1 Introduction

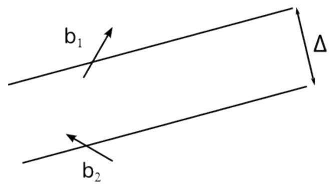


Figure 1: General representation of two parallel dislocation segments separated by a distance Δ

The general model for the elastic energy per unit length for a mixed dislocation dissociated into two partials can be given as [1]:

$$E_D(\theta) = E_S(\theta) + E_I(\theta, \Delta) + E_F(\Delta, \gamma) \tag{1}$$

"E_S" is the self-energy, "E_I" is the interaction energy, and "E_F" is the fault-energy. "θ" is the angle between the Burgers vector and the unit line vector, Δ is the separation between two line segments, γ is the stacking-fault energy.

A general expression can be given for each energy.

$$E_S(\theta) = \frac{\mu b^2}{4\pi(1-\nu)}\left(1 - \nu\cos^2\theta\right)\ln\left(\frac{R}{r_0}\right) \tag{2a}$$

$$E_I(\theta) = \frac{\mu b^2}{2\pi}\left(\alpha + \frac{\beta}{1-\nu}\right)\ln\left(\frac{R}{\Delta}\right) - \frac{\mu}{2\pi(1-\nu)}\psi \tag{2b}$$

$$E_F = \gamma\Delta \tag{2c}$$

r_0 and R are the inner and outer cutoff radii, respectively. μ, b, and ν are the shear modulus, the Burgers vector of the dislocation, and the Poisson ratio.

Equation 2b is the interaction energy between two parallel dislocation segments separated by a vector $\vec{\Delta}$. α, β, and ψ are related to the Burgers vectors and the line direction vectors of the two dislocations. Δ is the vector pointing from one dislocation segment to the second.

γ is the stacking-fault energy

2 Interaction energy between two parallel in-plane dislocation segments

The interaction energy between two parallel dislocations is defined from eq.(5-16)[2]. It has the same form as defined in eq.(2b). As such α, β, and ψ are defined as:

$$\alpha = \left(\vec{b}_1 \cdot \hat{l}\right)\left(\vec{b}_2 \cdot \hat{l}\right) \tag{3a}$$

$$\beta = \left(\vec{b}_1 \wedge \hat{l}\right) \cdot \left(\vec{b}_2 \wedge \hat{l}\right) \tag{3b}$$

$$\psi = \frac{1}{\Delta^2}\left[\left(\vec{b}_1 \wedge \hat{l}\right) \cdot \vec{\Delta}\right]\left[\left(\vec{b}_2 \wedge \hat{l}\right) \cdot \vec{\Delta}\right] \tag{3c}$$

For our case, the dislocations also exist in the same plane since they are partials. Hence $\vec{b}_i \wedge \hat{l} \perp \vec{\Delta} \Rightarrow \psi = 0$ for our model.

The form of the elastic energy is then

$$\begin{aligned} E_D(\theta) &= E_S(\theta) + E_I(\theta, \Delta) + \gamma\Delta \\ &= E_S(\theta) + \frac{\mu}{2\pi}\left(\alpha + \frac{\beta}{1-\nu}\right) \ln\frac{R}{\Delta} + \gamma\Delta \end{aligned}$$

Taking the partial derivative wrt Δ to find the equilibrium separation d

$$\begin{aligned} \left.\frac{\partial E_D}{\partial \Delta}\right|_{\Delta=d} &= \frac{\mu}{2\pi}\left(\alpha + \frac{\beta}{1-\nu}\right)\frac{-1}{d} + \gamma \\ 0 &= \frac{\mu}{2\pi}\left(\alpha + \frac{\beta}{1-\nu}\right)\frac{-1}{d} + \gamma \end{aligned}$$

Which gives the relation between the equilibrium separation and the interaction energy coefficients

$$\gamma d = \frac{\mu}{2\pi}\left(\alpha + \frac{\beta}{1-\nu}\right) \tag{6}$$

Replacing equation 6 in equation 1 we get the general form

$$\boxed{E_D(\theta) = E_S(\theta + \phi) + E_S(\theta - \phi) + \gamma d \ln\frac{R}{d} + \gamma d} \tag{7}$$

