1 Introduction

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.

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

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

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

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

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

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

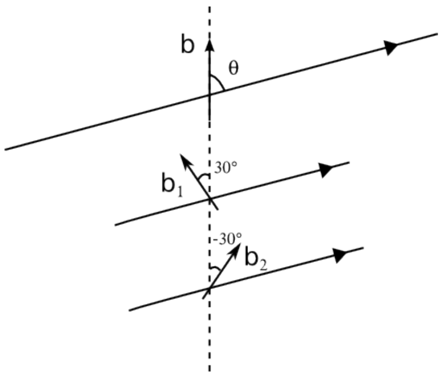

Figure 1: Representation of a Shockley pair

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

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

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

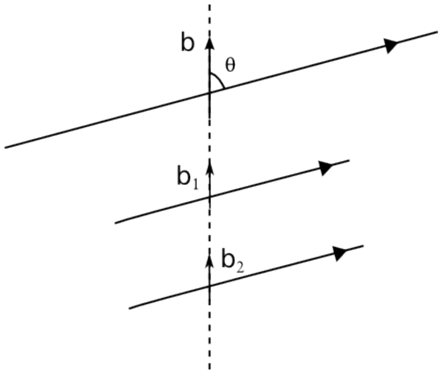

Figure 2: Representation of a prismatic pair

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

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 $E_0 = [\mu a^2/\pi] = [J/m]$ as units of energy and a as units of distance. This allows us to define the dimensionless stacking-fault energies γ' as

$$\gamma' = \frac{\gamma}{E_0/a} = \frac{\gamma\pi}{\mu a} \tag{17}$$

We use the parameters $\mu = 131$ GPa, $a = 3.232$ $\mathring{A}$ $\gamma_P = 135$ mJ/m^2, $\gamma_B = 198$ mJ/m^2 to define the prismatic and basal stacking fault-energies for zirconium

$$\begin{aligned} \gamma'_P &= 0.000100 \\ \gamma'_B &= 0.000147 \end{aligned} \tag{18}$$

For the radii let $r_0 = a$ and let $R = 10^n r_0$. We also specify $d = d'.a$. This choice of parameters allows to identify the dimensionless value d' and gives the following useful approximations to the natural logarithm:

$$\begin{aligned} \ln\frac{R}{r_0} &= \ln\frac{a\ 10^n}{a} = \ln 10^n = 2.3n \\ \ln\frac{R}{d} &= \ln\frac{10^n a}{d'\ a} = \ln 10^n - \ln(d') = 2.3n - \ln(d') \end{aligned} \tag{19}$$

Without any loss in generality we let $n = 3$ and using equations 19, 18, 16, and 13 we show in figure 3 the elastic energy of a dissociated dislocation in the basal plane as a function of θ and we compare with that of a dissociated dislocation in the prismatic plane.

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 $\Delta_{PB}(\theta = 0) = 504\ \frac{\mu a^2}{\pi}$. Using the same values for the parameters of zirconium listed above μ and a we get $\Delta_{PB}(\theta = 0) = 6753.6$ J/m

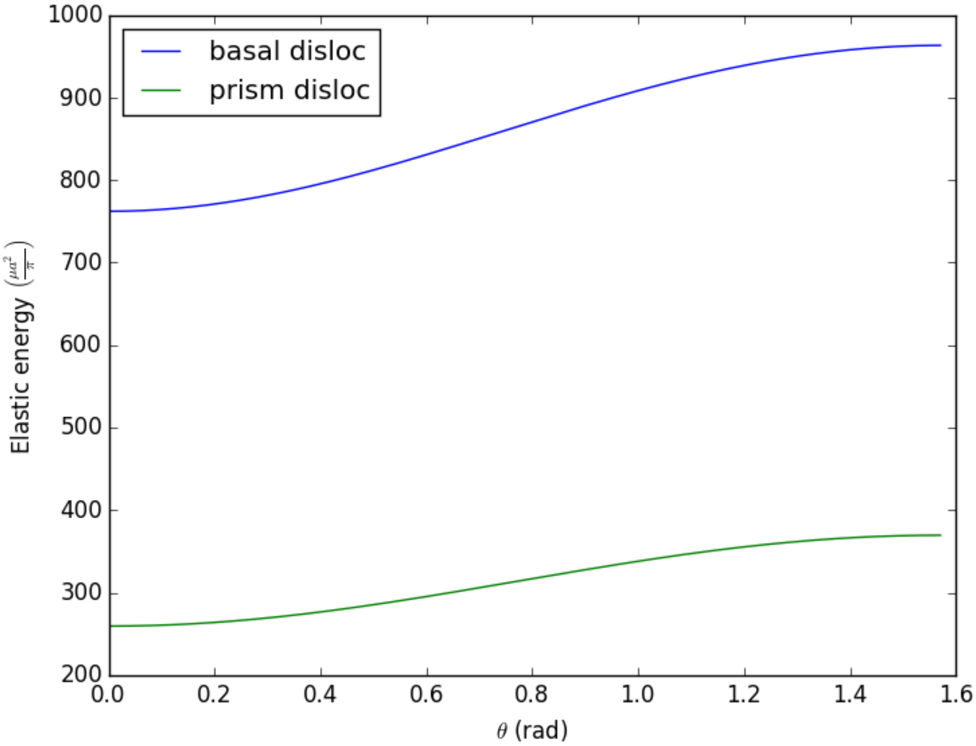

Figure 3: Elastic energy as a function of dislocation character. Case of zirconium. $\gamma'_P = 0.000100, \gamma'_B = 0.000147, \nu = 1/3$

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.