integral equation for h

$$-\frac{1}{4\pi D_v}\int_{\Gamma}\frac{h(x_1,y_1,z_1)}{\sqrt{(x-x_1)^2+(y-y_1)^2+(z-z_1)^2+r_d^2}}dl + c_\infty = c_0 e^{-\frac{f_{\mathrm{cl}}\Omega}{b_e k_B T}}\Big|_{(x,y,z)}$$

for all points *(x,y,z)* on dislocations.

Non-local formula

2. Calculate climb velocity from h

$$V_{cl}=h/b_e$$

for all non-screw points on dislocations.

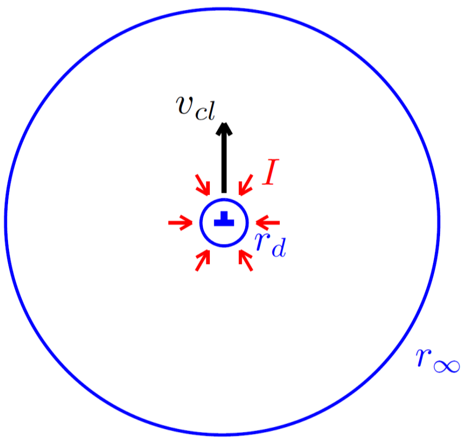
Cutoff and linear interpolation of f_{cl}/b_e near screw ($b_e=0$)

Applications of Green's Function Formulation

Single edge dislocation

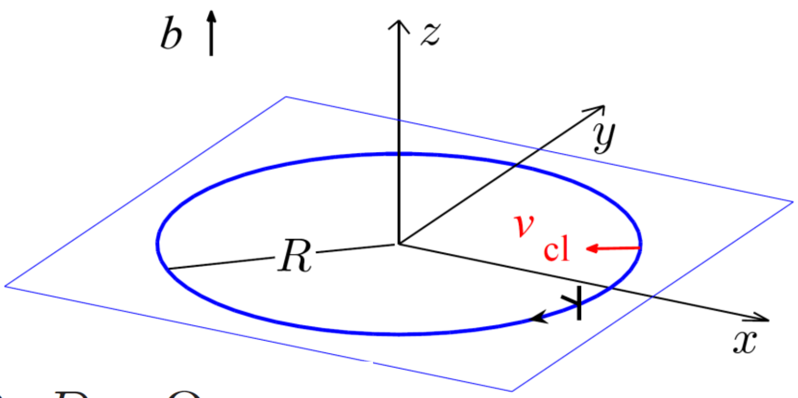
$$v_{\rm cl} = A\left(c_\infty - c_0 e^{-\frac{f_{\rm cl}\Omega}{bk_BT}}\right)$$

$$A = \frac{2\pi D_v}{b\ln(r_\infty/r_d)}$$



Agrees with Hirth & Lothe 1982, Mordehai et al 2008

Prismatic loop



$$f_{\rm cl} = \frac{\mu b^2}{4\pi(1-\nu)R}\left(\ln\frac{8R}{r_d} - 1\right)$$

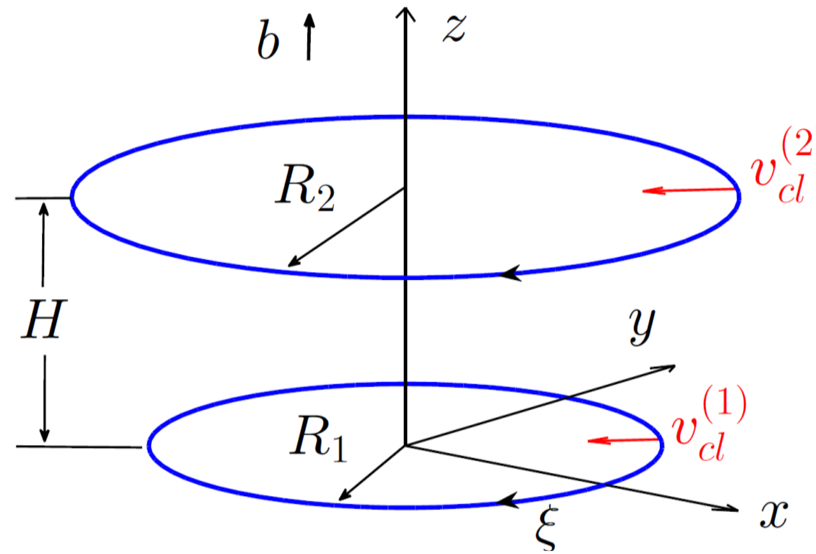
$$v_{\rm cl} = \frac{2\pi D_v}{b\ln(8R/r_d)}\left(c_\infty - c_0 e^{-\frac{f_{\rm cl}\Omega}{bk_BT}}\right) \approx \frac{2\pi D_v c_0\Omega}{b^2k_BT\ln(8R/r_d)}f_{\rm cl}$$

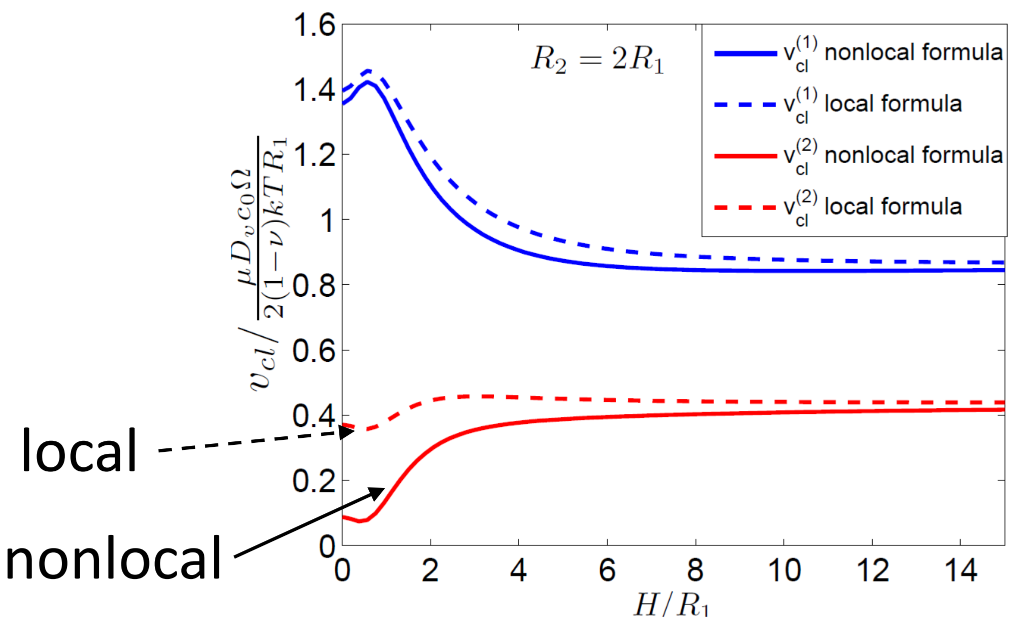
$$\approx \frac{\mu D_v c_0\Omega}{2(1-\nu)Rk_BT}$$

