Phase field model for dislocation self-climb of prismatic dislocation loops

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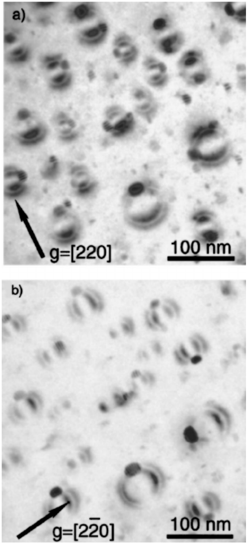
Prismatic loop images-pictures borrowed from web



Picture by Chaldyshev et al ’02

Dislocation loops in Sb-doped LT GaAs

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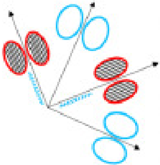

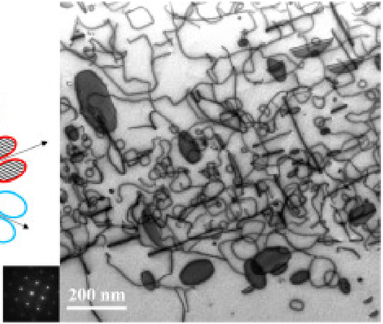

Picture by Xiu et al. ’20

Dislocation loops in irradiated FCC alloy

What is self-climb of dislocation loops

During the core diffusion process, atoms can be absorbed or emitted by the core region, leading to climb out of the original slip plane, known as dislocation self-climb.

- Driven by pipe diffusion of vacancies along the dislocations.
- Area enclosed by dislocation loop (projected perpendicular to Burgers vector) is preserved during the self climb motion.
- Dominant mechanism of prismatic motion at not very high temperatures (much faster diffusivity comparing to bulk diffusion)

Experimental observations of self-climb of prismatic loops

Self-climb motion of dislocations plays an important role in irradiated materials.

Johnson (1960), Silcox and Whelan (1960), Vendervoort and Washburn (1960), Krupa and Price (1961), Turnbull (1970), Narayan and Washburn (1972), Hirth and Lothe (1982), Burton and Speight (1986), Durarev (2013), Durarev et al (2014)Swinburne et al (2016), Okata et al (20160, Hayakawa et al (2016)

Previous models for self climb

- Johnson (1960) Proposed short circuit mechanism (self-climb) for coalescence of dislocation loops.
- Kroupa (1960)
  - Derived analytical formula for self-climb velocity for circular loops
  - Climb velocity of the circular loop satisfies linear mobility law $\mathbf{v_{cl}} \sim \mathbf{f}_{cl}$
  - Assume loop remain unchanged during evolution
- Turunen and Lindroos (1974)
  - Proposed a self-climb model for dislocation line
  - climb velocity $v \sim \frac{d^2}{ds^2} f_{cl}$

Previous models for self climb continued

- Niu et al (2017)
  - Discrete dislocation dynamics model via upscaling from stochastic self climb model.
  - $\mathbf{v} \sim \frac{d^2}{ds^2}\mathbf{f}_{cl}$
  - local velocity formula, works for any dislocation
- Niu et al (2019) Numerical simulations for the DDD model.
- Liu et al (2020) Finite element framework for self-climb.

Dislocation self-climb velocity formulation

- Niu-Luo-Lu-Xiang (2017): The climb velocity

$$v_{cl} = v_{cl}^{(b)} + v_{cl}^{(p)}$$

where $v_{cl}^{(b)}$ is the climb velocity due to bulk diffusion and $v_{cl}^{(p)}$ is climb velocity due to pipe diffusion. The self climb velocity is proportional to the second derivative of the vacancy concentration on the dislocation core.

$$v_{cl}^{(p)} = D_c b \frac{d^2}{ds^2} c_d^c = c_0 D_c b \frac{d^2}{ds^2} e^{-\frac{f_{cl}\Omega}{bK_B T}}$$

When $f_{cl} \ll \frac{bK_b T}{\Omega}$, the self climb velocity reduces to

$$v_{cl}^{(p)} = -\frac{c_0 D_c \Omega}{k_B T} \frac{d^2 f_{cl}}{ds^2}$$

Why Phase field model

- Common framework for evolution of interfaces.
- Can handle topological automatically and to avoid re-meshing during simulations.
- Phase field models for glide and climb by vacancy bulk diffusion have been developed. Core diffusion has been ignored in those models.

