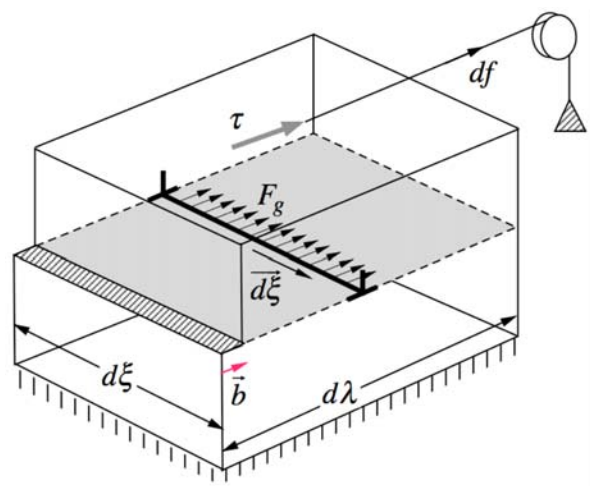
Forces on Dislocations

We consider now the forces that act on dislocations as a result of stresses acting in the crystal. We will derive the famous Peach-Koehler formula for computing forces on dislocations by first considering some special cases. Throughout this discussion we will note that the configurational forces acting on dislocations arise because the total energy of the system, including any applied stresses that might be present, changes as the position of the dislocation is changed. The force is then computed in the usual way by noting that $F_x = -(dE/dx)$, for example.

First consider an infinitesimal crystal element with dimensions $d\xi$ and $d\lambda$ through which an edge dislocation is passing by glide, as shown in the figure.



Thermodynamic system for calculation of Peach-Koehler glide force on an edge dislocation

The shear stress acting on the crystal element can be supplied by a weight, as shown, so that an infinitesimal force, $df = \tau(d\xi \cdot d\lambda)$, acts on the top face of the infinitesimal element. The applied stress causes a force per unit length, F_g, to act on the dislocation, tending to push it through the element. The shear stress created by the external weight can be represented by the distributed force on the dislocation. We make use of a reversible work argument wherein the dislocation is allowed to move reversibly through the crystal element. We consider the energy changes associated with allowing the dislocation segment to glide all the way through the crystal element. Note that the top part of the element moves in the direction of the Burgers vector using the RH/SF convention with the sense vector shown. When this happens, the work done by the external loading agent is

$$dW_\tau = b \cdot df = \tau b(d\xi \cdot d\lambda),$$

that is, the force on the top part of the element, df, times the distance it moves in the process, b. Equivalently we can express the work as the distributed force on the dislocation times the distance it moves in the process. This is

$$dW_{equivalent} = \left(F_g d\xi\right)\cdot d\lambda ,$$

where $F_g d\xi$ is the total force acting on the dislocation segment and $d\lambda$ is the distance through which it acts. Equating these equivalent work effects we have

$$dW_\tau = dW_{equivalent}$$
$$\tau b\left(d\xi \cdot d\lambda\right) = \left(F_g d\xi\right)\cdot d\lambda$$

so that

$$F_g = \tau b .$$

This is an elementary form of the Peach-Koehler formula; it indicates that the distributed force per unit length on a glide dislocation is simply the product of the shear stress resolved on the slip plane and in the direction of the Burgers vector and the magnitude of the Burgers vector. This simple relation for the glide force (per unit length) holds whatever the character of the dislocation (edge, screw, mixed..)

Another simple case involves the force on a climbing edge dislocation. Consider a crystal element through which an edge dislocation is climbing in response to a tensile stress, as shown in the diagram below. As the dislocation climbs through the element, the top part of the element moves in the direction of the Burgers vector (for the choice of the sense vector and using the RH/SF convention) by the amount b. The work done by the tensile stress on the element is then