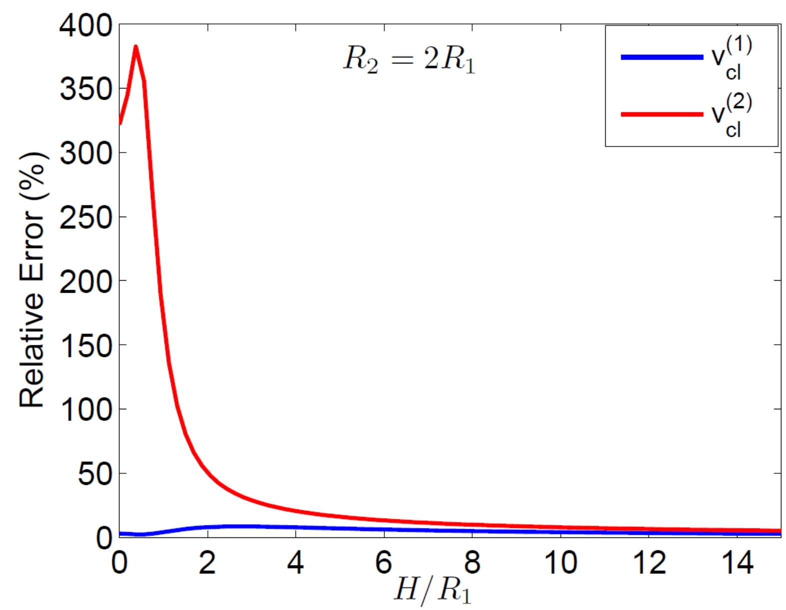
Agrees with Hirth & Lothe 1982

Two Prismatic Dislocation Loops

- Local climb mobility law only for well separated dislocations
- Long-range effect due to vacancy diffusion
- In addition to the long-range effect of PK force







Two Prismatic Dislocation Loops

Greens' function formulation leads to the linear system

$$\frac{b}{4\pi D_v}\left(\frac{4R_1K\left(\frac{2R_1}{\sqrt{4R_1^2+r_d^2}}\right)}{\sqrt{4R_1^2+r_d^2}}v_{\rm cl}^{(1)}+\frac{4R_2K\left(\frac{2\sqrt{R_1R_2}}{\sqrt{(R_1+R_2)^2+H^2+r_d^2}}\right)}{\sqrt{(R_1+R_2)^2+H^2+r_d^2}}v_{\rm cl}^{(2)}\right)=c_\infty-c_0e^{-\frac{f_{\rm cl}^{(1)}\Omega}{bk_BT}},$$

$$\frac{b}{4\pi D_v}\left(\frac{4R_1K\left(\frac{2\sqrt{R_1R_2}}{\sqrt{(R_1+R_2)^2+H^2+r_d^2}}\right)}{\sqrt{(R_1+R_2)^2+H^2+r_d^2}}v_{\rm cl}^{(1)}+\frac{4R_2K\left(\frac{2R_2}{\sqrt{4R_2^2+r_d^2}}\right)}{\sqrt{4R_2^2+r_d^2}}v_{\rm cl}^{(2)}\right)=c_\infty-c_0e^{-\frac{f_{\rm cl}^{(2)}\Omega}{bk_BT}}.$$

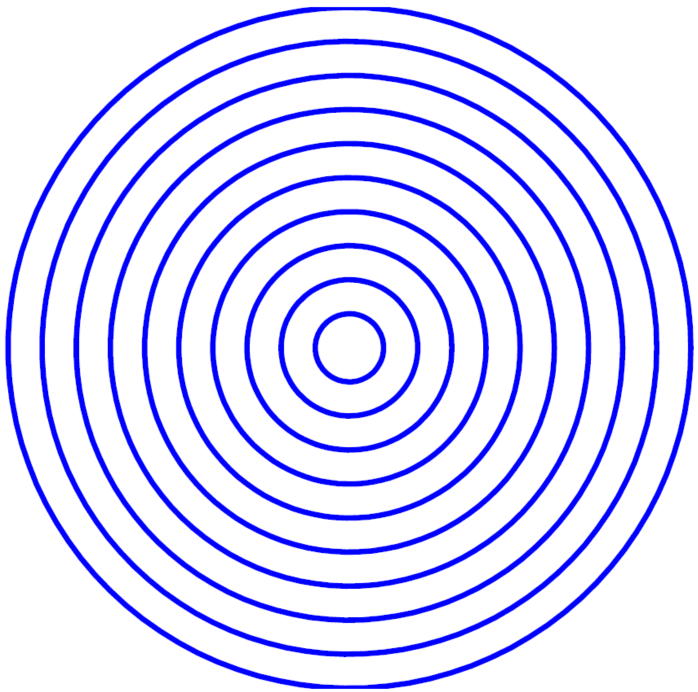
Solution

$$\begin{pmatrix} v_{\rm cl}^{(1)} \\ v_{\rm cl}^{(2)} \end{pmatrix}=\frac{2\pi D_v c_0\Omega}{b^2k_BT(A_{11}A_{22}-A_{12}A_{21})}\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} f_{\rm cl}^{(1)} \\ f_{\rm cl}^{(2)} \end{pmatrix}$$

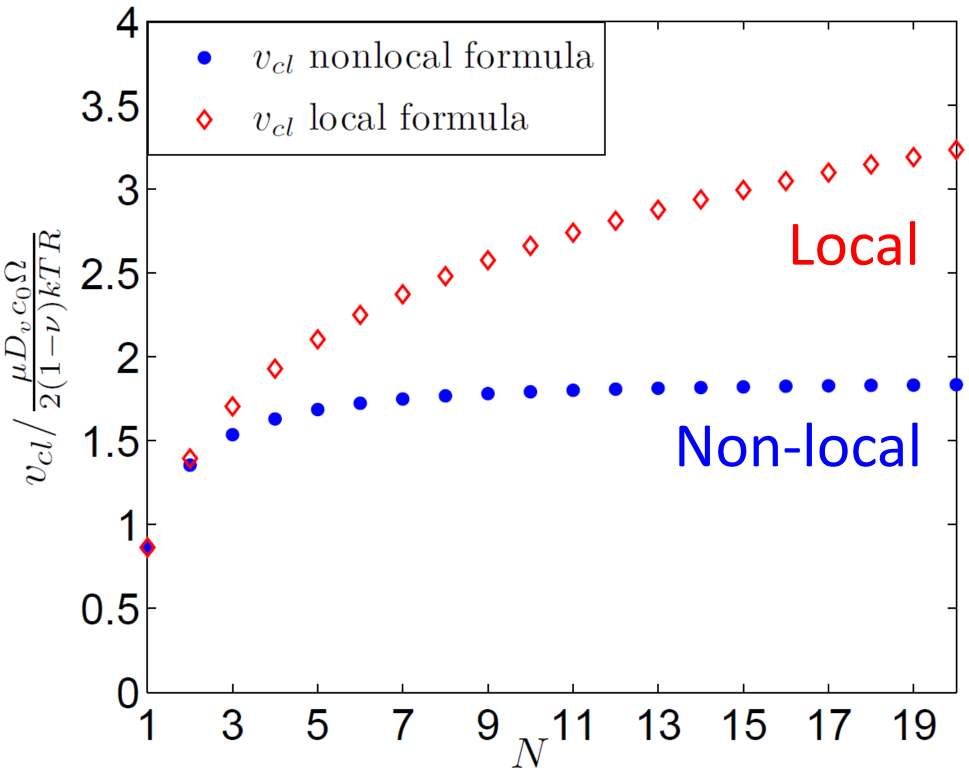
$$A_{11}=\ln\frac{8R_2}{r_d},\ \ A_{12}=-\frac{2R_2}{\sqrt{(R_1+R_2)^2+H^2}}K\left(\frac{2\sqrt{R_1R_2}}{\sqrt{(R_1+R_2)^2+H^2}}\right),$$