3 Shockley dislocation ($\theta, \phi = \pm\pi/6$)

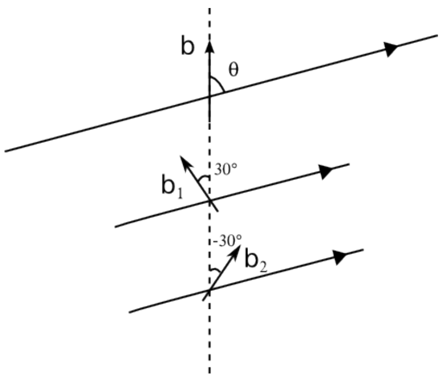


Figure 2: Representation of a Shockley pair

3.1 Self-energy

Using equation (2a) we can show that the self-energy for a pair of Shockley partials is given as

$$E_S\left(\theta+\frac{\pi}{6}\right)+E_S\left(\theta-\frac{\pi}{6}\right) \cong 2-\nu\cos^2\left(\theta+\frac{\pi}{6}\right)-\nu\cos^2\left(\theta-\frac{\pi}{6}\right) \tag{8}$$

Using the identity:

$$\cos^2(A+B)+\cos^2(A-B)=2(\cos^2 A\cos^2 B+\sin^2 A\sin^2 B) \tag{9}$$

And letting $A=\theta, B=\pi/6$ we get

$$\begin{aligned}\cos^2\left(\theta+\frac{\pi}{6}\right)+\cos^2\left(\theta-\frac{\pi}{6}\right) &= 2\left(\frac{3}{4}\cos^2\theta+\frac{1}{4}\sin^2\theta\right)\\ &= \frac{1}{2}(3\cos^2\theta+\sin^2\theta)\\ &= \frac{1}{2}(1+2\cos^2\theta)\end{aligned}$$

Replacing in equation 8 gives:

$$\begin{aligned}E_S\left(\theta+\frac{\pi}{6}\right)+E_S\left(\theta-\frac{\pi}{6}\right) &= \frac{\mu b^2}{4\pi}\ln\left(\frac{R}{r_0}\right)\frac{1}{1-\nu}\left[2-\frac{\nu}{2}(1+2\cos^2\theta)\right]\\ &= \frac{\mu b^2}{8\pi}(4-\nu-2\nu\cos^2\theta)\ln\frac{R}{r_0}\end{aligned} \tag{11}$$

3.2 Interaction energy

Hirth [2](eq.10-15) defines the equilibrium separation between two Shockley partials as:

$$\gamma_B d_B = \frac{\mu b^2}{8\pi}\frac{2-\nu}{1-\nu}\left(1-\frac{2\nu\cos 2\theta}{2-\nu}\right) \tag{12}$$

3.3 Full expression

Replacing equations 12 and 11 in equation 7 we get the elastic energy of a pair of Shockley partial dislocations

$$\begin{aligned}E_D^B(\theta,\nu,\gamma) &= \frac{\mu b^2}{8\pi}\frac{4-\nu-2\cos^2\theta}{1-\nu}\ln\frac{R}{r_0}\\ &+\frac{\mu b^2}{8\pi}\left(1-\frac{2\nu\cos 2\theta}{2-\nu}\right)\left(\ln\frac{R}{d_B}+1\right)\end{aligned} \tag{13}$$

where d_B is defined in equation 12.

4 Prismatic dislocation $(\theta, \phi=0)$

4.1 Self-energy

The self energy of a pair of dislocations with equal Burgers vectors ($\phi=0$) is just double that for a single

$$E_S(\theta)=2\cdot\frac{\mu b^2}{4\pi}\frac{1-\nu\cos^2\theta}{1-\nu}\ln\frac{R}{r_0} \tag{14}$$