$$dW_\sigma = b \cdot df = \sigma b\left(d\xi \cdot d\lambda\right),$$

while the equivalent work done by the distributed climb force is

$$dW_{equivalent} = \left(F_c d\xi\right)\cdot d\lambda \; .$$

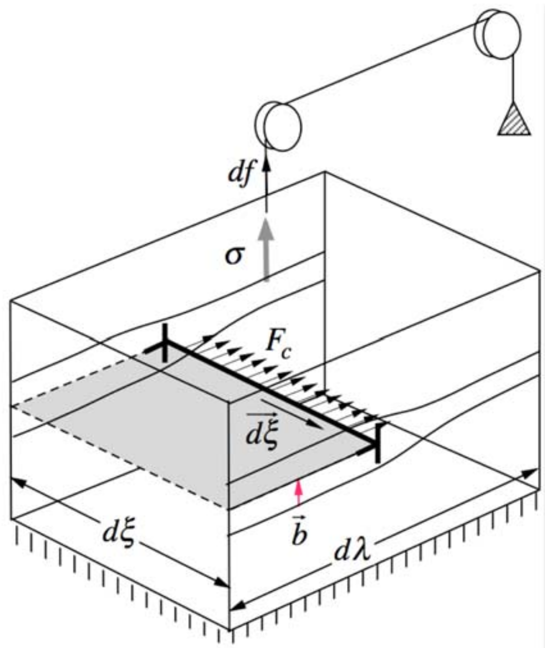
Equating these equivalent works we have

$$dW_\sigma = dW_{equivalent}$$
$$\sigma b\left(d\xi \cdot d\lambda\right) = \left(F_c d\xi\right)\cdot d\lambda$$

or

$$F_c = \sigma b .$$

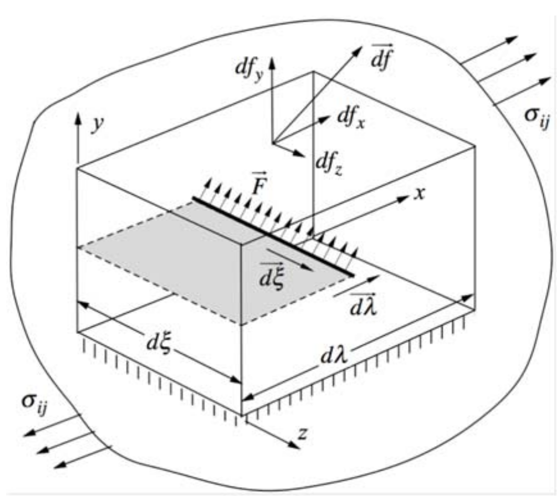
In this case the distributed climb force is the product of the tensile stress acting in the direction of the Burgers vector times the magnitude of the Burgers vector.



Thermodynamic system for calculation of Peach-Koehler climb force on an edge dislocation

Generalization of Peach-Koehler Formula

We may generalize the above derivations by allowing a mixed dislocation to move through a crystal element under a general state of stress, σ_{ij} .



Thermodynamic system for calculation of Peach-Koehler climb force on a mixed dislocation

Using the RH/SF convention and the sense vector shown, the top part of the element moves in the direction of the Burgers vector when the dislocation segment moved through the element in the $+x$ direction. The vector force (per unit length) acting on the dislocation is $\vec{F}$. The vector force acting on the top of the element is

$$\overrightarrow{df} = \sigma_{ij} \bullet \overrightarrow{dA} = \sigma_{ij} \bullet \left(\overrightarrow{d\xi} x \overrightarrow{d\lambda} \right)$$

where the stress is a second rank tensor

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}.$$

In the special case shown in the figure,

$$\overrightarrow{dA} = \overrightarrow{d\xi} x \overrightarrow{d\lambda} = dA[010]$$

so that the vector force on the top of the element is

$$\overrightarrow{df} = \sigma_{ij} \bullet \overrightarrow{dA} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} dA \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$
$$\overrightarrow{df} = dA \begin{bmatrix} \sigma_{xy} & \sigma_{yy} & \sigma_{zy} \end{bmatrix}.$$
$$\overrightarrow{df} = \begin{bmatrix} df_x & df_y & df_z \end{bmatrix}$$

