1.2.4 Stress fields of dislocations

For this description we apply continuum mechanics (i. e. we allow only elastic distortions introduced by the stress field of dislocations)
For this purpose we introduce the general form of Hooke's law:

$$\sigma_{ij} = \mathrm{C}\ \epsilon_{ij}$$

which derives from the fundamental physical law $\mathrm{F} = -\mathrm{D} \cdot \mathrm{x}$ where a force F applied on a material causes an elongation or compression x. D is the spring constantIn this general form σ_{ij} is a 3×3 matrix containing
- the normal principal stresses σ_{ii} (within the main diagonal)
- shear stresses τ_{ij} in the respective ij-planes

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

The stress matrix describes the stress fields (conditions) of any volume element in bulk material. As the matrix is symmetrical it holds:

$$\sigma_{ij} = \begin{vmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_{zz} \end{vmatrix}$$

The strain matrix is equivalentely given by:

$$\epsilon_{ij} = \begin{vmatrix} \epsilon_{xx} & \gamma_{xy} & \gamma_{xz} \\ \gamma_{xy} & \epsilon_{yy} & \gamma_{yz} \\ \gamma_{xz} & \gamma_{yz} & \epsilon_{zz} \end{vmatrix}$$

- with normal strains ϵ_{ii}
- and shear strains γ_{ij}

→ in scalar way: $\sigma = \mathrm{E}\epsilon$; $\tau = \mathrm{G}\gamma$
G is the stiffness matrix (containing the elastic constants). It is a fourth-rank tensor - containing 81 elements at most.

stress field of a screw dislocation

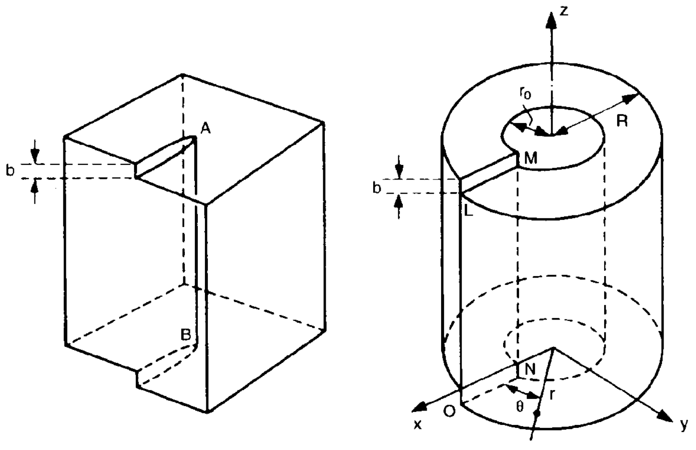


Figure 1.22: Screw dislocation and the corresponding eigenstate of stress

Consider a dislocation in a crystal and built a hollow cylinder around it. Use a hollow cylinder, because the plastic strains in the core are much to high, as one can calculate it in terms of continuum mechanics. Then consider the elastic distortion of this cylinder.
For screw dislocations it is useful to introduce cylindric coordinates:

$$\begin{aligned} x &= r\cos\theta \\ y &= r\sin\theta \\ z &= z \end{aligned}$$

For the example given (Fig.1.22) a pure shear stress in z-direction is obtained, hence:

$$\begin{aligned} \sigma_{xx} = \sigma_{yy} = \sigma_{zz} = 0 = \tau_{xy} \quad &\text{(carthesian coordinates)} \\ \sigma_{rr} = \sigma_{\theta\theta} = \sigma_{zz} = 0 = \tau_{r\theta} = \tau_{rz} \quad &\text{(cylindric coordinates)} \end{aligned}$$

Intersection: *cylindric coordinates*
$x = r\cos\theta$
$y = r\sin\theta$
$z = z$

$$\left.\begin{aligned} x^2 &= r^2\cos^2\theta \\ y^2 &= r^2\sin^2\theta \end{aligned}\right\} x^2 + y^2 = r^2 \underbrace{(\cos^2\theta + \sin^2\theta)}_{=1}$$