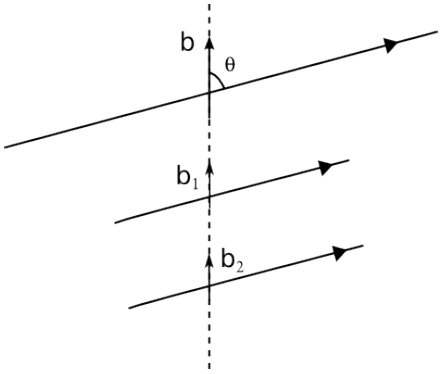


Figure 3: Representation of a prismatic pair

4.2 Interaction energy

There is no equation in [2] similar to that of 12, so we will derive it here. The equilibrium separation between the pair of dislocations in the prismatic plane can be obtained from equation 3

$$\alpha = b^2 \cos^2\theta$$
$$\beta = b^2 \sin^2\theta$$

Replacing in equation 6 gives

$$\begin{aligned}
\gamma d &= \frac{\mu b^2}{2\pi}\left(\cos^2\theta + \frac{\sin^2\theta}{1-\nu}\right) \\
&= \frac{\mu b^2}{2\pi}\frac{1}{1-\nu}(\cos^2\theta - \nu\cos^2\theta + \sin^2\theta) \\
&= \frac{\mu b^2}{2\pi}\frac{1}{1-\nu}(1 - \nu\cos^2\theta) \\
&= \frac{\mu b^2}{2\pi}\frac{1}{1-\nu}\left(1 - \nu\frac{\cos 2\theta + 1}{2}\right) \\
&= \frac{\mu b^2}{4\pi}\frac{1}{1-\nu}(2 - \nu\cos 2\theta - \nu)
\end{aligned}$$

And we get

$$\gamma_P d_P = \frac{\mu b^2}{4\pi}\frac{2-\nu}{1-\nu}\left(1 - \frac{\nu\cos 2\theta}{2-\nu}\right) \tag{15a}$$

which is quite similar to equation 12 up to the constant inside the paranthases.

4.3 Full expression

If we combine equations 15a and 14 we get

$$
\begin{aligned}
E_D^P(\theta,\nu,\gamma) = &\frac{\mu b^2}{4\pi}\frac{2}{1-\nu}(1-\nu\cos^2\theta)\ln\frac{R}{r_0} \\
&+\frac{\mu b^2}{4\pi}\frac{2-\nu}{1-\nu}\left(1-\frac{\nu\cos 2\theta}{2-\nu}\right)\left(\ln\frac{R}{d_P}+1\right)
\end{aligned}
\tag{16}
$$

where d_P is defined in equation 15a.

5 Implementation for the case of Zr

We will take $E_0 = [\mu a^2/\pi] = [\mathrm{J/m}]$ as units of energy and a as units of distance.

Paramter	value
μ (GPa)	34
λ (GPa)	131.143
ν	0.3970
a (Å)	3.232
γ_{prism} (mJ/m^2)	135
γ_{basal} (mJ/m^2)	198
R (A)	1000
r_0 (A)	1

This gives the following results:

		E_S	E_{I+F}	d_{eq}	E_D	$1-E_D^{\text{s}}/E_D^{\text{e}}$
prism	screw	0.8635	0.6949	3.239	1.5584	0.3716
	edge	1.3408	0.37714	0.9874	2.480	
basal	screw	1.341	0.37714	5.372	1.7180	0.35355
	edge	1.720	0.0.93773	2.9264	2.6576	

We note that the screw dislocation ($\theta = 0$) in the prismatic plane (green curve) has the lowest energy. The energy difference between the screw dislocation in the basal and the prismatic plane is roughly $\Delta_{PB}(\theta = 0) = 0.1596\ \frac{\mu a^2}{\pi} = 0.3538$ eV/Å (300 K $\approx$ 26 meV).