$$A_{21}=-\frac{2R_1}{\sqrt{(R_1+R_2)^2+H^2}}K\left(\frac{2\sqrt{R_1R_2}}{\sqrt{(R_1+R_2)^2+H^2}}\right),\ \ A_{22}=\ln\frac{8R_1}{r_d}.$$

Multiple Prismatic Loops



Climb velocity of the innermost loop



Our Green's function formulation provides a systematic tool to handle the long-range effect due to vacancy diffusion.

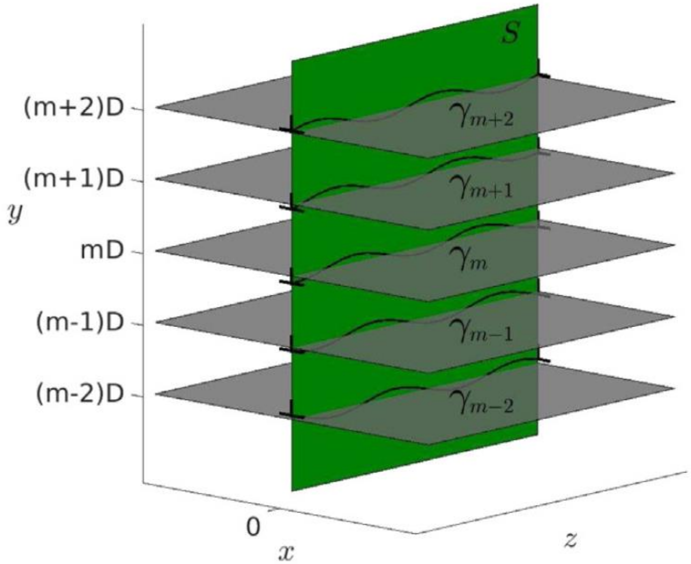
Stability of a Low Angle Tilt Boundary

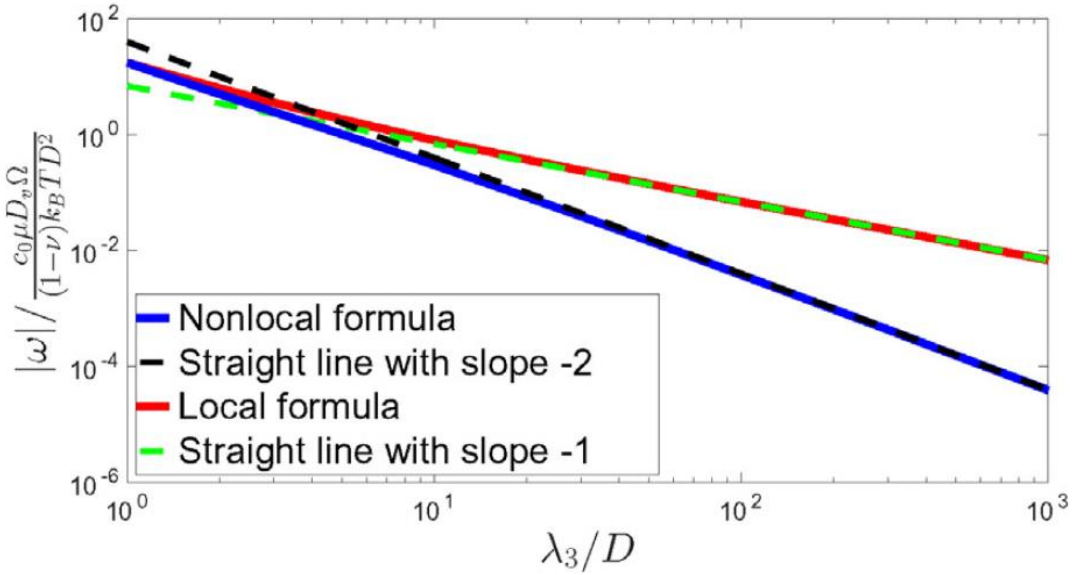
- Perturbation in inter-dislocation distance
- Perturbation wavelength λ=ND, $r_j(t) = jD + \varepsilon e^{\omega t} \cos\frac{2\pi j}{N}$
- Stabilized by dislocation climb

Yejun Gu, Xiang, Srolovitz, Scripta Mater 2016

Local mobility law, $\omega \sim 1/\lambda$

Green's function formulation $\omega \sim 1/\lambda^2$





Implementing Climb in Discrete Dislocation Dynamics

To solve integral equations along dislocations

$$-\frac{1}{4\pi D_v}\int_\Gamma \frac{h(x_1,y_1,z_1)}{\sqrt{(x-x_1)^2+(y-y_1)^2+(z-z_1)^2+r_d^2}}dl + c_\infty = c_0 e^{-\frac{f_{\mathrm{cl}}\Omega}{b_e k_B T}}\Big|_{(x,y,z)}$$

