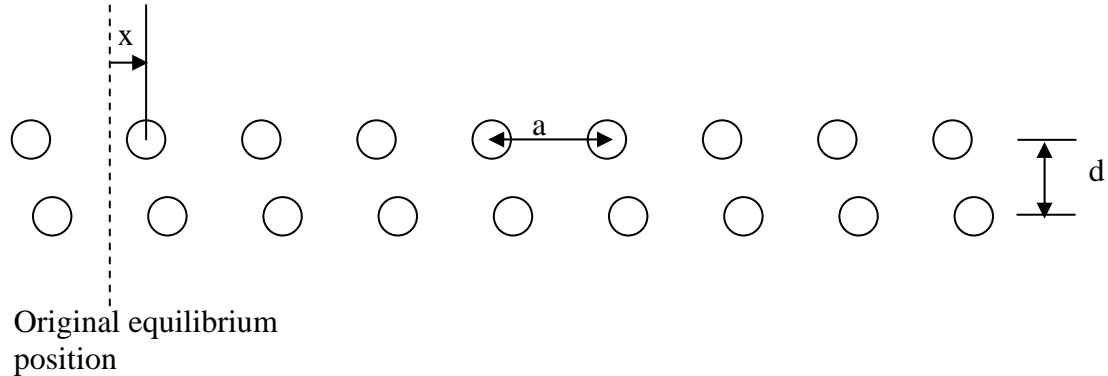


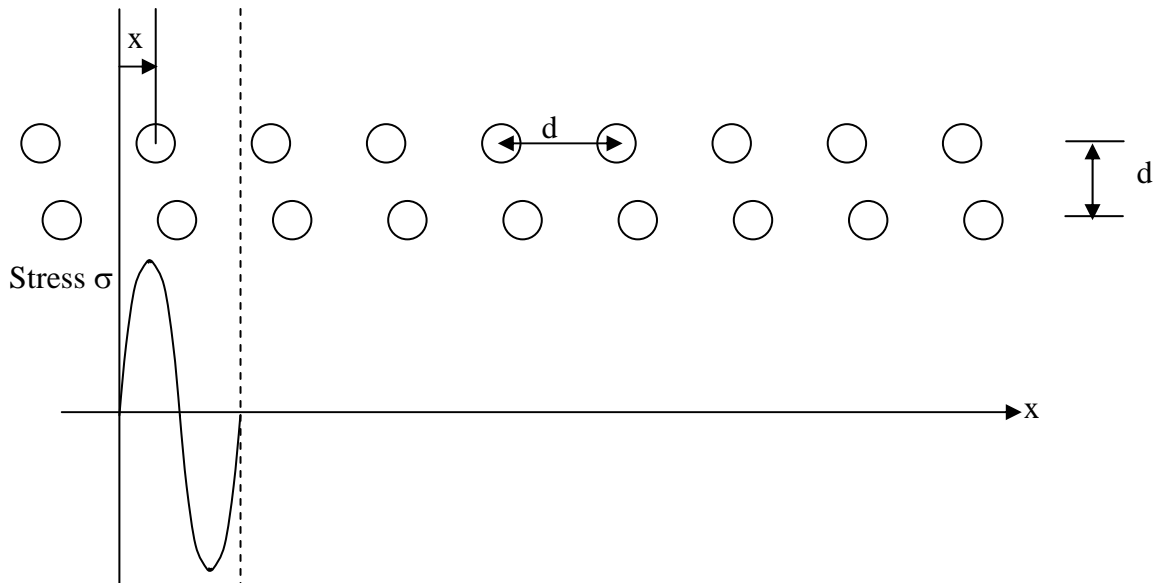
## Chapter 5. Dislocation

### I. Critical shear stress of perfect crystal

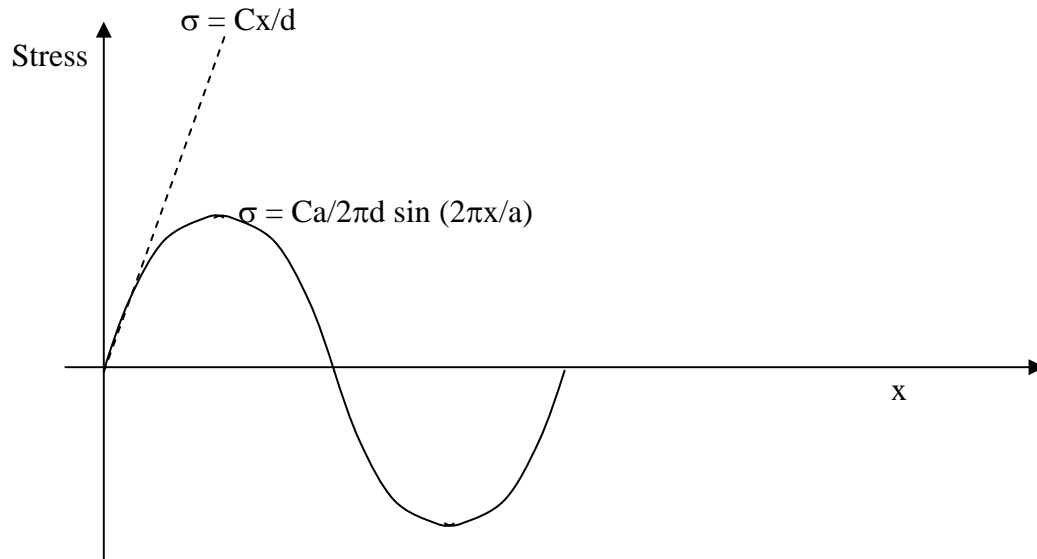
1. Consider displacement  $x$  of two atomic planes under a shear stress  $\sigma$ . For small displacement, the shear strain is given as  $e=x/d$ , where  $d$  is the distance between the layers.



2. The force (and hence the shear stress) required is periodic because of the lattice periodicity. The magnitude of force can be modeled as sinusoidal. So,  $\sigma = A \sin (2\pi x/a)$  where  $a$  is the lattice constant or distance between two atoms in the same plane.