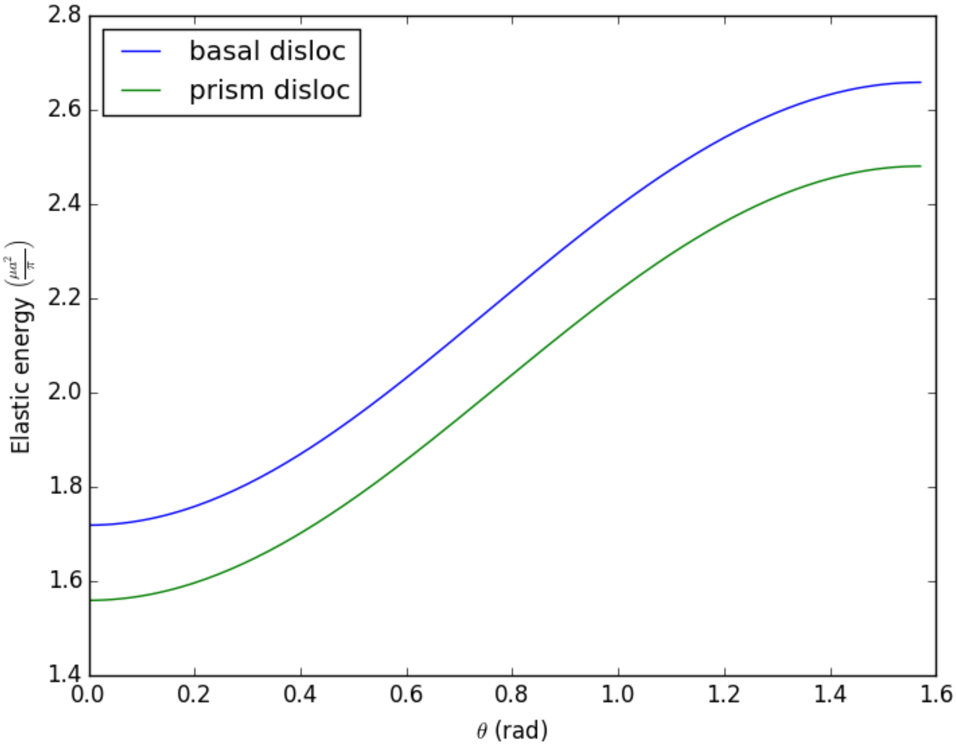
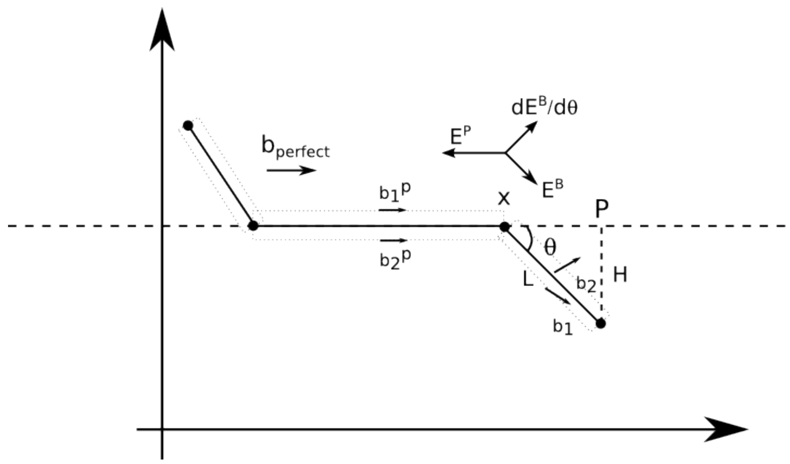


Figure 4: Elastic energy as a function of dislocation character. Case of zirconium. $\gamma'_P = 0.000100, \gamma'_B = 0.000147, \nu = 1/3$

6 Cross-slip of basal segment

We want to determine in this section the critical angle for which a basal segment is able to cross-slip into the prismatic plane and remain stable. We use the elastic energy per unit length determined in the previous sections to determine this angle. The approximation to the critical angle therefore neglects interactions between the segments in the two glide planes.



Consider for example the configuration shown in figure 6. We want to calculate the fornce on node 3. There are two sources of force: the force due to the prismatic section ($\theta = 0$) and due to the rotated basal section (θ). θ defined in this configuration is equivalent to the θ used in the definition of the elastic energy per unit length (equations 13 and 16).
The force in both cases is equal to

$$F_x^{P/B} = -\frac{dE_T}{dx} = -\frac{d}{dx}\left(L^{P/B}E^{P/B}(\theta)\right) \tag{17}$$