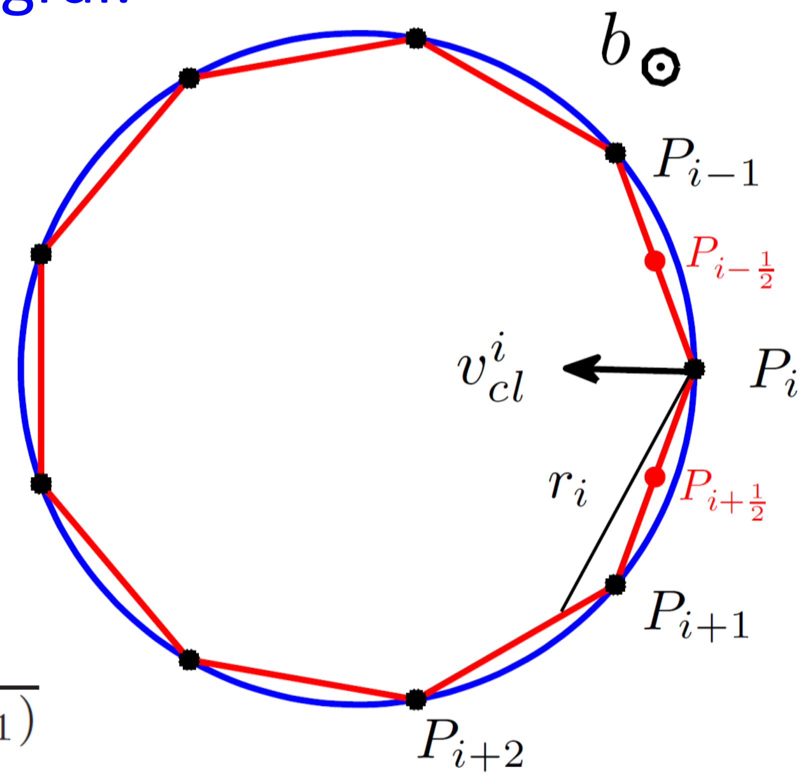
Numerical discretization for the integral:

$$\int_\Gamma \approx \sum_j \int_{P_j P_{j+1}}$$

$$\int_{P_j P_{j+1}} \frac{h(x_1,y_1,z_1)}{r_i(x_1,y_1,z_1)}dl \approx$$

$$h^j \int_{P_j P_{j+\frac{1}{2}}} \frac{dl}{r_i(x_1,y_1,z_1)}$$

$$+\, h^{j+1} \int_{P_{j+\frac{1}{2}} P_{j+1}} \frac{dl}{r_i(x_1,y_1,z_1)}$$



Numerical Algorithm to Implement Climb in Discrete Dislocation Dynamics

1. To solve the linear system

$$\sum_{j=1}^{N} a_{ij} h^j = 4\pi D_v \left(c_\infty - c_0 e^{-\frac{g^i \Omega}{k_B T}} \right)$$

$g=f_{cl}/b_e$ for nonscrew points and linear interpolation in between

$$a_{ii} = \ln \frac{\delta_1 \delta_2}{r_d^2}$$

$$a_{ij} = I_1 + I_2$$

with

$$I_k = \begin{cases} \ln \dfrac{\sqrt{A_k^2 + 4A_kB_k + 4A_kC} + A_k + 2B_k}{2(\sqrt{A_kC} + B_k)} & \text{if } \sqrt{A_kC} + B_k \neq 0 \\ \ln \dfrac{2(\sqrt{A_kC} - B_k)}{\sqrt{A_k^2 + 4A_kB_k + 4A_kC} - A_k - 2B_k} & \text{otherwise} \end{cases}$$

for $k = 1, 2$, and

$$A_1 = (x^j - x^{j-1})^2 + (y^j - y^{j-1})^2 + (z^j - z^{j-1})^2$$

$$A_2 = (x^j - x^{j+1})^2 + (y^j - y^{j+1})^2 + (z^j - z^{j+1})^2$$

$$B_1 = (x^j - x^{j-1})(x^i - x^j) + (y^j - y^{j-1})(y^i - y^j) + (z^j - z^{j-1})(z^i - z^j)$$

$$B_2 = (x^j - x^{j+1})(x^i - x^j) + (y^j - y^{j+1})(y^i - y^j) + (z^j - z^{j+1})(z^i - z^j)$$

$$C = (x^i - x^j)^2 + (y^i - y^j)^2 + (z^i - z^j)^2$$

$$P_i = (x^i, y^i, z^i),\ P_j = (x^j, y^j, z^j),\ P_{j\pm1} = (x^{j\pm1}, y^{j\pm1}, z^{j\pm1}).$$

2. Calculate v_{cl} from h

$$V_{cl}^{\,i} = h^i / b_e^{\,i}$$

for non-screw points

Implementing Climb in Discrete Dislocation Dynamics

Calculation of climb component of Peach-Koehler force (f_{cl})

Many methods available:

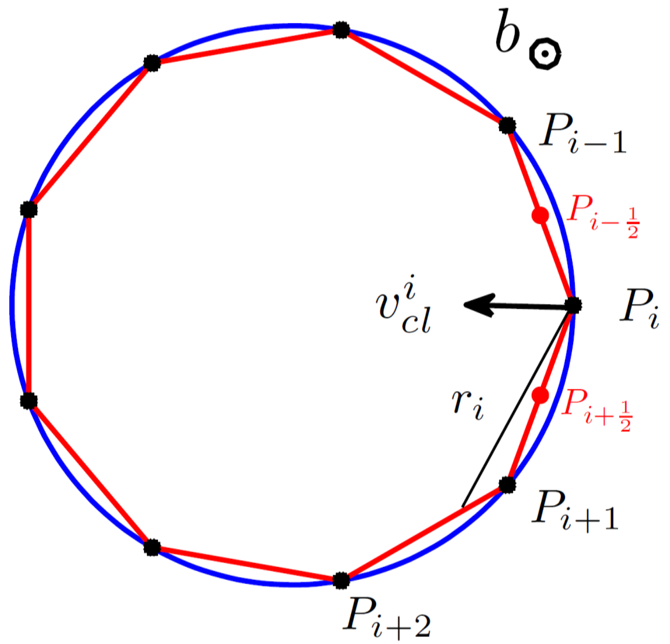
Kubin et al 1992; Zbib et al 1998; Schwarz 1999; Xiang et al 2003; Wang et al 2004; Cai et al 2006; Arsenlis et al 2007; Zhao, Huang & Xiang 2010 …

The climb velocity using our nonlocal Green's function formulation can be calculated with the **same order of computational cost** as that of calculation of the long-range Peach-Koehler force in the available DDD methods.

