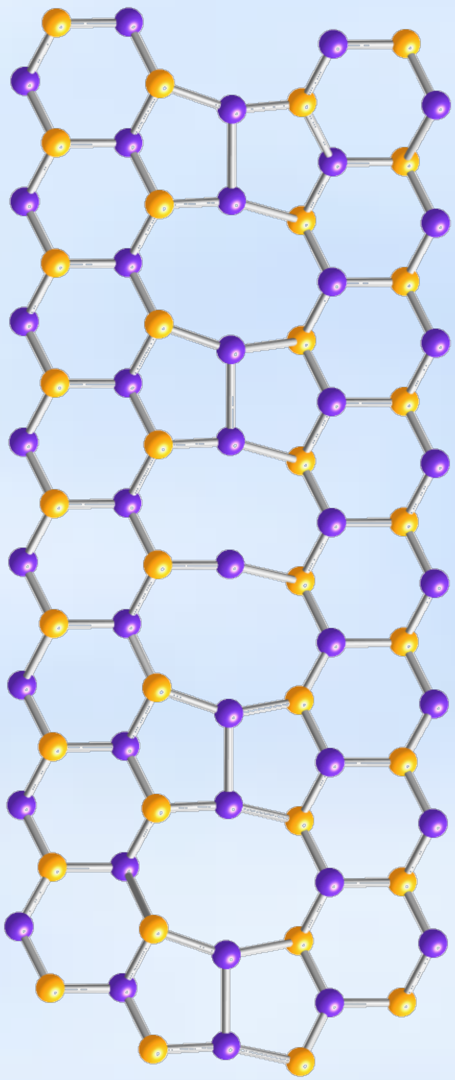
Hartmut S. Leipner: *Defects in imperfect materials*



3.2 Elasticity theory of dislocations

- Basics of linear elasticity theory
- Stress field of a straight dislocation
- Strain energy
- Forces on dislocations

Basics of linear elasticity theory

- Displacement vector $\boldsymbol{u} = (u_x, u_y, u_z)$
- Nine components of the strain tensor

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial u_y}{\partial y}, \quad \varepsilon_{zz} = \frac{\partial u_z}{\partial z}$$

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

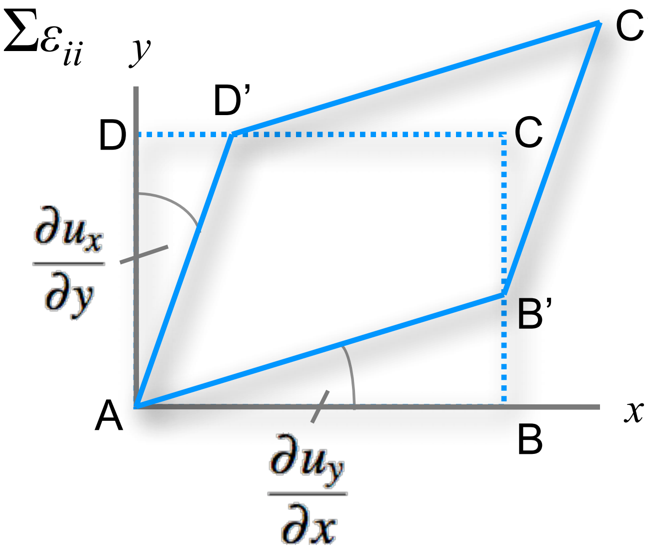
$$\varepsilon_{yz} = \varepsilon_{zy} = \frac{1}{2}\left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right)$$

$$\varepsilon_{zx} = \varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right)$$

- $\varepsilon_{ij} << 1$,

  ε_{ii} normal strain, ε_{ij} $(i \neq j)$ shear strain

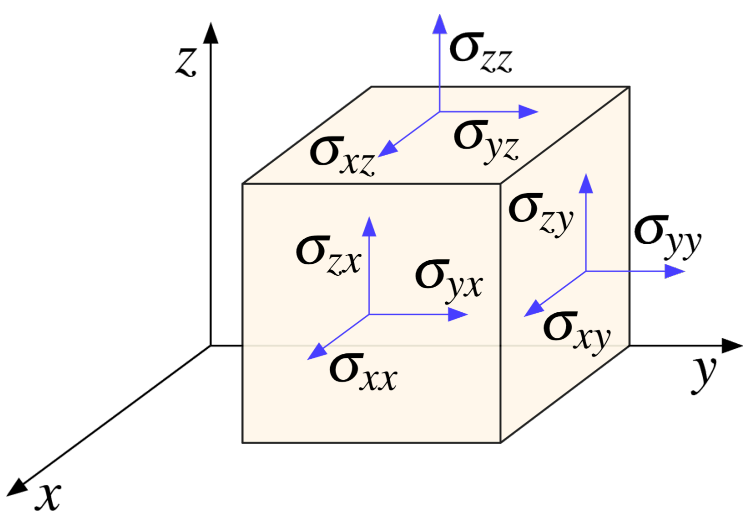
- Fractional change in volume $\Delta V/V = \Sigma\varepsilon_{ii}$



Stress in the solid

- Considering a small cubic volume element in a solid, the total stress state can be described by the forces perpendicular and parallel to the faces of the cube.
- On each face, three stresses:

  1 normal σ_{ii}, 2 shear σ_{ij} $(i \neq j;\ i, j = x, y, z)$
- All together nine components of the stress



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

Stress tensor

- Stress tensor is symmetrical, $\sigma_{ij} = \sigma_{ji}$ (rotational equilibrium).
- Magnitude of the individual components depends on the orientation of the coordinate system.
- A special coordinate system can always be found, where there are only normal stresses,