6.1 Force from prismatic

Using equation 17 and $L^P = x$

$$F_x^P = -\frac{d}{dx}\left(xE_D^P(0)\right) = -E_D^P(0) \tag{18}$$

6.2 Force from basal

Using equation 17 we find

$$F_x^B = -\frac{d}{dx}\left(LE_D(\theta)^B\right)$$

Using the chain rule we change variables $x(\theta, L)$

$$\frac{d}{dx} = \frac{d\theta}{dx}\frac{\partial}{\partial\theta} + \frac{dL}{dx}\frac{\partial}{\partial L}$$

Using $\tan\theta = (P-x)/H$

$$\begin{aligned}
P - x &= \frac{H}{\tan\theta} \\
-dx &= -\frac{H}{\sin^2\theta} \\
\frac{d\theta}{dx} &= \frac{\sin^2\theta}{H} \\
\frac{d\theta}{dx} &= \frac{\sin\theta}{L}
\end{aligned}$$

We also find for L

$$\begin{aligned}
(P-x)^2 + H^2 &= L^2 \\
-2(P-x)dx &= 2LdL \\
\frac{dL}{dx} &= -\frac{P-x}{L} \\
\frac{dL}{dx} &= -\cos\theta
\end{aligned}$$

Hence we can now write

$$\frac{d}{dx} = \frac{sin\theta}{L}\frac{\partial}{\partial\theta} - \cos\theta\frac{\partial}{\partial L} \tag{19}$$

Hence using equation 19 and 17

$$\begin{aligned}
F_x^B &= -\left(\frac{sin\theta}{L}\frac{\partial}{\partial\theta} - \cos\theta\frac{\partial}{\partial L}\right)\left(LE_D^B(\theta)\right) \\
F_x^B &= -\sin\theta\frac{\partial E_D^B(\theta)}{\partial\theta} + \cos\theta E_D^B(\theta) \qquad (20)
\end{aligned}$$

The condition for the stability of the node connecting the two dislocation segments can now be given as $F_x^P = F_x^B$ which using equations 20 and 18 is:

$$\boxed{\cos\theta E_D^B(\theta) - \sin\theta\frac{\partial E_D^B(\theta)}{\partial\theta} = E_D^P(\theta = 0)} \tag{21}$$

We plot the equation 21 in 5 and we find the root of the equation using numerical methods. We show that the critical angle $\theta_c = 65.32°$. For all angles below that the sum of forces is positive (positive direction of motion see figure), and the prismatic dislocation is stable.

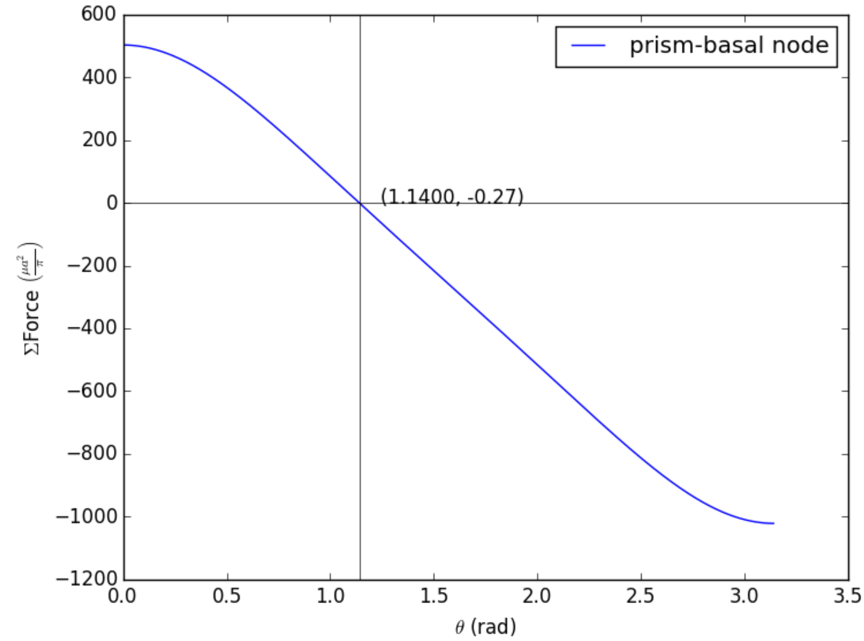


Figure 5: Sum of forces on node connecting a prismatic screw dislocation and a mixed basal dislocation in Zr

7 Implementation in NUMODIS

We want to implement the previous model in NUMODIS. The model needs to function for any type of dislocation in any crystal structure; however, to test it we will report results for zirconium only. We use the files ”linetension.C”, ”linetension.h”, and ”linetension.hpp” to write the code for our model.

baconlinetension.h Is an empty file.

baconlinetension.C Contains the declaration of a COREENERGY mode so that the class can be constructed from a keyword.

baconlinetension.hpp Contains the definitions of the main functions of the model: `ComputeForce` and `ComputeEnergy`

Warning! Unlike `linetension`, `baconlinetension` is implemented only for a `GSystem`.

