Microstructure Mechanics

Dislocation statics

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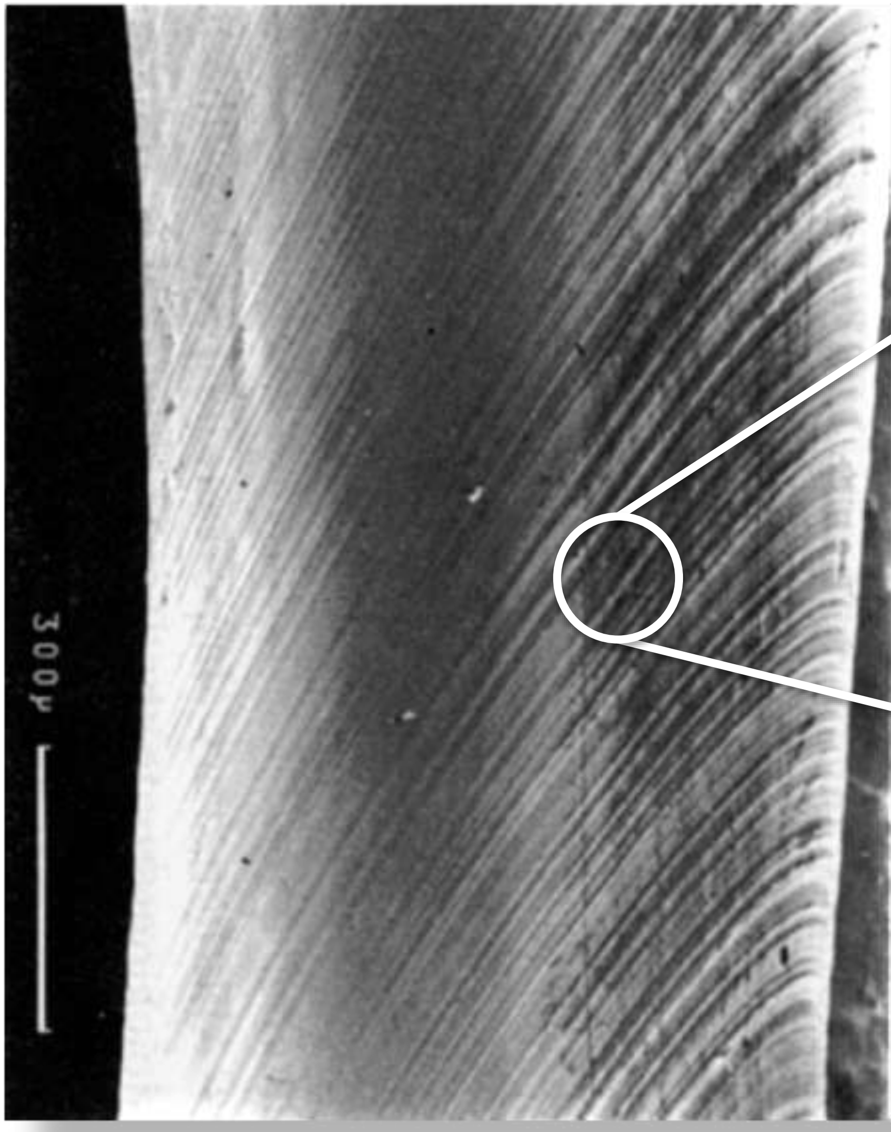
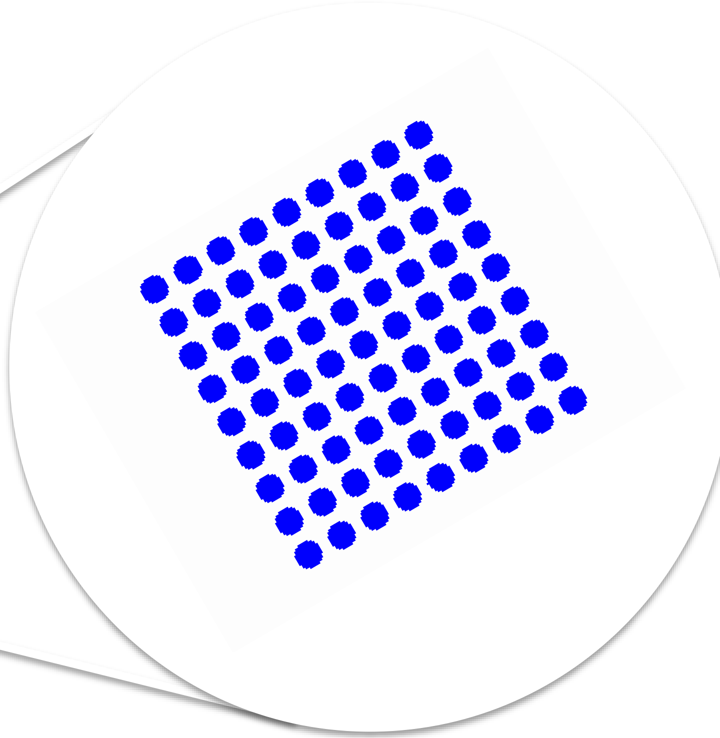
Plastic deformation of a single crystal by dislocation slip