Implementing Climb in Discrete Dislocation Dynamics

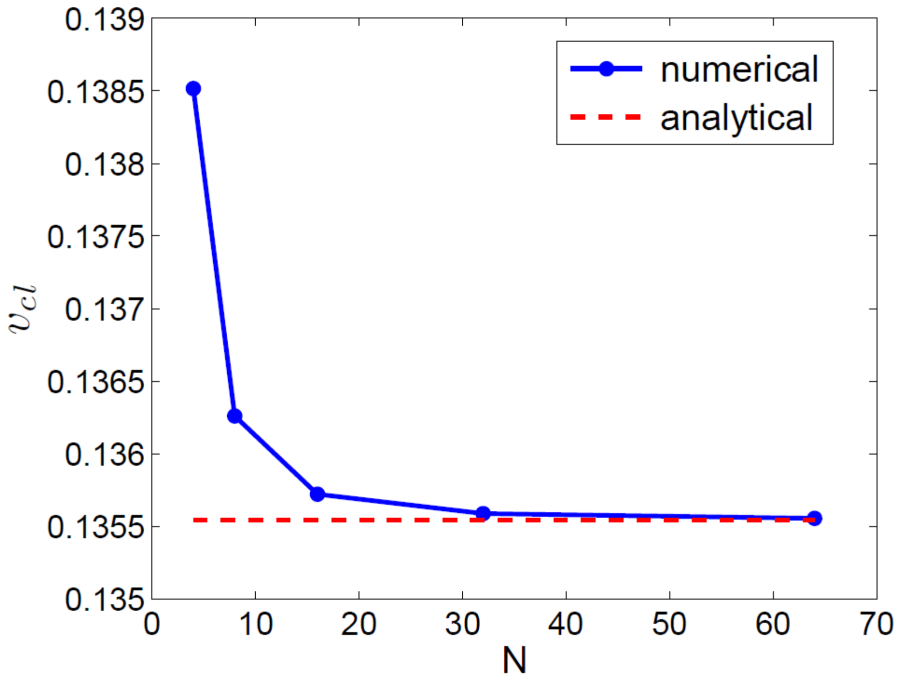
A single prismatic loop

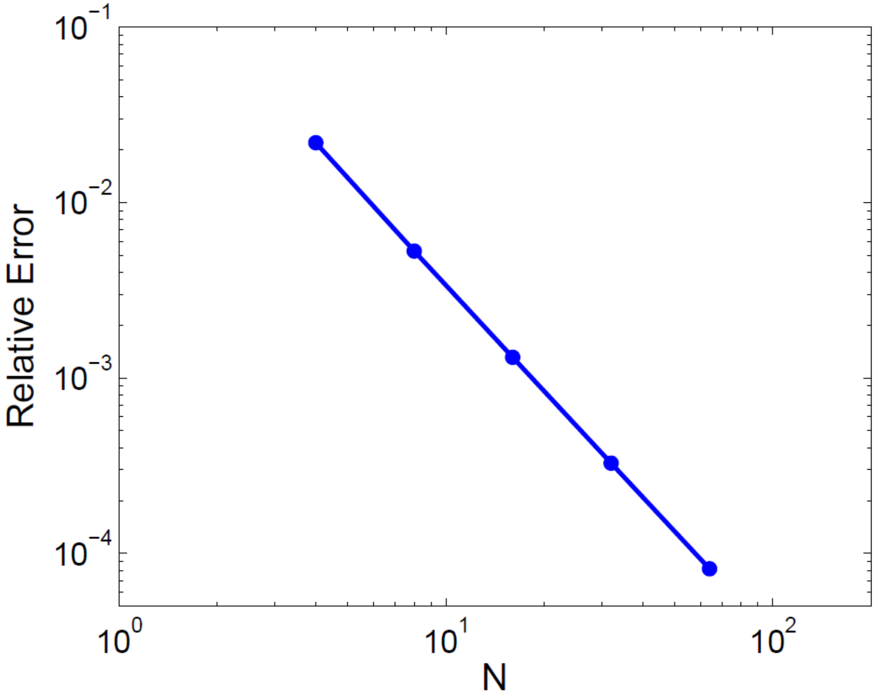
$$A \begin{pmatrix} v_{\mathrm{cl}}^1 \\ v_{\mathrm{cl}}^2 \\ v_{\mathrm{cl}}^3 \\ \vdots \\ v_{\mathrm{cl}}^N \end{pmatrix} = \frac{4\pi D_v}{b} \begin{pmatrix} c_\infty - c_0 e^{-\frac{f_{\mathrm{cl}}^1 \Omega}{b k_B T}} \\ c_\infty - c_0 e^{-\frac{f_{\mathrm{cl}}^2 \Omega}{b k_B T}} \\ c_\infty - c_0 e^{-\frac{f_{\mathrm{cl}}^3 \Omega}{b k_B T}} \\ \vdots \\ c_\infty - c_0 e^{-\frac{f_{\mathrm{cl}}^N \Omega}{b k_B T}} \end{pmatrix}$$



Implementing Climb in Discrete Dislocation Dynamics

Numerical solutions





Implementing Climb in Discrete Dislocation Dynamics

A single prismatic loop

N=6

$$A = \begin{pmatrix} 10.5966 & 1.1305 & 0.6151 & 0.5290 & 0.6151 & 1.1305 \\ 1.1305 & 10.5966 & 1.1305 & 0.6151 & 0.5290 & 0.6151 \\ 0.6151 & 1.1305 & 10.5966 & 1.1305 & 0.6151 & 0.5290 \\ 0.5290 & 0.6151 & 1.1305 & 10.5966 & 1.1305 & 0.6151 \\ 0.6151 & 0.5290 & 0.6151 & 1.1305 & 10.5966 & 1.1305 \\ 1.1305 & 0.6151 & 0.5290 & 0.6151 & 1.1305 & 10.5966 \end{pmatrix}$$