7.1 Expression for energy

The most general expression for the energy using this model is given in equation 7. The total energy for a segment with unit vector $\hat{\xi}$, length ξ, and dissociated burgers vectors $\vec{b}_1$ and $\vec{b}_2$ is given as

$$\begin{aligned} E_T = {} & \xi \cdot \frac{\mu b_1^2}{4\pi(1-\nu)} \left[1 - \nu(\hat{b}_1 \cdot \hat{\xi})^2\right] \log\left(\frac{R}{r0}\right) + \xi \cdot \frac{\mu b_2^2}{4\pi(1-\nu)} \left[1 - \nu(\hat{b}_2 \cdot \hat{\xi})^2\right] \log\left(\frac{r0}{R}\right) \\ & + \xi \cdot \gamma d \log\frac{R}{d} \\ & + \xi \cdot \gamma d \end{aligned} \tag{22}$$

where

$$\begin{aligned} \gamma d &= \frac{\mu}{2\pi}\left[\left(\vec{b}_1 \cdot \hat{\xi}\right)\left(\vec{b}_2 \cdot \hat{\xi}\right) + \frac{\left(\vec{b}_1 \times \hat{\xi}\right) \cdot \left(\vec{b}_2 \times \hat{\xi}\right)}{1-\nu}\right] \\ &= \frac{\mu}{2\pi(1-\nu)}\left[\left(\vec{b}_1 \cdot \hat{\xi}\right)\left(\vec{b}_2 \cdot \hat{\xi}\right)(1-\nu) + \left(\vec{b}_1 \cdot \vec{b}_2\right)\left(\hat{\xi} \cdot \hat{\xi}\right) - \left(\vec{b}_1 \cdot \hat{\xi}\right)\left(\hat{\xi} \cdot \vec{b}_2\right)\right] \\ &= \frac{\mu}{2\pi(1-\nu)}\left[\left(\vec{b}_1 \cdot \vec{b}_2\right) - \nu\left(\vec{b}_1 \cdot \hat{\xi}\right)\left(\vec{b}_2 \cdot \hat{\xi}\right)\right] \\ &= \frac{\mu b_1 b_2}{2\pi(1-\nu)}\left[\left(\hat{b}_1 \cdot \hat{b}_2\right) - \nu\left(\hat{b}_1 \cdot \hat{\xi}\right)\left(\hat{b}_2 \cdot \hat{\xi}\right)\right] \end{aligned} \tag{23}$$

7.2 Expression for force

The force acting on node 1 F_i is given by the derivative of the energy with respect to ξ_i. The derivative of the first line in equation 22 is already given by the line-tension model in `linetension.hpp:117`

$$\vec{F}_{\text{lt}} = E_0\left[1 + \nu\left(\hat{b} \cdot \hat{\xi}\right)\right]\hat{\xi} - 2E_0\nu\left(\hat{b} \cdot \hat{\xi}\right)\hat{b} \tag{24}$$

where $E_0 = \frac{\mu b^2}{4\pi(1-\nu)} \log \frac{R}{r_0}$

We will now find the derivative of the second and third line of equation 22 with the help of equation 23

$$\gamma d = \frac{\mu b_1 b_2}{2\pi(1-\nu)} \left[\left(\hat{b}_1 \cdot \hat{b}_2\right) - \nu \frac{\left(b_{1x}\xi_x + b_{1y}\xi_y + b_{1z}\xi_z\right)\left(b_{2x}\xi_x + b_{2y}\xi y + b_{2z}\xi_z\right)}{b_1 b_2 \left(\xi_x^2 + \xi_y^2 + \xi_z^2\right)} \right]$$