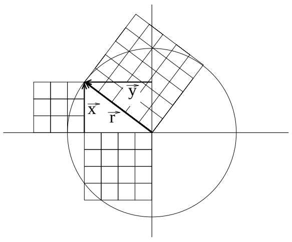


Illustration of cylindric coordinates by the use of karthesian coordinates on the basis of the stress fields of screw dislocations:

$$\tau_{\theta z} = \frac{Gb}{2\pi r} = -\tau_{xz}\sin\theta + \tau_{yz}\cos\theta \tag{1.1}$$

$$\tau_{rz} \overset{def}{=} 0 = \tau_{xz}\cos\theta + \tau_{yz}\sin\theta \tag{1.2}$$

eq.1.1/ $\sin\theta$: $\quad \tau_{yz} = -\tau_{xz}\frac{\cos\theta}{\sin\theta}$ in eq.1.2

$$\tau_{\theta z} = \tfrac{Gb}{2\pi r} = -\tau_{xz}\left(\sin\theta + \tfrac{cos^2\theta}{\sin\theta}\right) \qquad \cdot\sin\theta$$

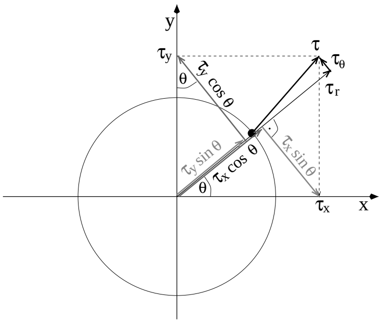
$$\tau_{\theta z} = \tfrac{Gb}{2\pi r}\sin\theta = -\tau_{xz}(\sin^2\theta + \cos^2\theta) \overset{def}{=} -\tau_{xz}$$

$\Rightarrow$

$$\tau_{xz} = -\tfrac{Gb}{2\pi r}\sin\theta \overset{y=r\sin\theta}{\overbrace{=}} -\tfrac{Gb}{2\pi r} \overset{x^2+y^2=r^2}{\overbrace{=}} -\tfrac{Gb}{2\pi}\tfrac{y}{x^2+y^2} \quad \text{o.k. !}$$

with the use of eq.1.2:

$$\tau_{yz} = -\tau_{xz}\tfrac{\cos\theta}{\sin\theta} = \tfrac{Gb}{2\pi r}\cos\theta \overset{x=r\cos\theta}{\overbrace{=}} \tfrac{Gb}{2\pi}\tfrac{x}{x^2+y^2} \quad \text{o.k. !}$$



$$\begin{aligned} \tau_r &= \tau_x\cos\theta + \tau_y\sin\theta \\ \tau_\theta &= -\tau_x\sin\theta + \tau_y\cos\theta \end{aligned}$$

shear stress in a radial plane (τ = const.) in z-direction: $\tau_{\theta z}$ =? Cut the hollow cylinder along the xz-plane and deconvolute it (middle and right in Fig.1.23). Compare this with an analogous cylinder which was around no dislocation.

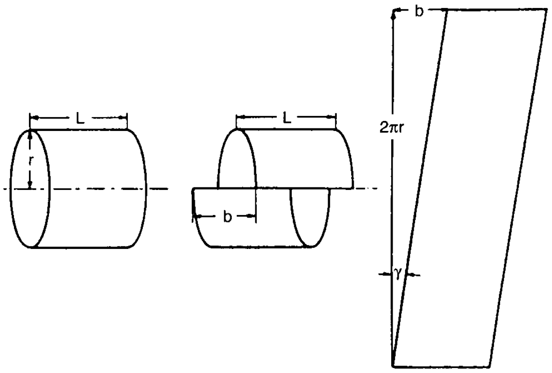


Figure 1.23: On the calculation of shearing and stress field of a screw dislocation by means of deconvoluting a infinitesimally thin zylinder section.