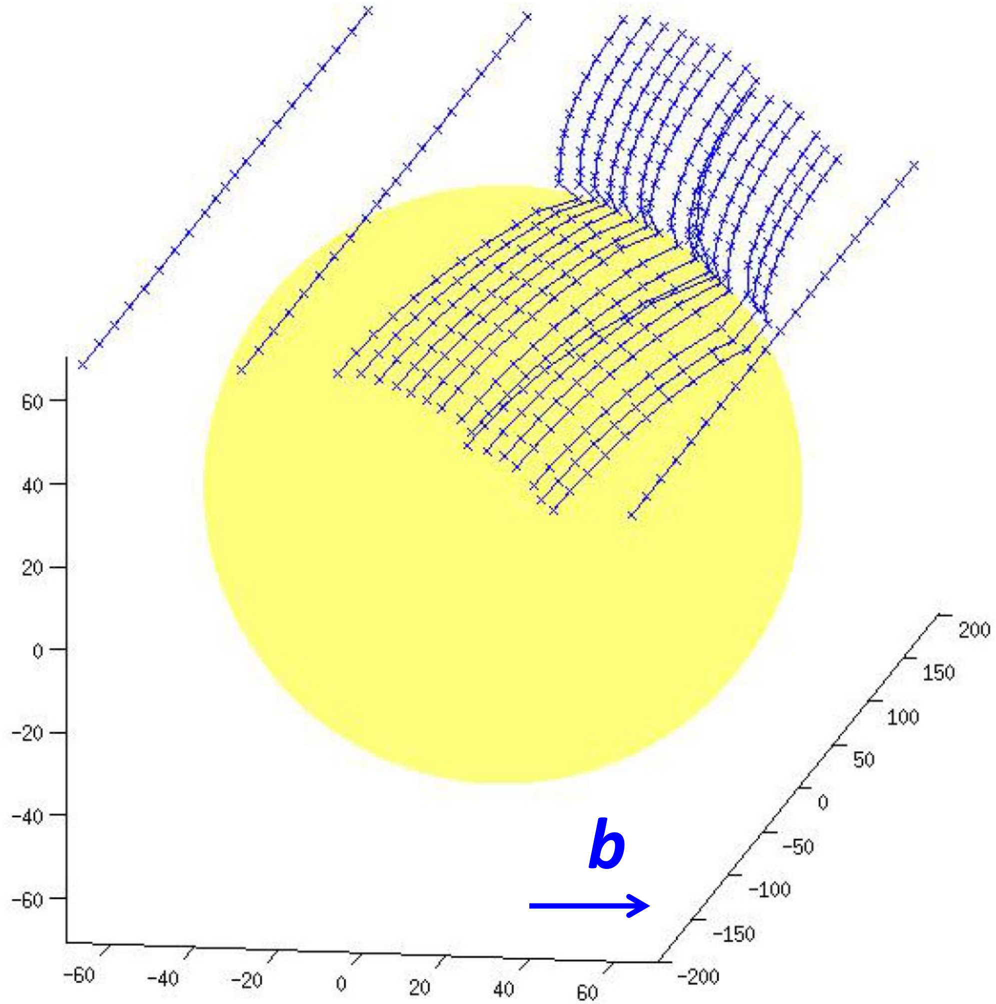
Condition number

1.8223 for N=10
4.2213 for N=100

Implementing Climb in Discrete Dislocation Dynamics

[Dislocation bypassing an impenetrable particle (test)]

- Edge dislocation, driven by applied stress
- Impenetrable particle
- Climbs when glide reaches equilibrium



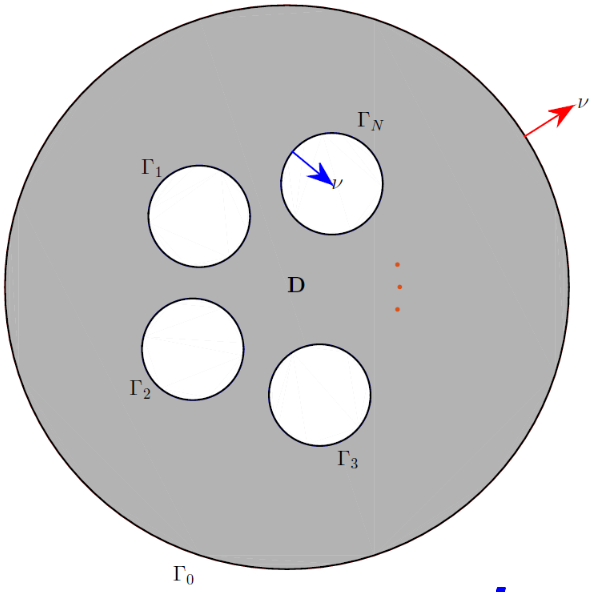
Second Kind Integral Equation Formulation in 2D

Jiang, Rachh, Xiang, *SIAM Multiscale Model. Simul.* 2017

$$\Delta c = 0, \quad \text{in } D,$$

$$c(\boldsymbol{r}) = g_i = c_0 e^{-\frac{f_{\mathrm{cl}}^{(i)}\Omega}{b k_B T}}, \quad \text{on } \Gamma_i, \quad i = 1, \ldots, N,$$

$$c(\boldsymbol{r}) = c_\infty, \quad \text{on } \Gamma_0.$$



$$\mathbf{f}_{PK} = (\boldsymbol{\sigma} \cdot \mathrm{b}) \times \boldsymbol{\tau}$$

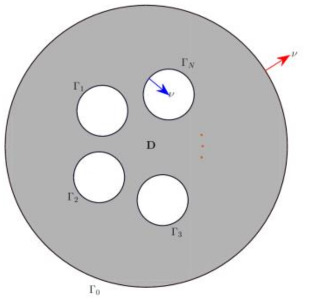
b

$$\sigma_{11}(x_i, y_i) = -\sum_{j \neq i} \mathrm{sgn}(j) \cdot \frac{\mu b}{2\pi(1-\nu)} \frac{(y_i - y_j)[3(x_i - x_j)^2 + (y_i - y_j)^2]}{[(x_i - x_j)^2 + (y_i - y_j)^2]^2}$$

$$v_{\mathrm{cl}}^{(i)} = \frac{D_v}{b} \int_{\Gamma_i} \frac{\partial c(\boldsymbol{r})}{\partial \boldsymbol{\nu}_{\boldsymbol{r}}} dS(\boldsymbol{r}), \quad i = 1, \ldots, N.$$

Second Kind Integral Equation Formulation in 2D

$$c(\boldsymbol{r}) = \sum_{i=1}^{N} \left(\mathcal{D}_{\Gamma_i}[\rho_i](\boldsymbol{r}) + \frac{1}{2\pi|\Gamma_i|} \left(\int_{\Gamma_i} \rho_i dS \right) \log|\boldsymbol{r} - \boldsymbol{r}_i| \right) + \mathcal{D}_{\Gamma_0}[\rho_0](\boldsymbol{r})$$



$$-\frac{1}{2}\rho_i(\boldsymbol{r}) + \mathcal{D}_{\Gamma_i}^{PV}[\rho_i](\boldsymbol{r}) + \mathcal{D}_{\Gamma_0}[\rho_0](\boldsymbol{r}) + \sum_{\substack{j=1 \\ j\neq i}}^{N} \mathcal{D}_{\Gamma_j}[\rho_j](\boldsymbol{r})$$

$$+ \sum_{j=1}^{N} \frac{1}{2\pi|\Gamma_j|} \left(\int_{\Gamma_j} \rho_j dS \right) \log|\boldsymbol{r} - \boldsymbol{r}_j| = g_i, \quad \boldsymbol{r} \in \Gamma_i, \quad i = 1, \ldots, N.$$

$$-\frac{1}{2}\rho_0(\boldsymbol{r}) + \mathcal{D}_{\Gamma_0}^{PV}[\rho_0](\boldsymbol{r})$$

$$+ \sum_{i=1}^{N} \left(\mathcal{D}_{\Gamma_i}[\rho_i](\boldsymbol{r}) + \frac{1}{2\pi|\Gamma_i|} \left(\int_{\Gamma_i} \rho_i dS \right) \log|\boldsymbol{r} - \boldsymbol{r}_i| \right) = c_\infty, \quad \boldsymbol{r} \in \Gamma_0,$$

Second Kind Integral Equation Formulation in 2D

(a) Algorithm 1: FMM+GMRES, i.e, use GMRES to solve the linear system iteratively with the FMM [4, 14] to accelerate the computation of the matrix-vector product.