3. “Hooke’s law”:  $\sigma = Ce$ , but this linear relationship applies only to small strain  $e$  (or small displacement  $x$ ). Since  $\sigma = A \sin (2\pi x/a) \Rightarrow \sigma = 2\pi Ax/a$   
 $\therefore Cx/d = 2\pi Ax/a \Rightarrow C = 2\pi dA/a \Rightarrow A = Ca/2\pi d$   
 $\therefore \sigma = Ca/2\pi d \sin (2\pi x/a)$



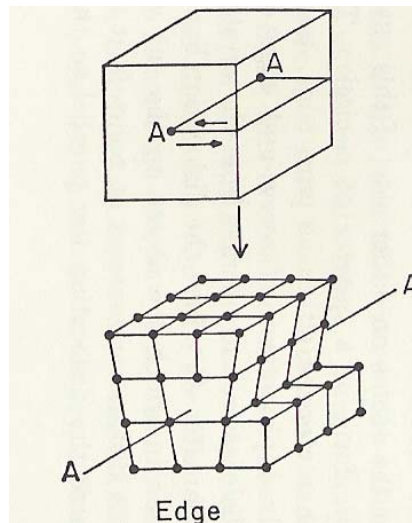
4. The amplitude  $\sigma_c = A = Ca/2\pi d$  is known as the critical shear stress at which the lattice becomes unstable and the top layer will slide into a new equilibrium position. For  $a \sim d$ , we have  $\sigma_c = C/2\pi$ . In other words, the critical shear stress is about 1/6 of the shear modulus.

5. In reality, the critical shear is much smaller and is only a few percent of the shear modulus. Such a discrepancy can only be explained by dislocation.