Phase field model

Phase field model for self-climb of prismatic dislocation loops

$$
\begin{aligned}
\phi_t &= \nabla \cdot \left(M(\phi) \nabla \frac{\mu_c}{g(\phi)} \right) \\
\mu_c &= -\Delta \phi + \frac{1}{\varepsilon^2} q'(\phi) + \frac{1}{\varepsilon} h(\phi) f_{cl} \\
&= \frac{\delta E_{CH}}{\delta \phi} + \frac{1}{\varepsilon} h(\phi) \frac{\delta E_{el}}{\delta \phi}
\end{aligned}
$$

where

$$
E_{CH}(\phi) = \int_\Omega \frac{1}{2} |\nabla \phi(x)|^2 + \frac{1}{\varepsilon^2} q(\phi(x)) dx
$$

is the classic Cahn-Hillard energy and

Proposed phase field model continued

elastic energy is

$$E_{el} = \int_{\Omega} \left(\frac{1}{2} \phi f_{cl}^{d} - \phi f_{cl}^{app} \right) dx$$

Here

$$M(\phi) = M_0 \phi^2 (1-\phi)^2 \qquad g(\phi) = \phi^2 (1-\phi)^2,$$

are degenerate mobility and stability function respectively, and

$$q(\phi) = 2\phi^2 (1-\phi)^2 \qquad h(\phi) = H_0 \phi^2 (1-\phi)^2.$$

$h(\phi)$ guarantee the climb force is only added to the C-H chemical potential only on the dislocations.

Proposed phase field model continued

We assume all prismatic loops have same Burgers vector $\mathbf{b} = (0, 0, b)$ and let σ denote the stress. Then

$$f_{cl} = -\sigma_{33} b = f_{cl}^{d} + f_{cl}^{app}$$

where

$$f_{cl}^{d} = -\sigma_{33}^{d} b, \qquad f_{cl}^{app} = -\sigma_{33}^{app} b$$

with σ_{33}^{d} is a stress component generated by all dislocations given by

$$\sigma_{33}^{d} = \frac{\mu b}{4\pi(1-\nu)} \int_C -\frac{x-\bar{x}}{R^3} d\bar{y} + \frac{y-\bar{y}}{R^3} d\bar{x}$$

Outer expansion

We first consider expansion with respect to ε in the region away from the dislocations. Assume

$$\phi(x,y,t) = \phi^{(0)}(x,y,t) + \varepsilon\phi^{(1)}(x,y,t) + \varepsilon^2\phi^{(2)}(x,y,t) + \cdots .$$

Accordingly, we have

$$\begin{aligned}
g(\phi) &= g(\phi^{(0)}) + g'(\phi^{(0)})\phi^{(1)}\varepsilon \\
&\quad + \left(g'(\phi^{(0)})\phi^{(2)} + \frac{1}{2}g''(\phi^{(0)})\left(\phi^{(1)}\right)^2 \right)\varepsilon^2 + \cdots , \\
h(\phi) &= h(\phi^{(0)}) + h'(\phi^{(0)})\phi^{(1)}\varepsilon \\
&\quad + \left(h'(\phi^{(0)})\phi^{(2)} + \frac{1}{2}h''(\phi^{(0)})\left(\phi^{(1)}\right)^2 \right)\varepsilon^2 + \cdots , \\
q(\phi) &= q(\phi^{(0)}) + g'(\phi^{(0)})\phi^{(1)}\varepsilon \\
&\quad + \left(q'(\phi^{(0)})\phi^{(2)} + \frac{1}{2}q''(\phi^{(0)})\left(\phi^{(1)}\right)^2 \right)\varepsilon^2 + \cdots
\end{aligned}$$