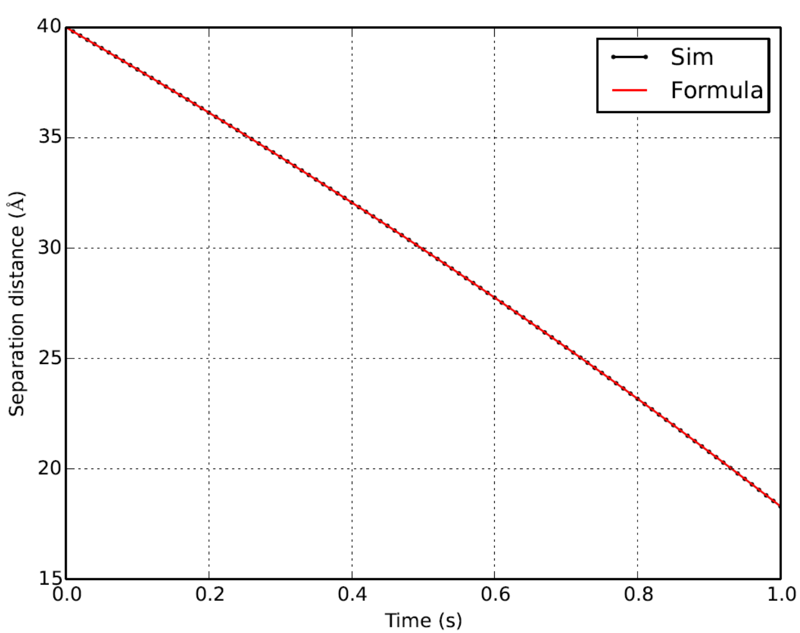
(b) Algorithm 2: FDS, i.e., use the fast direct solver [20, 22] to construct an efficient factorization for A^{-1} to high precision, then simply apply the compressed A^{-1} to b to obtain the solution vector.

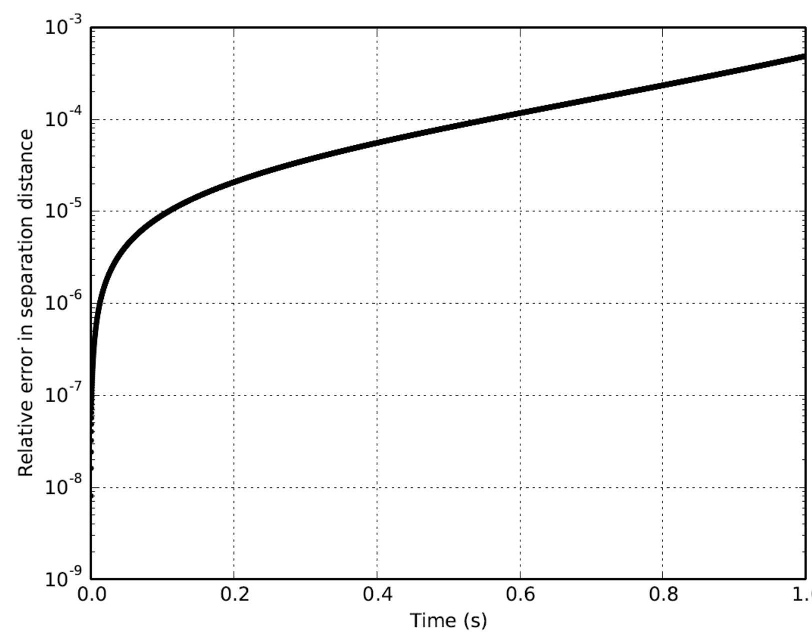
(c) Algorithm 3: FDS+FMM+GMRES, i.e., use the fast direct solver to constrct an efficient factorization for the matrix inverse with low accuracy, denoted by A_{la}^{-1}, then apply FMM accelerated iterative solve to solve the preconditioned linear system $A_{\text{la}}^{-1}Ax = A_{\text{la}}^{-1}b$.

Second Kind Integral Equation Formulation in 2D

Dynamics of dislocation dipole

$$v_{\mathrm{cl,a}}(r_a(t)) = \frac{\pi D_v}{b \ln(r_\infty / \sqrt{r_a(t) r_d})} \left(c_\infty - c_0 e^{-\frac{f_{\mathrm{cl}}(t)\Omega}{b k_B T}} \right)$$





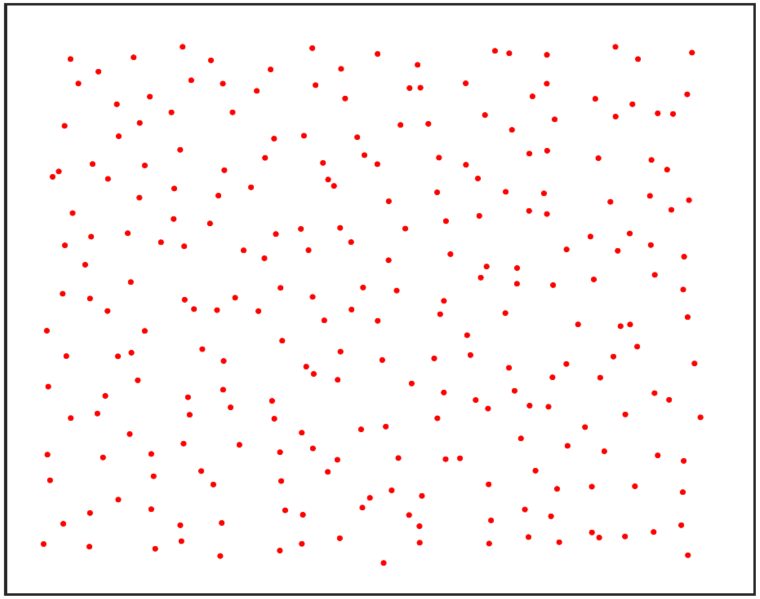
Second Kind Integral Equation Formulation in 2D

Number of GMRES iterations

stopping tolerance 10^{-10}

Algorithm 1

N	8^2	16^2	32^2	62^2	128^2
$p=2$	33	47	77	120	200
$p=4$	33	47	74	130	200
$p=6$	33	47	77	120	190
$p=8$	33	47	90	140	180



Algorithm 3

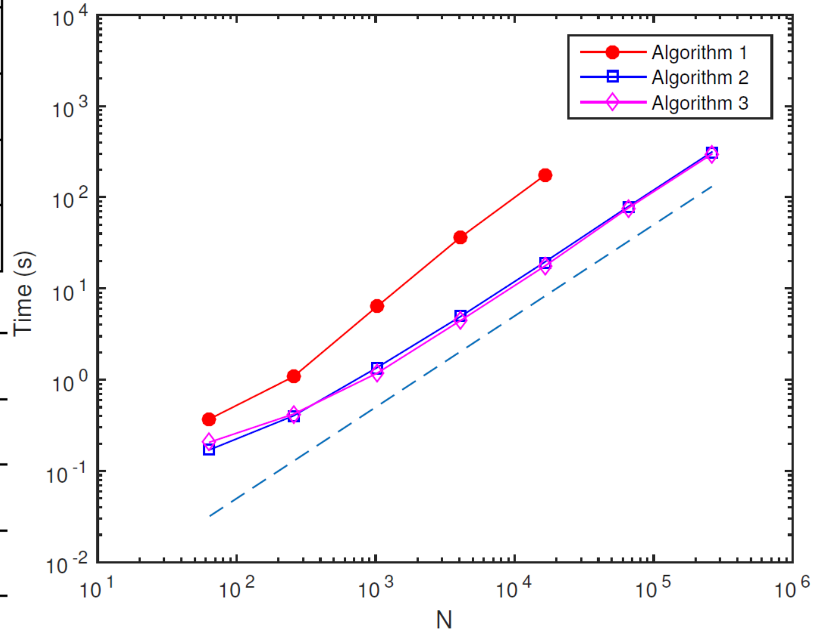
N	8^2	16^2	32^2	64^2	128^2	256^2	512^2
$p=2$	3	4	4	4	4	5	5
$p=4$	3	4	4	4	4	5	5
$p=6$	3	3	4	4	4	5	5
$p=8$	3	4	4	4	4	5	5