## II. Edge dislocation

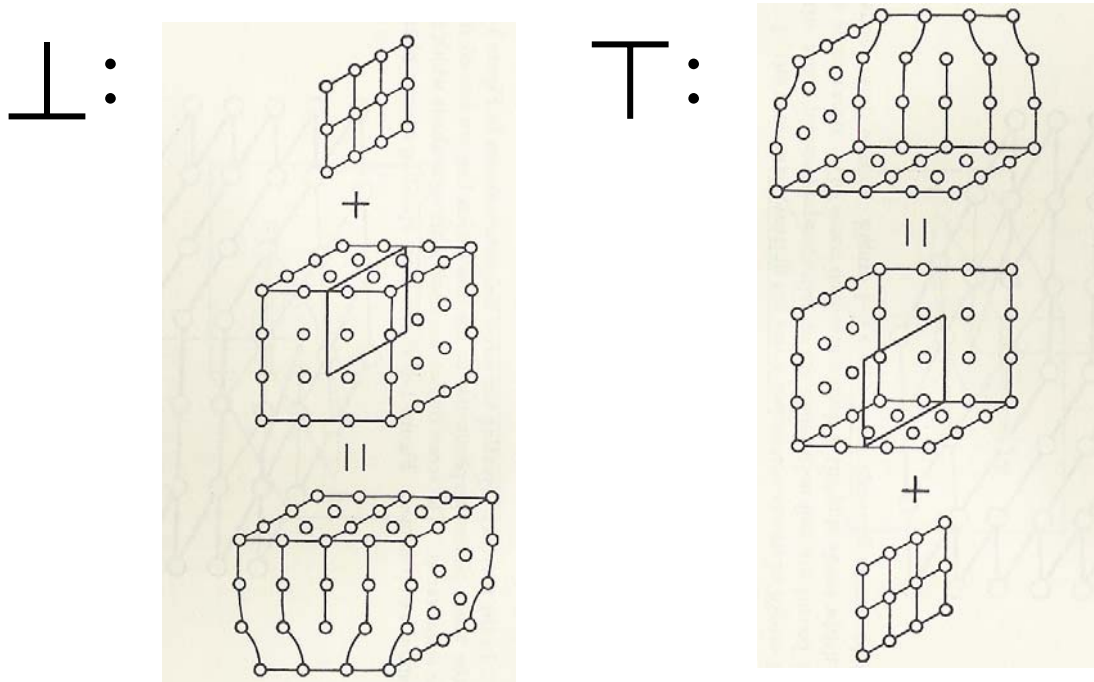
1. There are two types of dislocation: edge dislocation and screw dislocation (or a mixture of both).

2. To understand dislocation, we can imagine to start from a perfect, undeformed lattice and cut the lattice along any of the planes as shown in the figure.



3. If the cut stops at line AA, and let the atoms at one side of the plane slip over a distance with respect to the atoms at the other side. The cut plane is also known as a *slip plane*.

4. The above slipping is equivalent to inserting an extra plane vertical to the slip plane to the lattice (or removing one from the other side) as show in the figure below:



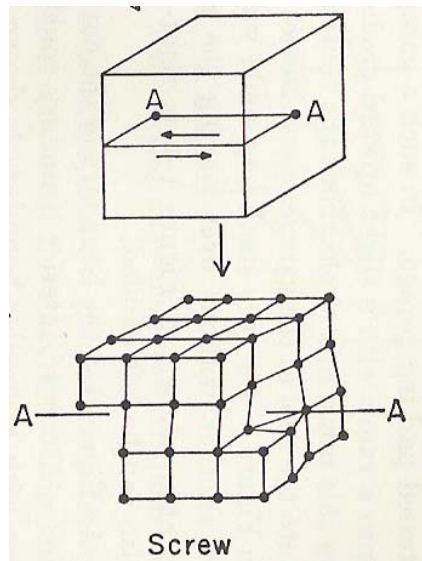
6. The lattice structure is near perfect except the line AA. The imperfection is concentrated around the line. For this reason, the line AA is known as the *line of dislocation*.

7. The type of dislocation discussed above is called edge *dislocation*. For edge dislocation, the slipping direction is *perpendicular* to the line of imperfection.

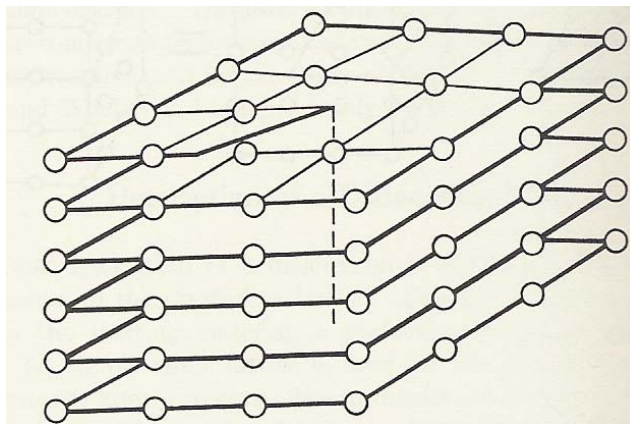
8. Edge dislocation has “sign” because the plane can slip in one of the two possible directions, either towards to or away from the dislocation line. We will use symbol  $\perp$  (as shown in above figure) to represent edge dislocation. The horizontal line represent the slip plane, and the vertical line represent the extra plane to be inserted to the lattice.