Outer expansion continued

We also expand the climb force and chemical potential as

$$\begin{aligned} f_{cl}^{d}(x,y,\phi) &= f_{cl}^{d}(x,y,\phi^{(0)}) + f_{cl}^{d}(x,y,\phi^{(1)})\varepsilon + f_{cl}^{d}(x,y,\phi^{(2)})\varepsilon^2 + \cdots, \\ \mu_c &= \frac{1}{\varepsilon^2}\left(\mu_c^{(0)} + \mu_c^{(1)}\varepsilon + \mu_c^{(2)}\varepsilon^2 + \cdots\right) \end{aligned}$$

For $M(\phi) = M_0 g(\phi)$, we rewrite our phase field equation as

$$\phi_t = M_0\left(\Delta\mu_c - \nabla\cdot\left(\mu_c\frac{g'(\phi)}{g(\phi)}\nabla\phi\right)\right)$$

Outer expansion -matching ε powers $O(\frac{1}{\varepsilon^2})$, $O(\frac{1}{\varepsilon})$

Comparing ε powers on both sides, we have

$$O(\frac{1}{\varepsilon^2}) \qquad 0 = \Delta\mu_c^{(0)} - \nabla\cdot\left(\left(\mu_c\frac{g'(\phi)}{g(\phi)}\right)^{(0)}\nabla\phi^{(0)}\right)$$

Here $\mu_c^{(0)} = q'(\phi^{(0)})$, $\left(\mu_c\frac{g'(\phi)}{g(\phi)}\right)^{(0)} = 8(1-2\phi^{(0)})^2$. $\phi^{(0)} = 1$ or 0 satisfies this equation.

$$O(\frac{1}{\varepsilon}) \qquad 0 = \Delta\mu_c^{(1)} - \nabla\cdot\left(\left(\mu_c\frac{g'(\phi)}{g(\phi)}\right)^{(0)}\nabla\phi^{(1)}\right) - \nabla\cdot\left(\left(\mu_c\frac{g'(\phi)}{g(\phi)}\right)^{(1)}\nabla\phi^{(0)}\right). \qquad (1)$$

Outer expansion -matching ε powers $O(1)$

Substituting $\mu_c^{(1)} = q''(\phi^{(0)})\phi^{(1)} + h(\phi^{(0)}) f_{cl}^d(x, y, \phi^{(0)})$ and $\phi^{(0)} = 1$ or 0 into (1), we have

$$\Delta \left(q''(\phi^{(0)})\phi^{(1)} \right) - \nabla \cdot \left(8(1 - 2\phi^{(0)})^2 \nabla \phi^{(1)} \right) = 0. \qquad (2)$$

Thus $\phi^{(1)} = 0$ satisfies (2).
The order $O(1)$ equation is

$$\begin{aligned} \phi_t^{(0)} &= M_0 \left[\Delta \mu_c^{(2)} - \nabla \cdot \left(\left(\mu_c \frac{g'(\phi)}{g(\phi)} \right)^{(2)} \nabla \phi^{(0)} \right) \right. \\ & \quad - \nabla \cdot \left(\left(\mu_c \frac{g'(\phi)}{g(\phi)} \right)^{(1)} \nabla \phi^{(1)} \right) \\ & \quad \left. - \nabla \cdot \left(\left(\mu_c \frac{g'(\phi)}{g(\phi)} \right)^{(0)} \nabla \phi^{(2)} \right) \right]. \end{aligned} \qquad (3)$$

Outer expansion $O(1)$ continued

Substituting $\phi^{(0)} = 1$ or 0, $\phi^{(1)} = 0$ and

$$\mu_c^{(2)} = -\Delta\phi^{(0)} + q''(\phi^{(0)})\phi^{(2)} + \frac{1}{2}q'''(\phi^{(0)})\left(\phi^{(1)}\right)^2 + h'(\phi^{(0)})f_{cl}^d(x,y,\phi^{(0)})\phi^{(1)} + h(\phi^{(0)}f_{cl}^d(x,y,\phi^{(1)})$$

into (3), we have

$$\Delta\left(''(\phi^{(0)}\phi^{(2)}-\right) - \nabla\cdot\left(\left(\mu_c\frac{g'(\phi)}{g(\phi)}\right)^{(0)}\nabla\phi^{(2)}\right) = 0. \qquad (4)$$

For which $\phi^{(2)} = 0$ is a solution.