Random

Second Kind Integral Equation Formulation in 2D

Timing (algorithms 1,2,3)

N	8^2	16^2	32^2	64^2	128^2
$p=2$	0.308	0.768	4.09	24.0	177
$p=4$	0.380	1.46	8.58	61.7	393
$p=6$	0.440	1.69	10.1	67.2	436
$p=8$	0.472	1.95	14.1	91.8	485



N	8^2	16^2	32^2	64^2	128^2
$p=2$	0.056	0.461	1.72	10.5	82.3
$p=4$	0.242	0.822	4.12	27.7	217
$p=6$	0.349	1.17	6.18	43.7	339
$p=8$	0.443	1.58	7.82	51.9	386

N	8^2	16^2	32^2	64^2	128^2	256^2	512^2
$p=2$	0.104	0.395	0.96	3.93	17.0	83.1	401
$p=4$	0.171	0.501	1.56	6.16	27.0	126	582
$p=6$	0.240	0.546	1.84	7.49	32.7	150	677
$p=8$	0.310	0.727	2.53	9.97	43.2	196	870

Upscaling from atomistic scheme to dislocation dynamics

Niu, Luo, Lu, Xiang, *J Mech Phys Solids* 2017

Vacancy diffusion

$$c_t = D_v(c_{xx} + c_{yy} + c_{zz}), \text{ in the bulk},$$

$$-\frac{\partial c}{\partial n} = \frac{1}{l_\phi}(c - k_v c_d)\Big|_{r=r_d},$$

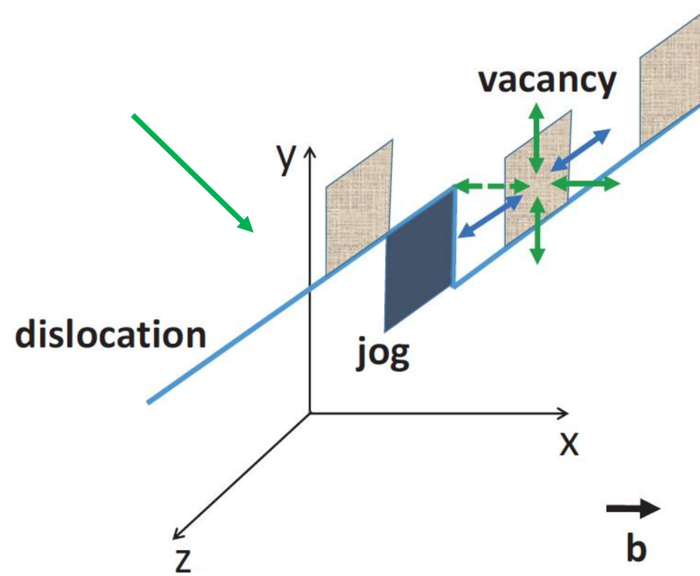
Finite exchange rates between dislocation sites and bulk sites

$$c = c_\infty\big|_{r=r_\infty}.$$

Climb velocity

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

Due to pipe diffusion



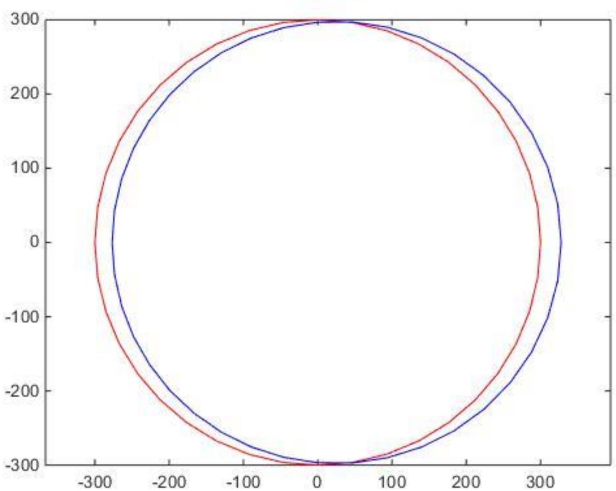
Conservative climb of prismatic loops by pipe diffusion

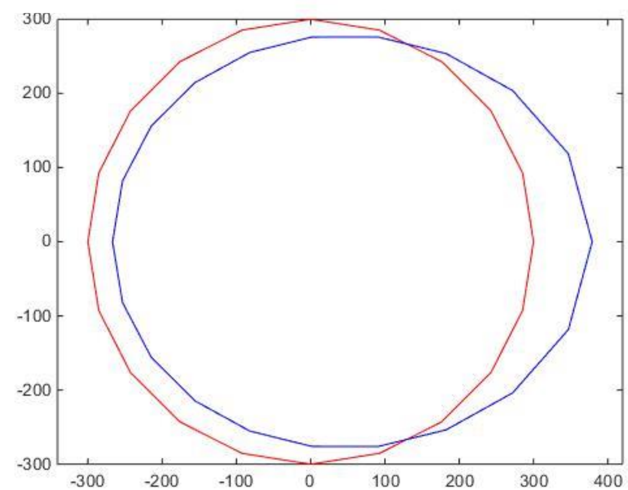
Experimental Observation: Kroupa & Prince 1961, Hirth & Lothe 1982.

- Not very high temperature; Under stress gradient
- Vacancy pipe diffusion dominates; Bulk diffusion is shut down

Our model in this case: $v_{\mathrm{cl}} = D_c b \frac{\mathrm{d}^2 c_d}{\mathrm{d}s^2}$ $\quad c_d(s) = c_0 e^{-\frac{f_{\mathrm{cl}}(s)\Omega}{bkT}}$

Enclosed area is conserved $\frac{\mathrm{d}S}{\mathrm{d}t} = \int_\gamma v_{\mathrm{cl}} \mathrm{d}s = 0.$





Other approach: translation of the whole loop with energy barrier
Swinburne et al, Scientific Report 2016, … .

Summary

- Green's function formulation for vacancy/interstitial diffusion assisted dislocation climb
- Nonlocal, incorporating new long-range effect of climb velocity due to vacancy diffusion
- Widely used local climb velocity formula applies only to some special cases.
- Numerical implementation method in DDD
- Applications and generalizations