$$\begin{aligned}
\frac{\partial \gamma d}{\partial \xi_x} &= -F_0 \nu \left\{ \frac{b_{1x}\left(\vec{b}_2 \cdot \vec{\xi}\right) + b_{2x}\left(\vec{b}_1 \cdot \vec{\xi}\right)}{\left(b_1 b_2 \xi^2\right)^2} b_1 b_2 \xi^2 - \frac{2\xi_x b_1 b_2}{\left(b_1 b_2 \xi^2\right)^2} \left(\vec{b}_1 \cdot \vec{\xi}\right)\left(\vec{b}_2 \cdot \vec{\xi}\right) \right\} \\
&= -F_0 \nu \left\{ \frac{1}{\xi} \frac{\vec{b}_2 \cdot \vec{\xi}}{b_2 \xi} \frac{b_{1x}}{b_1} + \frac{1}{\xi} \frac{\vec{b}_1 \cdot \vec{\xi}}{b_1 \xi} \frac{b_{2x}}{b_2} - 2 \frac{\left(\vec{b}_1 \cdot \vec{\xi}\right)\left(\vec{b}_2 \cdot \vec{\xi}\right)}{b_1 b_2 \xi^2} \frac{\xi_x b_1 b_2}{\xi^2 b_1 b_2} \right\} \\
&= -F_0 \nu \left\{ \frac{1}{\xi} \left(\hat{b}_2 \cdot \hat{\xi}\right) \frac{b_{1x}}{b_1} + \frac{1}{\xi} \left(\hat{b}_1 \cdot \hat{\xi}\right) \frac{b_{2x}}{b_2} - 2\frac{1}{\xi} \left(\hat{b}_1 \cdot \hat{\xi}\right)\left(\hat{b}_2 \cdot \hat{\xi}\right) \frac{\xi_x}{\xi} \right\}
\end{aligned}$$

where $F_0 = \frac{\mu b_1 b_2}{2\pi(1-\nu)}$ Which implies that

$$\frac{\partial \gamma d}{\partial \xi_i} = -\frac{F_0 \nu}{\xi} \left\{ \left(\hat{b}_2 \cdot \hat{\xi}\right) \hat{b}_1 + \left(\hat{b}_1 \cdot \hat{\xi}\right) \hat{b}_2 - 2\left(\hat{b}_1 \cdot \hat{\xi}\right)\left(\hat{b}_2 \cdot \hat{\xi}\right) \hat{\xi} \right\} \tag{25}$$

We can now write the complete expression for the dissociated-line tension

$$\begin{aligned}
\vec{F}_{bacon} &= \vec{F}_{\mathrm{lt}}(\vec{b}_1) + \vec{F}_{\mathrm{lt}}(\vec{b}_2) + \frac{\partial}{\partial \xi_i} \left[\xi \gamma d \ln \frac{R}{d} + \gamma d \xi \right] \\
&= \vec{F}_{\mathrm{lt}}(\vec{b}_1) + \vec{F}_{\mathrm{lt}}(\vec{b}_2) + \left(\gamma d \ln \frac{R}{d} + \gamma d \right) \hat{\xi} + \frac{\partial \gamma d}{\partial \xi_i} \ln \frac{R}{d} \xi + \frac{\xi \gamma d}{d} \frac{\partial d}{\partial \xi_i} + \xi \frac{\partial \gamma d}{\partial \xi_i}
\end{aligned}$$

Hence,

$$\boxed{\vec{F}_{bacon} = \vec{F}_{\mathrm{lt}}(\vec{b}_1) + \vec{F}_{\mathrm{lt}}(\vec{b}_2) + \gamma d \left(1 + \ln \frac{R}{d}\right) \hat{\xi} + \left(2 + \ln \frac{R}{d}\right) \xi \frac{\partial \gamma d}{\partial \xi_i}} \tag{26}$$

References

[1] D. J. Bacon. The effect of dissociation on dislocation energy and line tension. *Philosophical Magazine A*, 38(3):333–339, 1978.

[2] J.P. Hirth and J. Lothe. *Theory of Dislocations*. Krieger Publishing Company, 1982.