The work done by the external stress when the dislocations segment moves though the element is the dot product of the vector force, $\overrightarrow{df}$, and the Burgers vector, $\vec{b}$,

$$dW_{\sigma_{ij}} = \overrightarrow{df} \bullet \vec{b} = \vec{b} \bullet \sigma_{ij} \bullet \left(\overrightarrow{d\xi} x \overrightarrow{d\lambda} \right).$$

The equivalent work done by the vector force (per unit length) on the dislocation is

$$dW_{equivalent} = \left(d\xi \cdot \vec{F} \right) \bullet \overrightarrow{d\lambda}.$$

Equating these equivalent work effects we have

$$dW_{\sigma_{ij}} = dW_{equivalent}$$

$$\vec{b} \bullet \sigma_{ij} \bullet \left(\overrightarrow{d\xi} x \overrightarrow{d\lambda}\right) = \left(d\xi \cdot \vec{F}\right) \bullet \overrightarrow{d\lambda} \; .$$

Since the order of the multiplication is irrelevant this can be written as

$$\left(\vec{b} \bullet \sigma_{ij}\right) \bullet \left(\overrightarrow{d\xi} x \overrightarrow{d\lambda}\right) = \left(d\xi \cdot \vec{F}\right) \bullet \overrightarrow{d\lambda}$$

and using the triple vector product rule

$$\left(\left(\vec{b} \bullet \sigma_{ij}\right) x \overrightarrow{d\xi}\right) \bullet \overrightarrow{d\lambda} = \left(d\xi \cdot \vec{F}\right) \bullet \overrightarrow{d\lambda} ,$$

so that

$$\left(\vec{b} \bullet \sigma_{ij}\right) x \overrightarrow{d\xi} = d\xi \cdot \vec{F} \, .$$

If we let $\overrightarrow{d\xi} = d\xi \cdot \vec{\xi}$, where $\vec{\xi}$ is the unit sense vector, then we can write

$$\vec{F} = -\vec{\xi} x \left(\vec{b} \bullet \sigma_{ij}\right)$$

the Peach-Koehler formula.

Computational Form of the Peach-Koehler Formula

For computation it is sometimes preferable to write the Peach-Koehler formula in a way that can be easily coded, especially if one is interested in only glide, which is the primary mode of motion except at very high temperatures. For glide the relevant force is the force (per unit length) acting normal to the dislocation line and in the slip plane, as shown in the figure below. If $\vec{n}$ is a unit vector normal to the slip plane and $\vec{\xi}$ is the unit sense vector along the dislocation line, then using the RH/SF rule, the vector force in the $\vec{n} x \vec{\xi}$ direction is

$$F = \sigma_{ij} n_j b_i$$

where n_j are the three components of the slip plane normal, b_i are the components of the Burgers vector and σ_{ij} are the components of the applied stress tensor.

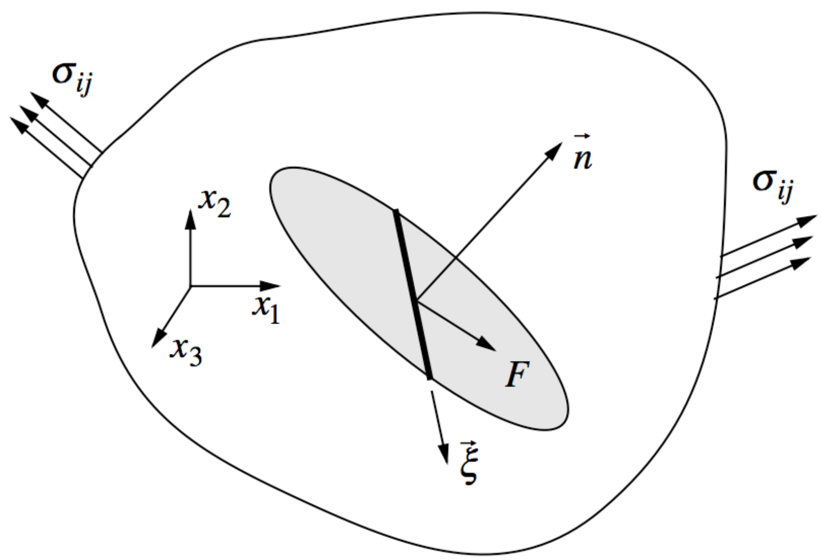
As an example consider a dislocation segment lying in the $x_1 x_3$ plane as shown in the figure below. As shown, the slip plane normal is $n_1 = 0, \; n_2 = 1, \; n_3 = 0$ so the computation of the force is