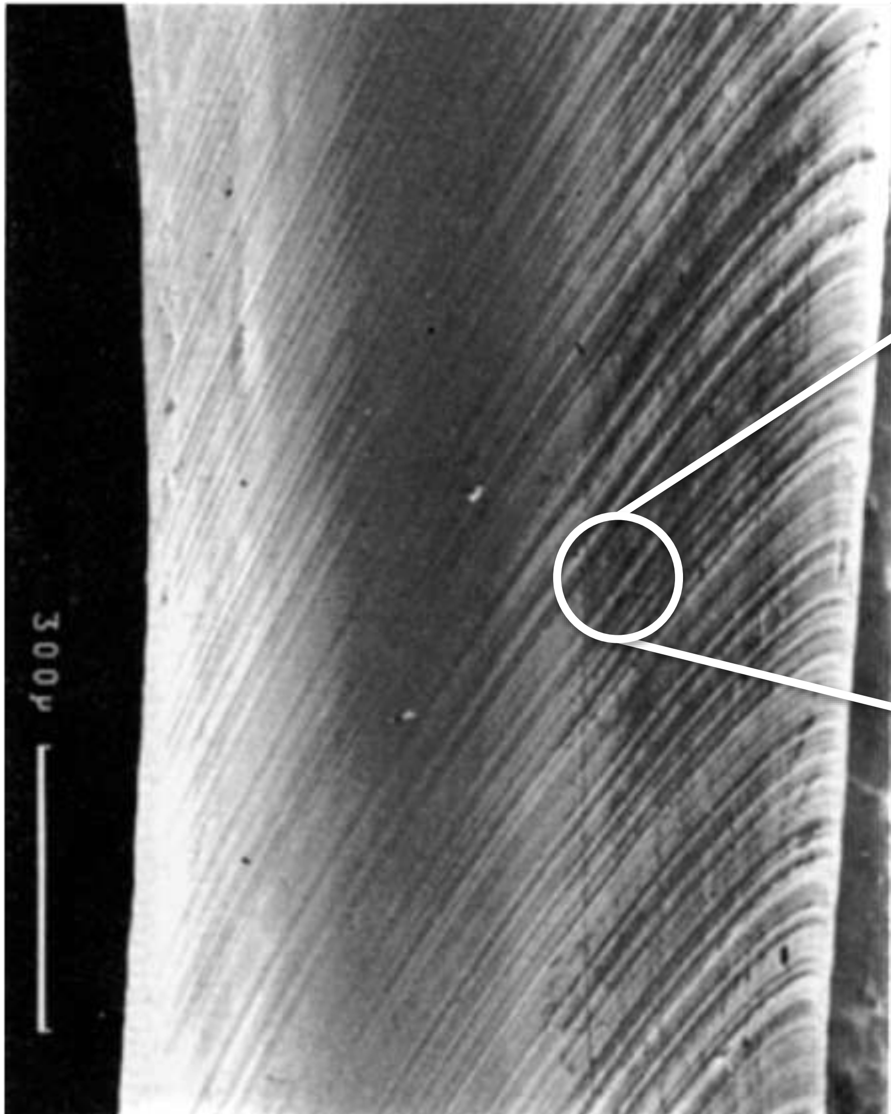


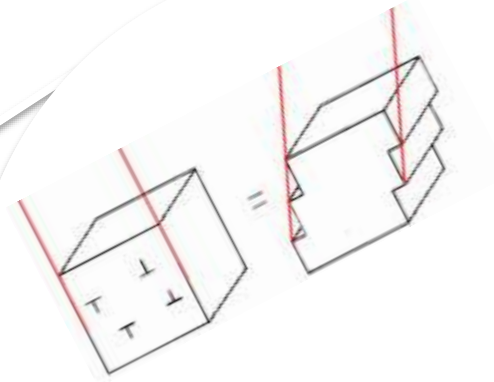
single slip in a single crystal



plastic anisotropy

Plastic deformation of a single crystal by dislocation slip





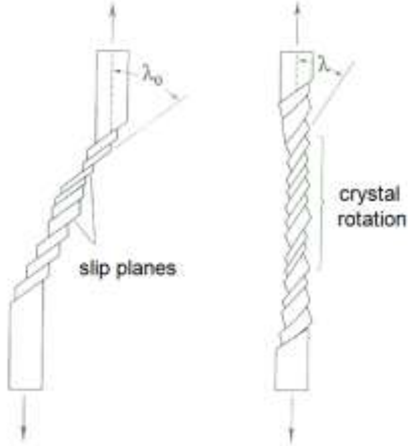
$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

Boundary condition: determines lab frame constraints

Constraints lead to specific crystal rotations

Non-symmetric dislocation shear leads to rotation

Symmetric-shear can lead to shape change without rotation



Change in local constraints leads to heterogeneity

Roters et al. Acta Mater.58 (2010)