Outer expansion $O(\varepsilon^k)$

In general, the $O(\varepsilon^k)$ ($k \geq 1$) equation is

$$\phi_t^{(k)} = M_0 \left[\Delta\mu_c^{(2+k)} - \sum_{i=1}^{k+2} \nabla \cdot \left(\left(\mu_c \frac{g'(\phi)}{g(\phi)} \right)^{(i)} \nabla\phi^{(k+2-i)} \right) \right]$$

Substituting $\phi^{(0)} = 1$ or 0, $\phi^{(1)} = \cdots = \phi^{(k+1)} = 0$ and

$$\mu_c^{(k+2)} = -\Delta\phi^{(k)} + \left(q'(\phi)\right)^{(k+2)} + \left(h(\phi) f_{cl}^{d}(x, y, \phi)\right)^{(k+1)}$$

into (5) , yields

$$\Delta \left(''(\phi^{(0)}\phi^{(k+2)} - \right) - \nabla \cdot \left(\left(\mu_c \frac{g'(\phi)}{g(\phi)} \right)^{(0)} \nabla\phi^{(k+2)} \right) = 0. \quad (5)$$

thus $\phi^{(k+2)} = 0$ is a solution.

Outer expansion-summary

The outer expansion shows

$$\phi^{(0)} = 1 \text{ or } 0; \phi^{(k)} = 0.$$

i.e $\phi = 0$ or 0 in the outer region.

Inner region-coordinates

For a point in the small region near the dislocation, we can write

$$\mathbf{r}(s,d) = \mathbf{r}_0(s) + d\mathbf{n}(s)$$

where s be the arc length parameter of the dislocation, $\mathbf{r}_0(s)$ represents point on the dislocation and d is the signed distance from point $\mathbf{r}$ to the dislocation.
Let $\rho = d/\varepsilon$, under coordinate system (s,ρ) with coordinate axes $(\mathbf{t}(s), \mathbf{n}(s))$, we have

$$\nabla = \frac{1}{1-\varepsilon\rho\kappa}\mathbf{t}\partial_s + \frac{1}{\varepsilon}\mathbf{n}\partial_\rho$$

Inner region-coordinates continued

Write $\phi(x, y, t) = \Phi(s, \rho, t)$, the phase field equation can be written as

$$\begin{aligned}\Phi_t + \frac{1}{\varepsilon} v_n \partial_\rho \Phi &= \frac{M_0}{1-\varepsilon\rho\kappa}\partial_s\left(\frac{1}{1-\varepsilon\rho\kappa}\left(\partial_s\mu_c - \frac{g'(\Phi)}{g(\Phi)}\mu_c\partial_s\Phi\right)\right) \\ &+ \frac{1}{\varepsilon^2}\frac{M_0}{1-\varepsilon\rho\kappa}\partial_\rho\left(\frac{1}{1-\varepsilon\rho\kappa}\left(\partial_\rho\mu_c - \frac{g'(\Phi)}{g(\Phi)}\mu_c\partial_\rho\Phi\right)\right)\end{aligned}$$

$$\begin{aligned}\mu_c &= -\frac{1}{1-\varepsilon\rho\kappa}\partial_s\left(\frac{1}{1-\varepsilon\rho\kappa}\partial_s\Phi\right) - \frac{1}{\varepsilon^2}\frac{1}{1-\varepsilon\rho\kappa}\partial_\rho\left((1-\varepsilon\rho\kappa)\partial_\rho\Phi\right) \\ &+ \frac{1}{\varepsilon^2}q'(\Phi) + \frac{1}{\varepsilon}h(\Phi)f^d_{cl}(s, \rho, \Phi)\end{aligned}$$