### III. Screw dislocation and mixed dislocation

1. If the slipping direction is *parallel* to the dislocation line, the dislocation is known as *screw* dislocation.

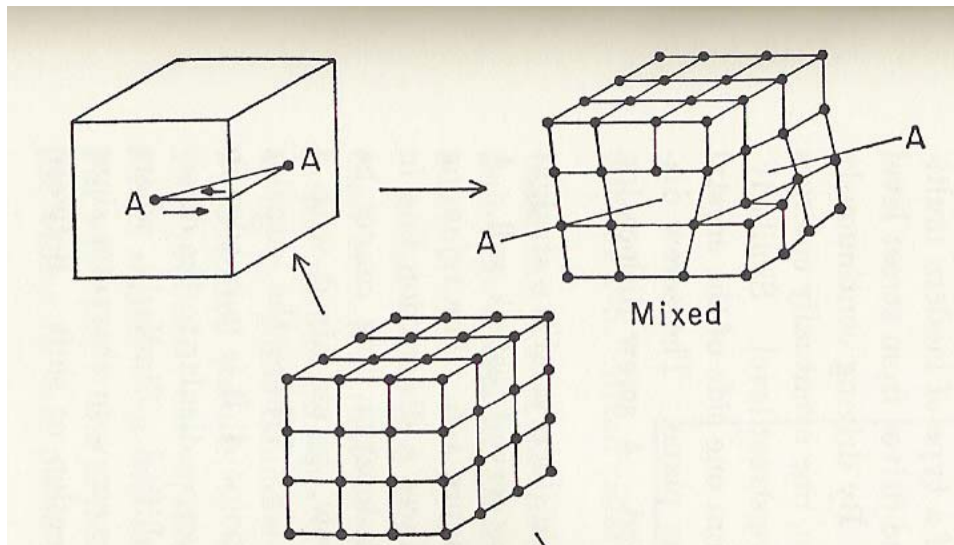


2. If one looks at the plane perpendicular to the dislocation line, the planes look like a spiral ramp.



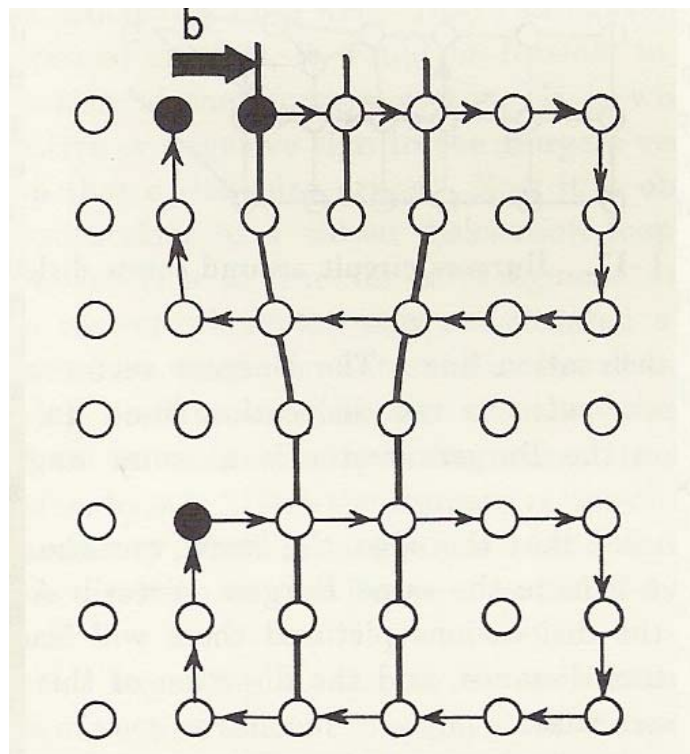
This is the reason why this is called screw dislocation. Again, there are two directions of screw dislocation – right hand and left hand. Note that the “handedness” of a screw is independent of the direction at which it is looked at.