$$F = \sigma_{11}n_1b_1 + \sigma_{12}n_2b_1 + \sigma_{13}n_3b_1$$
$$+\sigma_{21}n_1b_2 + \sigma_{22}n_2b_2 + \sigma_{23}n_3b_2$$
$$+\sigma_{31}n_1b_3 + \sigma_{32}n_2b_3 + \sigma_{33}n_3b_3$$

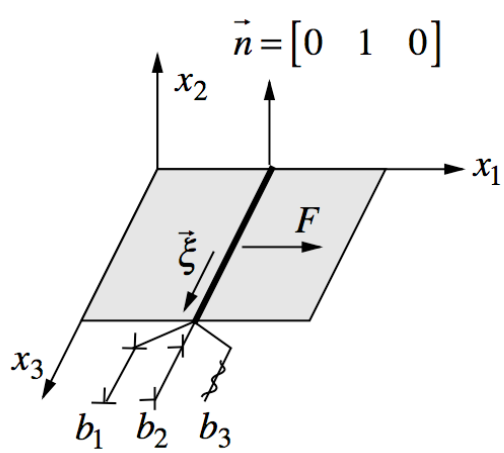
which, using the $n_2 = 1$ terms only, becomes

$$F = \sigma_{12}b_1 + \sigma_{22}b_2 + \sigma_{32}b_3 \,.$$

The first term in this expression is the glide force on a positive edge component, the second term is the climb force on an edge component and the last term is a glide force on a screw component, as shown schematically in the figure.



Computation of glide force by Peach-Koehler formula



Example of computation of Peach-Koehler force

Applications

We consider first some simple cases for which the Peach-Koehler force can be determined using basic formulas derived earlier and intuition. Indeed, the intuitive approach described here can be quite useful because many problems are sufficiently simple that the full tensor multiplication in the Peach-Koehler is not necessary. Suppose a positive edge dislocation lies along the z axis and the crystal is subjected to a pure shear stress, as shown in the figure. In this case the shear stress is the resolved shear stress in the slip plane of the dislocation and in the diretion of the Burgers vector. So the simple formula, $F_g = \tau b$, can be used to write the vector force (per unit length) on the dislocation:

$$\vec{F} = \left[\sigma_{xy} b \quad 0 \quad 0\right],$$

and the full tensor multiplication is not required. But as a tutorial exercise we use the full PK formula to obtain the same result. As shown in the figure, the sense vector can be chosen to be $\vec{\xi} = \left[0 \quad 0 \quad 1\right]$ so that the Burgers vector is $\vec{b} = b\left[1 \quad 0 \quad 0\right]$. Notice that is is convenient t write the Burgers vector as the product of the magnitude of the Burgers vector, b, and a unit vector, in this case, $\left[1 \quad 0 \quad 0\right]$. We will use this practice throughout these notes. The applied stress is simply

$$\sigma_{ij} = \begin{bmatrix} 0 & \sigma_{xy} & 0 \\ \sigma_{yx} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

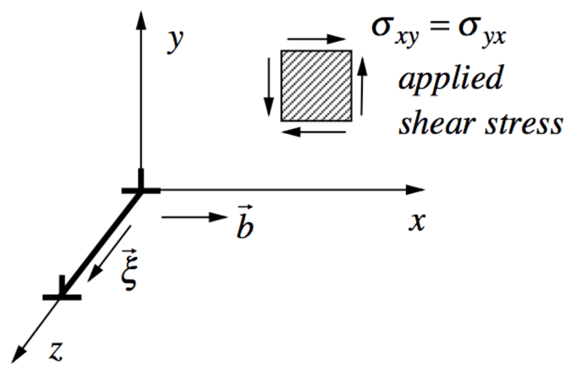
We now use the Peach-Koehler formula to obtain the vector force (per unit length) acting on the dislocation

$$\vec{F} = -\vec{\xi} x \left(\vec{b} \bullet \sigma_{ij}\right)$$

$$\vec{F} = -\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} x \left(b\left[1 \quad 0 \quad 0\right] \bullet \begin{pmatrix} 0 & \sigma_{xy} & 0 \\ \sigma_{yx} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right) = -b \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} x \begin{bmatrix} 0 \\ \sigma_{xy} \\ 0 \end{bmatrix}.$$