Kinematics: displacement vector in continuum space

$\underline{u}=u(x,y,z)$

$\underline{u}_{(1)}(x,y,z)=\underline{u}_{(2)}(x,y,z)$

Kinematics: displacement vector in continuum space

$\underline{u}=u(x,y,z)$

$\underline{u}_{(1)}(x,y,z)\neq\underline{u}_{(2)}(x,y,z)$

Roters et al. Acta Mater.58 (2010)

Kinematics, displacement, displacement gradient: general

Distorsions come from gradients in the displacement fields

Displacement vector:

$$\mathbf{u} = [u_x, u_y, u_z]$$

Strain tensor:

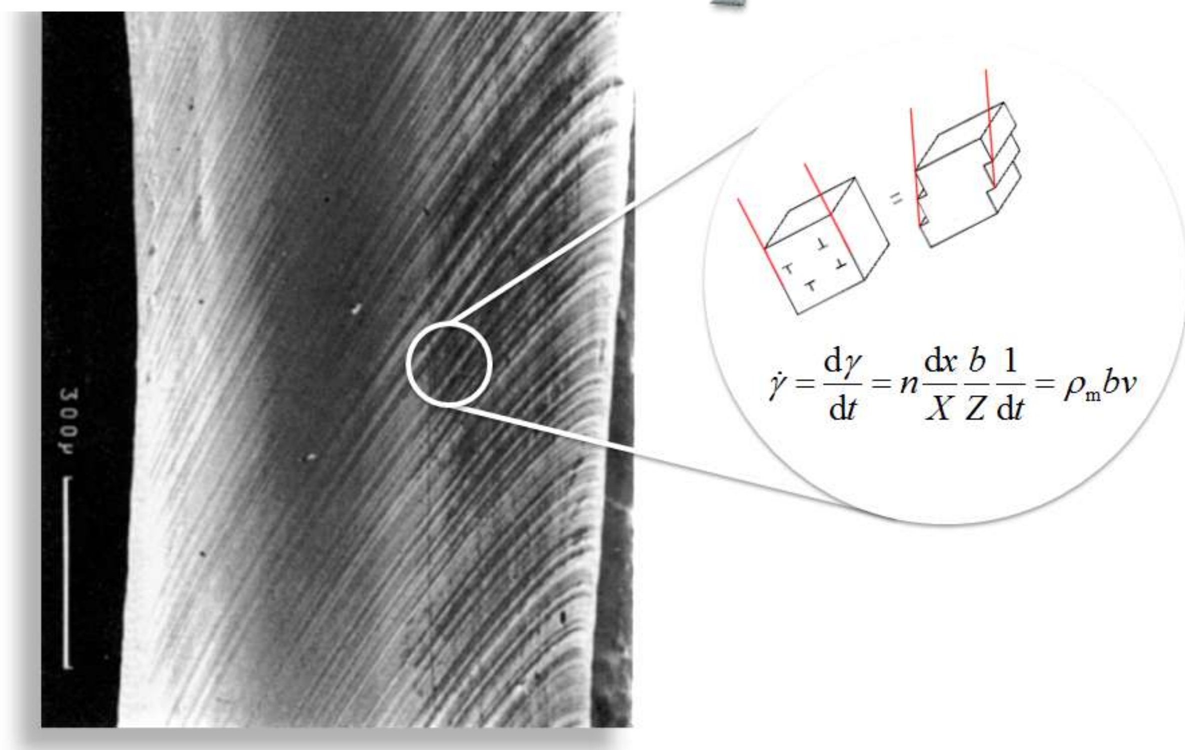
$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}$$