Inner expansion

Expand in ε powers,

$$\Phi(s,\rho,t) = \Phi^{(0)}(\rho) + \varepsilon\Phi^{(1)}(s,\rho,t) + \varepsilon^2\Phi^{(2)}(s,\rho,t) + \cdots$$

$$f_{cl}(s,\rho,\Phi) = \frac{1}{\varepsilon} f^{(-1)}(\rho,\Phi^{(0)}) + f_{cl}^{(0)}(s) + O(\varepsilon)$$

where the force due to stress field $\frac{1}{\varepsilon} f^{(-1)}(\rho,\Phi^{(0)})$ and climb force on the dislocation $f_{cl}^{(0)}(s)$ are

$$\begin{aligned}
f^{(-1)}(\rho,\Phi^{(0)}) &= \frac{\mu b}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\partial_\rho \Phi^{(0)}(\rho_1)}{\rho - \rho_1} d\rho_1 \\
f_{cl}^{(0)}(s) &= f_{cl}^{d}(s) + f_{cl}^{app}(s) \\
f_{cl}^{d}(s) &= \frac{\mu b^2}{4\pi(1-\nu)} \kappa \ln \varepsilon + O(1)
\end{aligned}$$

Asymptotic matching-$O(\varepsilon^{-4})$

Matching the ε powers on both sides, we have The $O(\varepsilon^{-4})$ equation is

$$\partial_{\rho\rho}\mu_c^{(0)} - \partial_\rho \left(\mu_c^{(0)} \frac{g'(\Phi^{(0)})}{g(\Phi^{(0)})} \partial_\rho \Phi^{(0)} \right) = 0 \tag{6}$$

$$\mu_c^{(0)} = -\partial_{\rho\rho}\Phi^{(0)} + q'(\Phi^{(0)}) + h(\Phi^{(0)}) f_{cl}^{(-1)}(\rho, \Phi^{(0)}).$$

Integrating (6), we have

$$\partial_\rho \mu_c^{(0)} - \mu_c^{(0)} \partial_\rho \ln g \left(\Phi^{(0)} \right) = C_1(s) \tag{7}$$

Recall $\mu_c^{(0)} = 0$ in the outer region, the asymptotic matching gives $\mu_c^{(0)}, \partial_\rho \mu_c^{(0)}$ both $\to 0$ as $\rho \to \pm\infty$. Thus $C_1(s) = 0$.

Asymptotic matching $O(\varepsilon^{-4})$-continued

Divide (7) by $\mu_c^{(0)}$ and integrate, we have

$$\mu_c^{(0)} = C_2(s)g(\Phi^{(0)}).$$

Since $\mu_c^{(0)}$ is independent of s and goes to 0 as $\rho \to \pm\infty$, we must have $C_2(s) = 0$. i.e.

$$-\partial_{\rho\rho}\Phi^{(0)} + q'(\Phi^{(0)}) + h(\Phi^{(0)}f_{cl}^{(-1)}(\rho, \Phi^{(0)}) = 0. \tag{8}$$

Solution to (8) with far field condition $\Phi^{(0)}(+\infty) = 0$, $\Phi^{(0)}(-\infty) = 1$ can found numerically.

Graph of $\Phi^{(0)}(\rho)$

$$H_0 = 56.25\,\left(2(1-\nu)/\mu b^2\right),$$

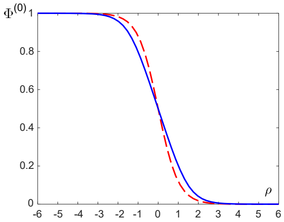

Figure 2: Profile of $\Phi^{(0)}(\rho)$ by solving Eq. (4.28) (solid blue line), and comparison with that in the classical Cahn-Hilliard equation (dashed red lne).

Asymptotic matching-$O(\varepsilon^{-3})$

The $O(\varepsilon^{-3})$ equation is

$$\partial_{\rho\rho}\mu_c^{(1)} - \partial_\rho\left(\mu_c^{(1)}\frac{g'(\Phi^{(0)})}{g(\Phi^{(0)})}\partial_\rho\Phi^{(0)}\right) = 0 \tag{9}$$

$$\mu_c^{(1)} = -\partial_{\rho\rho}\Phi^{(1)} + \kappa\partial_\rho\Phi^{(0)} + q''\left(\Phi^{(0)}\right)\Phi^{(1)} + h(\Phi^{(0)})f_{cl}^0(s) + h'(\Phi^{(0)})f_{cl}^{(-1)}(\rho,\Phi^{(0)})\Phi^{(1)} \tag{10}$$

$$\partial_\rho\mu_c^{(1)} - \mu_c^{(1)}\partial_\rho \ln g\left(\Phi^{(0)}\right) = C_3(s) \tag{11}$$