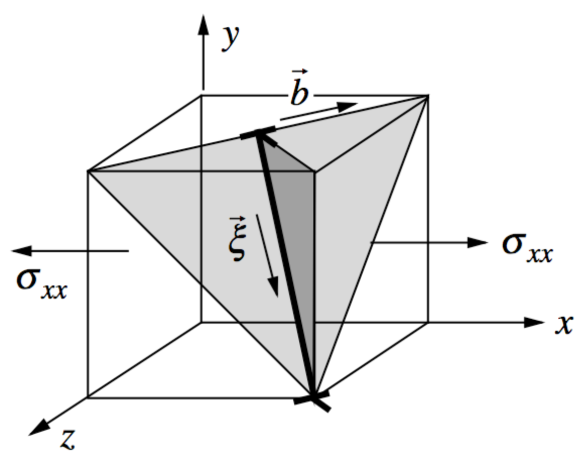
$$\vec{F} = -b \begin{bmatrix} x & y & z \\ 0 & 0 & 1 \\ 0 & \sigma_{xy} & 0 \end{bmatrix} = \left[\sigma_{xy} b \quad 0 \quad 0\right]$$

This is, of course, identical to the result obtained using the simple formula and intuition.



Positive edge dislocation subjected to a shear stress

Now we consider a simple Peach-Koehler problem for which the solution cannot be easily guessed using the simple formulas. An edge dislocation lies along a $<112>$ direction in a crystal element subjected to a pure tensile stress, σ_{xx}.



Edge dislocation subjected to tension stress

The sense vector in the diagram is a unit vector, $\vec{\xi} = \left(1/\sqrt{6}\right)\left[1 \quad \bar{2} \quad 1\right]$ and the corresponding Burgers vector is $\vec{b} = b\left(1/\sqrt{2}\right)\left[1 \quad 0 \quad \bar{1}\right]$. Notice that it is convenient to express the Burgers vector as the product of the magnitude of the Burgers vector, b, times a unit vector in the direction of the Burgers vector, $\left(1/\sqrt{2}\right)\left[1 \quad 0 \quad \bar{1}\right]$. The applied stress is simply

$$\sigma_{ij} = \begin{bmatrix} \sigma_{xx} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Now using the Peach-Koehler formula we can compute the vector force (per unit length) on the dislocations line.

$$\vec{F} = -\vec{\xi} x \left(\vec{b} \bullet \sigma_{ij} \right)$$

$$\vec{F} = -\frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ \bar{2} \\ 1 \end{bmatrix} x \left(\frac{b}{\sqrt{2}} \begin{bmatrix} 1 & 0 & \bar{1} \end{bmatrix} \bullet \begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right) = -\frac{b}{\sqrt{12}} \begin{bmatrix} 1 \\ \bar{2} \\ 1 \end{bmatrix} x \begin{bmatrix} \sigma_{xx} \\ 0 \\ 0 \end{bmatrix}.$$

$$\vec{F} = -\frac{b}{\sqrt{12}} \begin{bmatrix} x & y & z \\ 1 & \bar{2} & 1 \\ \sigma_{xx} & 0 & 0 \end{bmatrix} = -\frac{b}{\sqrt{12}} \begin{bmatrix} 0 & \sigma_{xx} & 2\sigma_{xx} \end{bmatrix}$$

So the final result is

$$\vec{F} = \begin{bmatrix} 0 & -\frac{\sigma_{xx} b}{2\sqrt{3}} & -\frac{\sigma_{xx} b}{\sqrt{3}} \end{bmatrix},$$

which agrees with intuition (if your intuition is good).