3. The slip can occur in general in any direction, neither parallel nor perpendicular to the dislocation line. This is the case of a mixed (of edge and screw) dislocation:

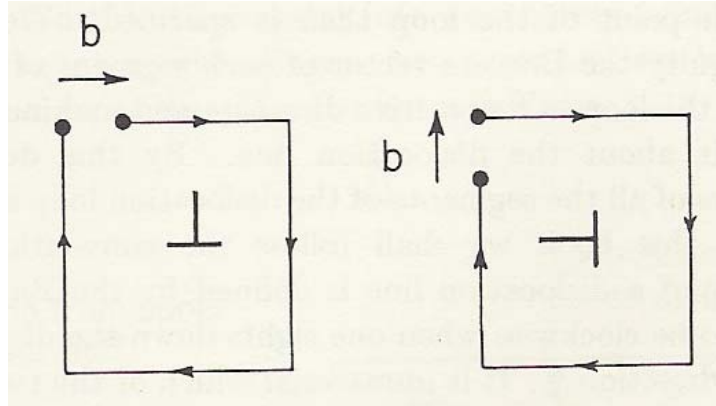


#### IV. Burgers vector

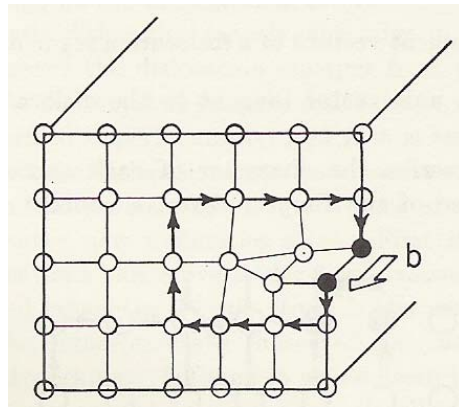
1. In a lattice, if we draw a closed circuit loop by going right  $x$  lattice point, up  $y$  lattice points, and then left the same  $x$  lattice points and down  $y$  lattice points. If the lattice is perfect, we will come back to the same lattice points (bottom loop in the figure below).
2. If the lattice is not perfect (i.e. with dislocation), we will not come back to the same lattice point (top loop in the figure below).



3. Burgers vector  $\mathbf{B}$  is defined as the vector from the end of the “loop” to the beginning of the “loop”.  $\mathbf{B}=\mathbf{0}$  if the loop encloses a perfect vector.  $\mathbf{B}\neq\mathbf{0}$  if the loop encloses some dislocation.
4. The Burgers vector is parallel to the slipping direction. So the Burgers vector of edge dislocation is perpendicular to the dislocation line, and the Burgers vector of a screw dislocation is parallel to the dislocation line.
5. Burgers vector of an edge dislocation:



6. Burgers vector around a screw dislocation:



## V. Motion of dislocations

1. Atoms on one side of the slip plane experience repulsive forces from some neighbors and attractive forces from others across the slip plane. These forces cancel to a first approximation.
2. As a result, the stress required to move a dislocation is quite small, below  $10^5$  dyne/cm. This explains why the critical stress is much smaller than the expected value.
3. If an edge dislocation moves completely across its slip plane:

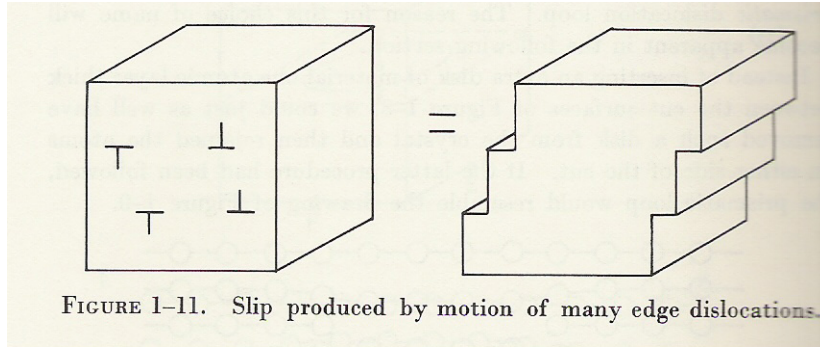


FIGURE 1-11. Slip produced by motion of many edge dislocations.

Similarly, if a screw dislocation moves completely across its slip plane:

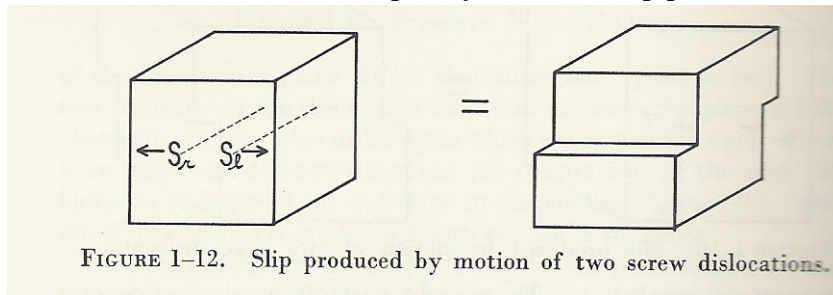


FIGURE 1-12. Slip produced by motion of two screw dislocations.