Matching with outer solutions, we have $\mu_c^{(1)}$, $\partial_\rho\mu_c^{(1)} \to 0$ as $\rho \to \pm\infty$, therefore $C_3(s) = 0$. (11) yields

$$\partial_\rho \ln\left(\mu_c^{(1)}/g(\Phi^{(0)})\right) = 0,$$

thus

$$\mu_c^{(1)} = D_1(s)g(\Phi^{(0)})$$

Asymptotic matching-$O(\varepsilon^{-3})$: $\mu_c^{(1)}$

i.e

$$\begin{aligned} D_1(s)g(\Phi^{(0)} &= -\partial_{\rho\rho}\Phi^{(01)} + \kappa\partial_\rho\Phi^{(0)} + q''\left(\Phi^{(0)}\right)\Phi^{(1)} \qquad (12) \\ &+h(\Phi^{(0)})f_{cl}^{0}(s) + h'(\Phi^{(0)})f_{cl}^{(-1)}(\rho, \Phi^{(0)})\Phi^{(1)} \end{aligned}$$

Multiply $\partial_\rho\Phi^{(0)}$ to (12) and integrate with respect to ρ from $-\infty$ to ∞, we have

$$\begin{aligned} &\int_{-\infty}^{\infty}\left(-\partial_{\rho\rho}\Phi^{(1)} + q''\left(\Phi^{(0)}\right)\Phi^{(1)}\right)\partial_\rho\Phi^{(0)}d\rho \\ &+\int_{-\infty}^{\infty} h'(\Phi^{(0)})f_{cl}^{(-1)}(\rho, \Phi^{(0)})\Phi^{(1)}\partial_\rho\Phi^{(0)}d\rho \\ = &\int_{-\infty}^{\infty}\left(-\partial_{\rho\rho}\Phi^{(1)} - q''\left(\Phi^{(0)}\right) - h(\Phi^{(0)})f_{cl}^{(-1)}(\rho, \Phi^{(0)})\right)\partial_\rho\Phi^{(1)}d\rho \\ = &\ 0 \end{aligned}$$

Asymptotic matching-$O(\varepsilon^{-3})$: $\mu_c^{(1)}$

The remaining terms are

$$\int_{-\infty}^{\infty} \left(\kappa\partial_\rho\Phi^{(0)} + h(\Phi^{(0)})f_{cl}^0(s)\right)\partial_\rho\Phi^{(0)}d\rho = \int_{-\infty}^{\infty} D_1(s)g(\Phi^{(0)})\partial_\rho\Phi^{(0)}d\rho$$

thus

$$D_1(s) = -\alpha_0\kappa + H_0 f_{cl}^0(s)$$

where

$$-\alpha_0 = \frac{\int_{-\infty}^{\infty}\left(\partial_\rho\Phi^{(0)}\right)^2 d\rho}{\int_{-\infty}^{\infty} g(\Phi^{(0)})\partial_\rho\Phi^{(0)}d\rho}$$

hence

$$\mu_c^{(1)} = g(\Phi^{(0)})\left(-\alpha_0\kappa + H_0 f_{cl}^0(s)\right)$$

Asymptotic matching-$O(\varepsilon^{-2})$

Let $\overline{\mu} = \frac{\mu_c}{g(\Phi)}$, the $O(\varepsilon^{-2})$ equation becomes

$$\partial_\rho \left(g(\Phi^{(0)}) \partial_\rho \overline{\mu}^{(2)} \right) = 0$$

thus $g(\Phi^{(0)}) \partial_\rho \overline{\mu}^{(2)} = C_4(s)$, the matching condition at $\rho = \pm\infty$ gives $C_4(s) = 0$. Therefore

$$\overline{\mu}^{(2)} = \left(\frac{\mu_c}{g(\Phi)} \right)^{(2)} = D_2(s)$$

Asymptotic matching-$O(\varepsilon^{-1})$

The $O(\varepsilon^{-1})$ equation is

$$v_n \partial_\rho \Phi^{(0)} = M_0 \partial_\rho \left(g(\Phi^{(0)}) \partial_\rho \overline{\mu}^{(3)} \right) + M_0 \partial_s \left(g(\Phi^{(0)}) \partial_s \overline{\mu}^{(1)} \right)$$