$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)_{etc.}$$

Strain tensor: symmetrical part of displacement gradient tensor

strain rates and displacement gradients in crystals

$$\dot{\varepsilon}^{K}_{ij} = D^{K}_{ij} = \frac{1}{2}\left(\dot{u}^{\mathrm{K}}_{i,j} + \dot{u}^{\mathrm{K}}_{j,i}\right) = \sum_{s=1}^{N} m^{\mathrm{sym},s}_{ij}\,\dot{\gamma}^{s} \qquad \text{mit} \qquad m^{\mathrm{sym}}_{ij} = m^{\mathrm{sym}}_{ji} = \frac{1}{2}\left(n_i b_j + n_j b_i\right)$$



$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

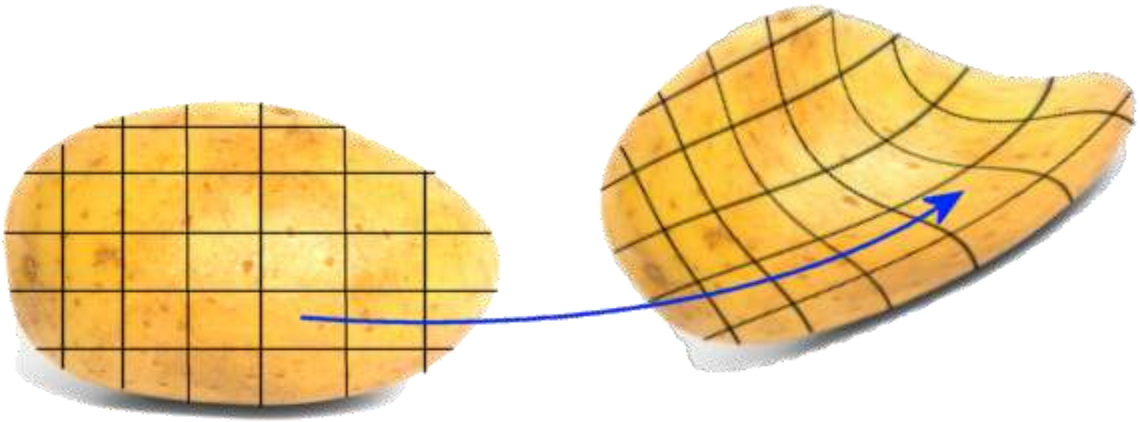
Geometrical interpretation

strain rates and displacement gradients in crystals

$$\dot{\varepsilon}_{ij}^{K} = D_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} + \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{sym},s}\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{sym}} = m_{ji}^{\mathrm{sym}} = \frac{1}{2}\left(n_i b_j + n_j b_i\right)$$