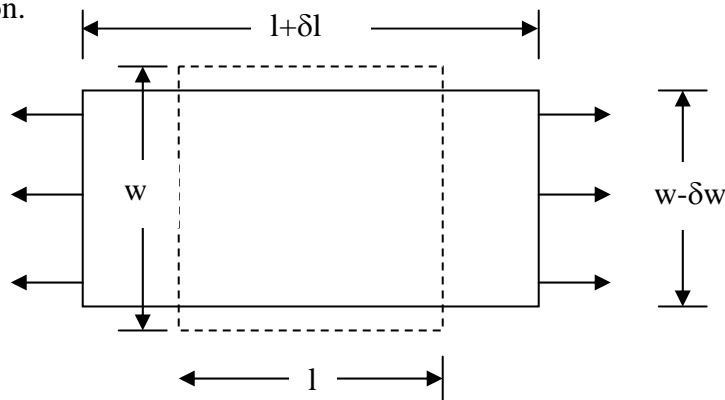
Movement of dislocations results in plastic deformation.

4. As the dislocations move, plastic deformation causes a very great increase in dislocation density, typically from  $10^8$  to  $10^{11}$  dislocations/cm<sup>2</sup>. Dislocations multiply during deformation!

5. For the strength of a material, the dislocations have to be “pinned” so that they cannot move freely to generate more dislocations. Examples: particles of iron carbide are precipitated in the hardening of steel, and particles of  $\text{Al}_2\text{Cu}$  are precipitated in the hardening of aluminum.

## VI. Stress fields of dislocations

1. Young’s modulus ( $E$ ) is defined as stress/strain for a tensile stress acting in one direction, with the specimen sides left free. Poisson’s ratio ( $\nu$ ) is defined as  $(\delta w/w)(\delta l/l)$  for this situation.



2. For isotropic materials,

$$\begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{pmatrix} = \begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix}$$

G is the rigidity modulus and it is related to E and  $\nu$  as:

$$G = \frac{E}{2(1+\nu)}$$

Reversing this matrix, we have:

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{pmatrix} \begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{pmatrix}$$

$\lambda$  and  $\mu$  are related to the Young's modulus and Poisson Ratio as

$$E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \text{ and } \nu = \frac{\lambda}{2(\lambda + \mu)}$$

3. In particular, let us look at the x-axis:

$$\begin{aligned} & \left[ \sigma_{xx} - \frac{1}{2} \frac{\partial \sigma_{xx}}{\partial x} \delta x \right] \delta y \delta z \\ & + \left[ \sigma_{xy} - \frac{1}{2} \frac{\partial \sigma_{yx}}{\partial y} \delta y \right] \delta x \delta z \\ & + \left[ \sigma_{xz} - \frac{1}{2} \frac{\partial \sigma_{zx}}{\partial z} \delta z \right] \delta y \delta x \end{aligned} \quad \begin{array}{c} \leftarrow \\ \square \\ \rightarrow \end{array} \quad \begin{aligned} & \left[ \sigma_{xx} + \frac{1}{2} \frac{\partial \sigma_{xx}}{\partial x} \delta x \right] \delta y \delta z \\ & + \left[ \sigma_{xy} + \frac{1}{2} \frac{\partial \sigma_{yx}}{\partial y} \delta y \right] \delta x \delta z \\ & + \left[ \sigma_{xz} + \frac{1}{2} \frac{\partial \sigma_{zx}}{\partial z} \delta z \right] \delta y \delta x \end{aligned}$$



Net force (in the x-direction) is

$$\delta F_x = \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \right) \delta x \delta y \delta z$$

Therefore equation of motion in the x-direction is

$$\begin{aligned} m \frac{\partial^2 u}{\partial x^2} &= \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \right) \delta x \delta y \delta z \\ \Rightarrow \rho \frac{\partial^2 u}{\partial t^2} &= \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \right) \quad \text{Density } \rho = \frac{m}{\delta x \delta y \delta z} \end{aligned}$$

Similarly, in y and z directions:

$$\begin{aligned} \rho \frac{\partial^2 v}{\partial t^2} &= \left( \frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} \right) \\ \rho \frac{\partial^2 w}{\partial t^2} &= \left( \frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zy}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) \end{aligned}$$