Integrating w.r.t ρ from $-\infty$ to ∞, we have

$$v_n = M_0 \partial_{ss} \overline{\mu}^{(1)} \int_{-\infty}^{\infty} g(\Phi^{(0)}) d\rho$$

Since $\overline{\mu}^{(1)} = \frac{\mu_c^{(1)}}{g(\Phi^{(0)})} = -\alpha_0 \kappa + H_0 f_{cl}^0(s)$, we arrive at our sharp interface equation

$$v_n = M_0 \alpha H_0 \frac{d^2}{ds^2} \left(\frac{-\alpha_0}{H_0} \kappa + f_{cl}^{(0)}(s) \right)$$

Numerical Simulations

In our simulations, the domain is chosen as $\Omega = [-\pi, \pi]^2$, mesh size $dx = dy = 2\pi/M$ with $M = 64$. Periodic boundary conditions are used. Small parameter in the phase field model is taken as $\varepsilon = dx$. $b = 2\pi/300$. $H_0 = 52.65(2(1-\nu)/\mu b^2$.

In the numerical simulations, we use the pseudospectral method: All the spatial partial derivatives are calculated in the Fourier space using FFT. For the time discretization, we use the forward Euler method. The climb force generated by dislocations f_{cl}^d is calculated by FFT using Eq. (3.8). $g(\phi)$ is regularized by $\sqrt{g(\phi)^2 + \varepsilon_0^2}$ with $\varepsilon_0 = 0.005$. In the initial configuaration of a simulation, ϕin the dislocation core region is set to be a `tanh` function with width 3ε, the location of the dislocation loop is the contour $\phi = 0.5$.

Evolution of an elliptic prismatic loop

$l_1 = 80b$ and $l_2 = 40b$. Radius for the ending circle is $R = 54.9b$. Theoretical value for R is $R = \sqrt{l_1 l_2} = 56.6b$. Evolution time is $t = 1.21 \times 10^7 (\frac{1}{2(1-\nu)} \cdot \frac{\mu\Omega}{k_B T} \cdot \frac{c_0 D_c}{b^2})^{-1}$.

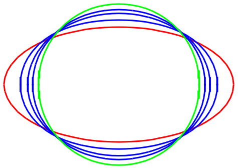

Figure 3: Evolution of an elliptic prismatic loop by self-climb using the phase field model. Red ellipse is the initial state, and green circle is the final state.

Comparison with DDD simulations

Radius for the ending circle is $R = 56.6b$. Theoretical value for R is $R = \sqrt{l_1 l_2} = 56.6b$. $t = 1.13 \times 10^7 \left(\frac{1}{2(1-\nu)} \cdot \frac{\mu\Omega}{k_B T} \cdot \frac{c_0 D_c}{b^2}\right)^{-1}$

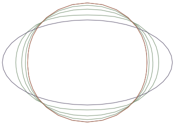

Fig. 4. Numerical simulation of self-climb of an elliptic prismatic loop (in blue), which converges to a circular loop (in red). Some snapshots of the loop in equal time intervals during the evolution are also shown (in green). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Translation of circular prismatic loop under constant stress gradient

The initial radius $R = 100b$. The applied stress field is $\sigma_{33}^{\text{app}} = -px$ with $p = 10^{-5}\mu/b$. $v = 1.95 \times 10^{-5} c_0 D_c/b$.

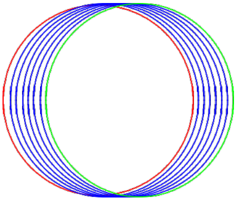

Figure 4: Translation of a circular prismatic loop under constant stress gradient using the phase field model. The leftmost, red circle is the initial configuration of the loop.

Comparison with DDD simulations

$v = 1.94 \times 10^{-5} c_0 D_c / b$. Theorectical value of v is $v = 1.85 \times 10^{-5} c_0 D_c / b$.