plastic spin from polar decomposition

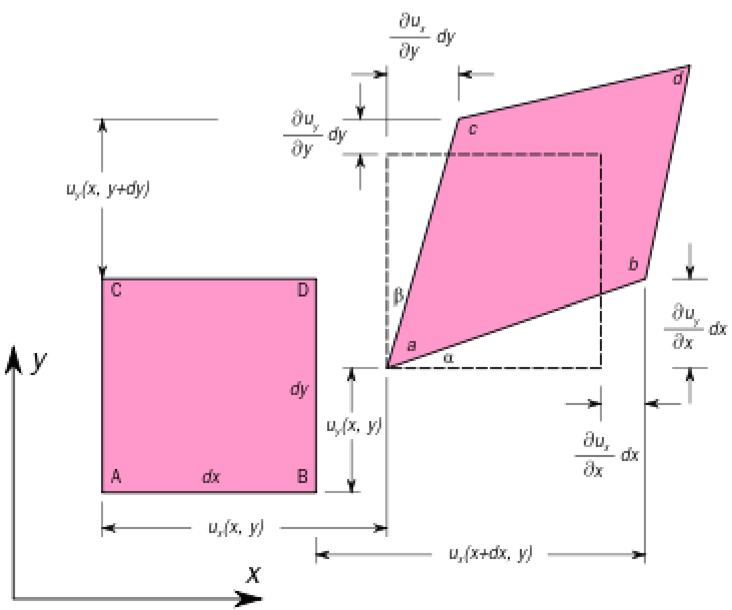
$$\dot{\omega}_{ij}^{K} = W_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} - \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{asym},s}\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{asym}} = \text{-}m_{ji}^{\mathrm{asym}} = \frac{1}{2}\left(n_i b_j - n_j b_i\right)$$



Displacement gradient

The tensor $\frac{\partial u_i}{\partial x_j}$ is called **displacement gradient tensor** and may be written as

$$\frac{\partial u_i}{\partial x_j} = u_{i,j} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}$$



Roters et al. Acta Mater.58 (2010)

Displacement gradient tensor

The displacement gradient tensor in general is a non-symmetric tensor and can be decomposed into symmetric and antisymmetric part. Hence the displacement is

$$u_i = \underbrace{u_i^0}_{\text{translation vector}} + \underbrace{\frac{1}{2}\left(u_{i,j} + u_{j,i}\right)}_{\text{strain tensor}} \mathrm{d}x_j + \underbrace{\frac{1}{2}\left(u_{i,j} - u_{j,i}\right)}_{\text{rotation tensor}} \mathrm{d}x_j$$

$$= u_i^0 + \varepsilon_{ij}\mathrm{d}x_j + \omega_{ij}\mathrm{d}x_j$$

Strain tensor

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$$

In matrix form

$$\varepsilon = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)$$

The above strain tensor is called **Caushy strain tensor**

Displacement gradient tensor: the Cauchy strain

$$
\begin{aligned}
\varepsilon_{ij} &= \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \\
&= \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right) \\ \frac{1}{2}\left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}\right) & \frac{\partial u_2}{\partial x_2} & \frac{1}{2}\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right) \\ \frac{1}{2}\left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3}\right) & \frac{1}{2}\left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3}\right) & \frac{\partial u_3}{\partial x_3} \end{bmatrix}
\end{aligned}
$$

Displacement gradient tensor: the rotation

Rotation tensor

$$\omega_{ij} = \frac{1}{2}(u_{i,j} - u_{j,i})$$

In matrix form

$$\omega = \frac{1}{2}\left(\nabla \mathbf{u} - (\nabla \mathbf{u})^T\right)$$

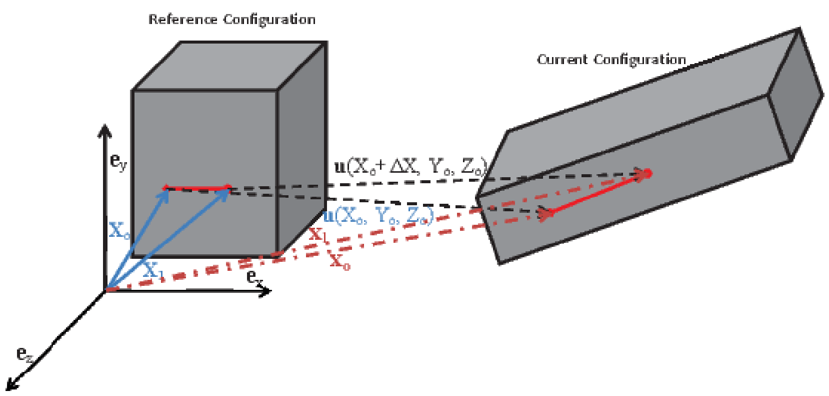
Displacement gradient tensor

Matrix expression of the strain tensor

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix}$$

Matrix expression of the rotation tensor

$$\omega = \begin{bmatrix} 0 & \omega_{xy} & \omega_{xz} \\ -\omega_{xy} & 0 & \omega_{yz} \\ -\omega_{xz} & -\omega_{yz} & 0 \end{bmatrix}$$