Obviously one obtains a pure shear in z-direction. The amount of shear γ is defined by the amount of the Burger's vector and the length $2\pi r$ which is the perimeter of a circle with given radius r:

$$\gamma_{\theta z} = \frac{b}{2\pi r} \underbrace{\Rightarrow}_{\tau=G\gamma} \tau_{\theta z} = \frac{Gb}{2\pi r}$$

The stress matrix (in cylindric coordinates) is then:

$$\sigma^{r\theta z} = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & \tau_{\theta z} \\ 0 & \tau_{\theta z} & 0 \end{vmatrix}$$

For a screw dislocation only two scalar components in the matrix are not zero. The result in carthesian coordinates would have been (see intersection for a full derivation):

$$\sigma^{xyz} = \begin{vmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & 0 \end{vmatrix} \qquad \text{with:} \qquad \underbrace{\begin{aligned} \tau_{xz} &= -\tfrac{Gb}{2\pi}\tfrac{y}{x^2+y^2} \\ \tau_{yz} &= +\tfrac{Gb}{2\pi}\tfrac{x}{x^2+y^2} \end{aligned}}_{x^2+y^2=r^2}$$

stress field of edge dislocations

Again built a hollow cylinder around the dislocation and exclude the core due to plastic strains. It is obvious from the plot, that there is no shear in z-direction.

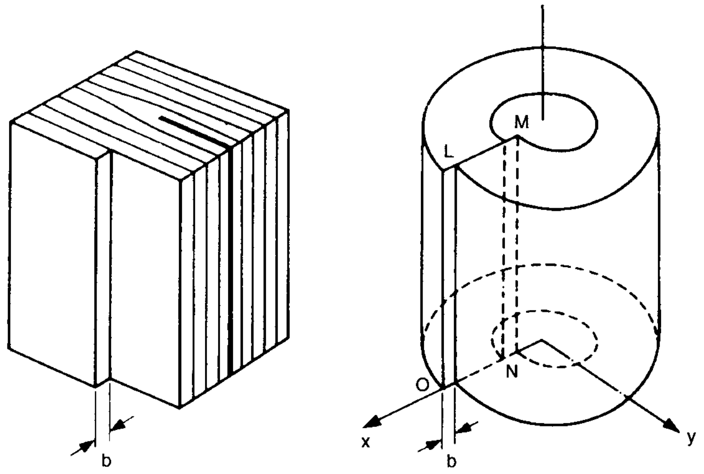
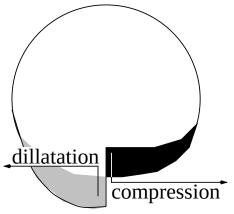


Figure 1.24: Edge dislocation and the corresponding eigenstate of stress

An edge dislocation has an extra half plane → there must be a zone of compression and dilatation (as illustrated right).



⇒ normal stresses must be present
⇒ no shearing in z-direction! → $\tau_{xz} = \tau_{yz} = 0$

⇒ stress matrix

$$\sigma^{xyz} = \begin{vmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{vmatrix}$$

Herein is (without proof):

- $\sigma_{xx} = -\frac{Gb}{2\pi(1-\nu} \frac{y(3x^2+y^2)}{(x^2+y^2)^2} = -\frac{Gb}{2\pi(1-\nu)} \frac{sin\theta(2+\cos(2\theta))}{r}$

  $\nu = 0 \ldots 0.5$ is the Poisson's ratio
- $\sigma_{yy} = -\frac{Gb}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2} = \frac{Gb}{2\pi(1-\nu)} \frac{\sin\theta\cos(2\theta)}{r}$
- $\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$

There is a normal stress in z-direction, because any compression of a body causes an elongation of the body in the other two directions!

- $\tau_{xy} = \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2} = \frac{Gb}{2\pi(1-\nu)} \frac{\cos\theta\cos(2\theta)}{r}$

Up to now, we did not consider the core of the dislocation. We estimate the stress existing next to the dislocation core of a screw dislocation: $r_0 = b$.

$$\tau_{\theta z}(r_0) = \frac{Gb}{2\pi r_0} = \frac{Gb}{2\pi b} = \frac{G}{2\pi}$$

⇒ this is the limit theoretical shear strength, i. e. the limit of validity of elastic continuum mechanics.