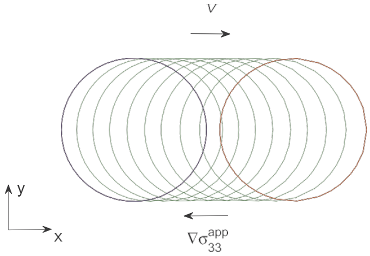

Fig. 5. Simulation of translation of a circular prismatic loop under constant stress gradient. Snapshots of the loop at $n\Delta t$, n 0,1, …, N, are shown. The blue circle is the initial loop, and the red circle is the loop at $N\Delta t$. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Coalescence of prismatic loops

$R_1 = 60b$ and $R_2 = 35b$, $d = 110b$. Final radius $R = 69.6b$. Theorectical value of $R = 69.5b$.

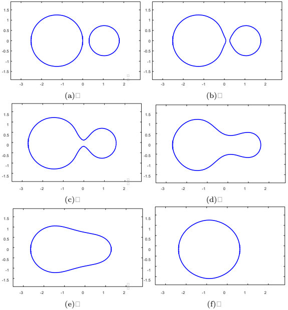

Figure 5: Coalescence of two prismatic loops by self-climb under their elastic interaction obtained by the phase field model.

Comparison with DDD simulations

$R_1 = 81b$ and $R_2 = 48b$, $d = 149b$. Final radius $R = 94.3b$.
Theorectical value of $R = 94.2b$.

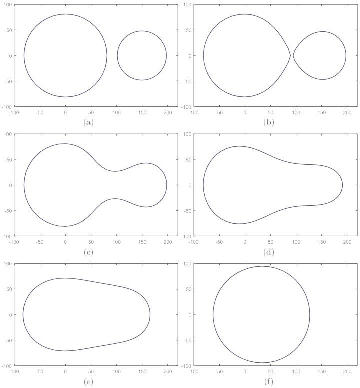

Fig. 6. Coalescence of two interstitial loops by self-climb under their elastic interaction obtained by our DDD simulation. The length unit is *b*. These images show the simulation results at time 0s, 0.47s, 0.49s, 0.70s, 1.04s, and 4.10s, respectively.

Coalescence of several prismatic loops

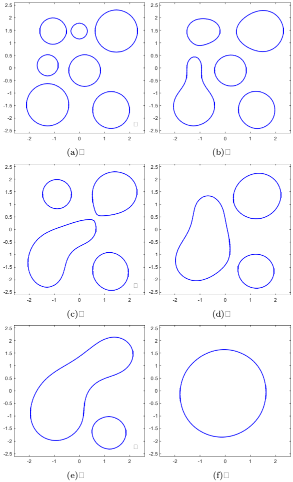

Figure 6: Coalescence of seven prismatic loops by self-climb under their elastic interaction obtained by the phase field model.

Repelling of two circular prismatic loops with opposite directions

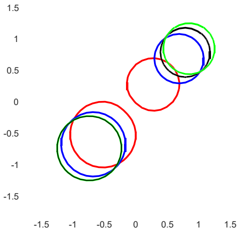

Figure 7: Repelling of two circular prismatic loops by self-climb under their elastic interaction obtained by our phase field model. The two red loops are the initial locations. Configurations of the two loops at different times during the evolution are shown by different colors.

dislocation climb coupled with self-climb of prismatic loops

$$
\begin{aligned}
\phi_t &= \nabla \cdot \left(M(\phi) \nabla \frac{\mu_c}{g(\phi)} \right) - \beta \mu_c \\
\mu_c &= -\Delta \phi + \frac{1}{\varepsilon^2} q'(\phi) + \frac{1}{\varepsilon} h(\phi) f_{cl} \\
&= \frac{\delta E_{CH}}{\delta \phi} + \frac{1}{\varepsilon} h(\phi) \frac{\delta E_{el}}{\delta \phi}
\end{aligned}
$$

Asymptotic analysis gives sharp interface limit equation

$$
v_n = \alpha H_0 \left(-M_0 \left(-\frac{\alpha_0}{H_0} \kappa + f_{cl}^{(0)}(s) \right) + \beta \left(-\frac{\alpha_0}{H_0} \kappa + f_{cl}^{(0)}(s) \right) \right).
$$

Future question: What about rigorous analysis? Existence? Uniqueness? Rigorous analysis for sharp interface limit?

Thank you!