Displacement gradient tensor: strain components

Normal strains

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial v}{\partial y}, \quad \varepsilon_{zz} = \frac{\partial w}{\partial z}$$

Shear strains

$$\varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

$$\varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)$$

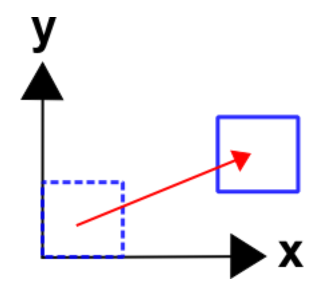
$$\varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)$$

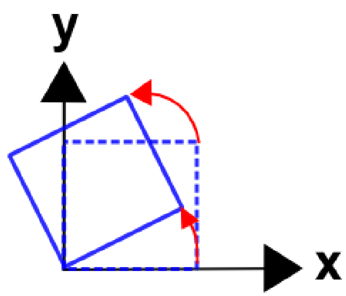
Engineering shear strains

$$\gamma_{xy} = 2\varepsilon_{xy}, \quad \gamma_{xz} = 2\varepsilon_{xz}, \quad \gamma_{yz} = 2\varepsilon_{yz}$$

Displacement gradient tensor: special cases

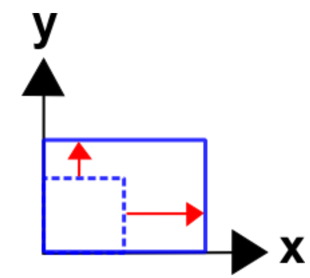
Rigid Body Displacements

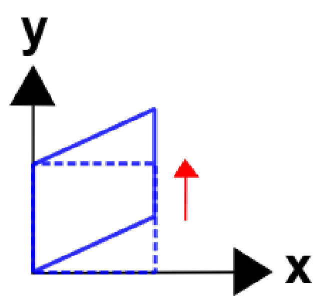




Rigid Body Rotations

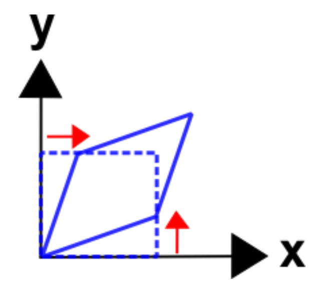
Stretching



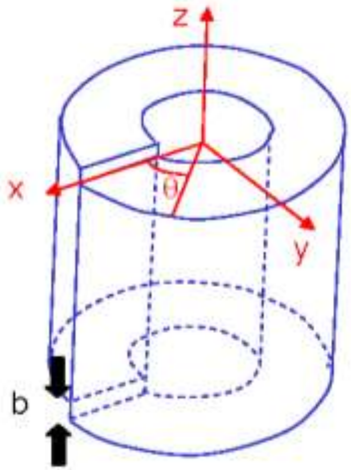


Shear (with Rotation)

Pure Shear



Displacement and strain field: infinite straight screw dislocation



"Recipe" :
- take a hollow cylinder, axis along z:
- cut on a plane parallel to the z-axis;
-displace the free surfaces by **b** in the z-direction.

By inspection:

$$u_x = u_y = 0$$

$$u_z = \frac{b\theta}{2\pi} = \frac{b}{2\pi}\tan^{-1}\left(\frac{y}{x}\right)$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0$$

$$\varepsilon_{xz} = \tfrac{1}{2}\frac{\partial u_z}{\partial x} = \frac{b}{4\pi}\frac{\partial}{\partial x}\tan^{-1}\left(\frac{y}{x}\right) = -\frac{b}{4\pi}\frac{1}{1+\left(y/x\right)^2}\frac{y}{x^2} = -\frac{b}{4\pi}\frac{y}{x^2+y^2} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{yz} = \tfrac{1}{2}\frac{\partial u_z}{\partial y} = \frac{b}{4\pi}\frac{\partial}{\partial y}\tan^{-1}\left(\frac{y}{x}\right) = \frac{b}{4\pi}\frac{1}{1+\left(y/x\right)^2}\frac{1}{x} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