4. Now assume the dislocation line is infinite long along the z- axis. By symmetry argument, the stresses do not depend on the z component and all stress derivatives with respect to z equal to 0.

$$\begin{aligned} \rho \frac{\partial^2 u}{\partial t^2} &= \left( \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \right) \\ \Rightarrow \rho \frac{\partial^2 u}{\partial t^2} &= \frac{\partial[(\lambda + 2\mu)e_{xx} + \lambda e_{yy}]}{\partial x} + \frac{\partial[\mu e_{xy}]}{\partial y} \end{aligned}$$

Note that  $e_{xx} = \frac{\partial u}{\partial x}$ ,  $e_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}$

$$\begin{aligned} \therefore \rho \frac{\partial^2 u}{\partial t^2} &= (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} + \lambda \frac{\partial^2 v}{\partial x \partial y} + \mu \left( \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial x \partial y} \right) \\ \Rightarrow \rho \frac{\partial^2 u}{\partial t^2} &= (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 v}{\partial x \partial y} \end{aligned}$$

Similarly, in y and z direction :

$$\begin{aligned} \rho \frac{\partial^2 v}{\partial t^2} &= \mu \frac{\partial^2 v}{\partial x^2} + (\lambda + 2\mu) \frac{\partial^2 v}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 u}{\partial x \partial y} \\ \rho \frac{\partial^2 w}{\partial t^2} &= \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) \end{aligned}$$

6. For stationary dislocations:

$$\begin{aligned}
 (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 v}{\partial x \partial y} &= 0 \\
 \mu \frac{\partial^2 v}{\partial x^2} + (\lambda + 2\mu) \frac{\partial^2 v}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 u}{\partial x \partial y} &= 0 \\
 \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) &= 0
 \end{aligned}$$

7. Consider the case of pure screw dislocation, with Burgers vector  $\mathbf{b} = b\mathbf{k}$ . For screw dislocation,  $u=v=0$ .

Guess solution of  $\mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) = 0$ :

$$w = -\frac{b}{2\pi} \tan^{-1} \frac{y}{x}$$

Notes: If a circuit is made about the dislocation line, the arc tan function changed by  $2\pi$  and thus  $w$  changed by the amount  $-b$ .

8. From this relation, we can calculate the strain of the screw dislocation:

$$\begin{aligned}
 e_{xz} &= \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} = \frac{b}{2\pi} \frac{y}{x^2 + y^2} \\
 e_{yz} &= \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} = -\frac{b}{2\pi} \frac{x}{x^2 + y^2} \\
 e_{xx} &= e_{yy} = e_{zz} = e_{xy} = 0
 \end{aligned}$$

And then stress follows:

$$\begin{aligned}
 \sigma_{xz} &= \frac{\mu b}{2\pi} \frac{y}{x^2 + y^2} \\
 \sigma_{yz} &= -\frac{\mu b}{2\pi} \frac{x}{x^2 + y^2} \\
 \sigma_{xx} &= \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = 0
 \end{aligned}$$

9. In cylindrical coordinates,  $r^2 = x^2 + y^2$ ,  $\tan \theta = y/x$ ,  $z=z$ . Above results can be transformed into simpler form:

$$\begin{aligned}
w &= -\frac{b\theta}{2\pi}, u_r = u_\theta = 0 \\
e_{\theta z} &= -\frac{b}{2\pi}, e_{rr} = e_{\theta\theta} = e_{zz} = e_{r\theta} = e_{rz} = 0 \\
\sigma_{\theta z} &= -\frac{b}{2\pi}, \sigma_{rr} = \sigma_{\theta\theta} = \sigma_{zz} = \sigma_{r\theta} = \sigma_{rz} = 0
\end{aligned}$$

10. Consider the case of pure edge dislocation, solution of the equations of motion are given as:

$$\begin{aligned}
u &= -\frac{b}{2\pi} \left[ \tan^{-1} \frac{y}{x} + \frac{\lambda + \mu}{\lambda + 2\mu} \frac{x^2}{x^2 + y^2} \right] \\
v &= -\frac{b}{2\pi} \left[ -\frac{\mu}{2(\lambda + 2\mu)} \log \frac{x^2 + y^2}{C} + \frac{\lambda + \mu}{\lambda + 2\mu} \frac{y^2}{x^2 + y^2} \right] \\
w &= 0
\end{aligned}$$