Stress field of straight screw dislocation

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0$$

$$\varepsilon_{xz} = -\frac{b}{4\pi}\frac{y}{x^2+y^2} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{yz} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

$$\Downarrow$$

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

$$\Delta = 0$$

$$\sigma_{xz} = 2G\varepsilon_{xz} = -\frac{Gb}{2\pi}\frac{y}{x^2+y^2} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = 2G\varepsilon_{yz} = \frac{Gb}{2\pi}\frac{x}{x^2+y^2} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

In Polar coordinates:

(either by direct inspection, or by transforming the strains and stresses from Cartesian co-ordinates)

$$\varepsilon_{\theta z} = \varepsilon_{z\theta} = \frac{b}{4\pi r}$$

$$\sigma_{\theta z} = \sigma_{z\theta} = \frac{Gb}{2\pi r}$$

All other components of the stress tensor are zero.

Note:

- Stress and strain fields are pure shear
- Fields have radial symmetry
- Stresses and strains are proportional to 1/r:
  - extend to infinity
  - tend to infinite values as $r \Rightarrow 0$

Infinite stresses cannot exist in real materials: the dislocation core radius r_0 is that within which our assumption of linear elastic behaviour breaks down. Typically $r_0 \approx 1$ nm.

Summary: infinite straight screw dislocation

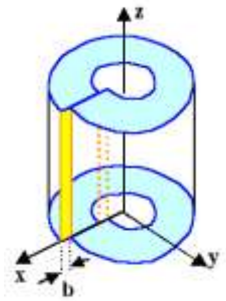
$$\underline{u}(\underline{x}) = \begin{pmatrix} 0 \\ 0 \\ \frac{b}{2\pi} \arctan \frac{y}{x} \end{pmatrix}$$

$$\underline{\underline{\varepsilon}}(\underline{x}) = \begin{pmatrix} 0 & 0 & -\frac{b}{4\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{b}{4\pi}\frac{x}{x^2+y^2} \\ -\frac{b}{4\pi}\frac{y}{x^2+y^2} & \frac{b}{4\pi}\frac{x}{x^2+y^2} & 0 \end{pmatrix}$$

$$\underline{\underline{\sigma}}(\underline{x}) = \frac{Gb}{2\pi} \begin{pmatrix} 0 & 0 & -\frac{b}{4\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{b}{4\pi}\frac{x}{x^2+y^2} \\ -\frac{b}{4\pi}\frac{y}{x^2+y^2} & \frac{b}{4\pi}\frac{x}{x^2+y^2} & 0 \end{pmatrix}$$

Summary: infinite straight edge dislocation

$$
\begin{aligned}
u_x &= \frac{b}{2\pi}(\arctan\frac{y}{x} + \frac{1}{2(1-\nu)}\frac{xy}{x^2+y^2}) \\
u_y &= \frac{b}{2\pi}(-\frac{1-2\nu}{2(1-\nu)}\log\sqrt{x^2+y^2} + \frac{1}{2(1-\nu)}\frac{y^2}{x^2+y^2}) \\
u_z &= 0
\end{aligned}
$$



$$
\varepsilon_{xx} = \frac{\partial u_x}{\partial x} = \frac{b\, y\, ((3-2\,\nu)\, x^2 + (1-2\,\nu)\, y^2)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}
$$

$$
\varepsilon_{yy} = \frac{\partial u_y}{\partial y} = \frac{-(b\, y\, ((1+2\,\nu)\, x^2 + (-1+2\,\nu)\, y^2))}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}
$$

$$
\varepsilon_{xy} = \frac{1}{2}(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}) = \frac{b\, x\, (-x^2+y^2)}{4\,(-1+\nu)\,\pi\,(x^2+y^2)^2}
$$

Summary: infinite straight edge dislocation

$$\sigma_{xx} = \frac{b\,G\,y\,(3\,x^2 + y^2)}{2\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

$$\sigma_{yy} = \frac{b\,G\,y\,(-x^2 + y^2)}{2\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

$$\sigma_{zz} = \frac{b\,G\,\nu\,y}{(-1+\nu)\,\pi\,(x^2+y^2)}$$

$$\sigma_{xy} = \frac{b\,G\,x\,(-x^2 + y^2)}{2\,(-1+\nu)\,\pi\,(x^2+y^2)^2}$$

Forces and stress field: infinite straight edge dislocation