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix}$$

- Positive normal stress as tension
- Hydrostatic pressure is the average normal stress,

$$p = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)$$

Strain

- Generally, the elastic deviation of the shape of the solid can be expressed as a strain tensor,

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}$$

- ε_{ii} elongations, ε_{ij} shear ($i \neq j$)
- Strain tensor also symmetrical

$$\frac{V - V_0}{V_0} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

Stress–strain relationships

- Stress as force per unit area of surface; consider orientation of the surface and direction of the force
- Uniaxial tension $\sigma = \tilde{E}\varepsilon$, shear $\tau = G\gamma$
- Special cases of Hooke's law $\boldsymbol{\sigma} = \boldsymbol{C\varepsilon}$
- Relation between stress and strain tensors

- Expression of 9 equation like $\sigma_{ij} = \sum_{i,j,k,l=1}^{3} C_{ijkl}\varepsilon_{kl}$
- $\boldsymbol{C}$ has $3^4 = 81$ components C_{ijkl} (4th rank tensor)

Elastic constants C

- *In praxi,* number of constants is reduced due to symmetry.
- For isotropic solids only two parameters (*e.g.* G and Lamé constant $\tilde{\lambda}$)

$$\sigma_{xx} = 2G\varepsilon_{xx} + \tilde{\lambda} \sum \varepsilon_{ii}$$
$$\sigma_{yy} = 2G\varepsilon_{yy} + \tilde{\lambda} \sum \varepsilon_{ii}$$
$$\sigma_{zz} = 2G\varepsilon_{zz} + \tilde{\lambda} \sum \varepsilon_{ii}$$
$$\sigma_{xy} = 2G\varepsilon_{xy} \qquad \sigma_{yz} = 2G\varepsilon_{yz} \qquad \sigma_{zx} = 2G\varepsilon_{zx}$$

- In cubic crystals, three constants are needed.

Elastic moduls

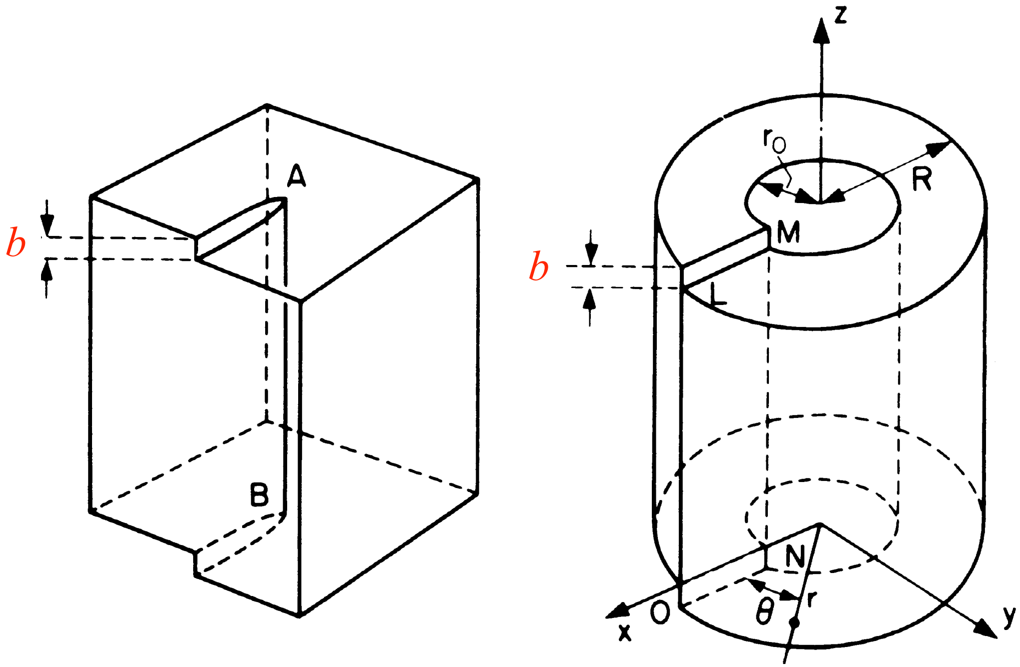
- Constants used for isotropic solids: Young's modulus $\tilde{E}$, Poisson's constant ν, and bulk modulus $\tilde{K}$,

$$\tilde{E} = 2G(1+\nu) \qquad \nu = \frac{1}{2(1+G)} \qquad \tilde{K} = \frac{\tilde{E}}{3(1-2\nu)}$$

- **Poisson's constant**
  Elongation in x-direction connected with reduction of cross section

$$\varepsilon_{yy} = \varepsilon_{zz} = -\nu\varepsilon_{xx}$$

Strain field of a straight screw dislocation



Volterra screw dislocation

[Hull, Bacon 1992]

- Representation as a cylinder of elastic material
- Slit LMNO || z axis, surface displaced by b

Displacements:

$$u_x = u_y = 0$$

$$u_z = \frac{b\theta}{2\pi} = \frac{b}{2\pi} \arctan \frac{y}{x}$$

- Cylinder with radius r_0 not taken into account: assumptions of *linear* elasticity theory not valid

Straight screw dislocation

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

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

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

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

$$\sigma_{xz} = \sigma_{zx} = -\frac{Gb}{2\pi}\frac{y}{(x^2+y^2)} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = \sigma_{zy} = -\frac{Gb}{2\pi}\frac{x}{(x^2+y^2)} = -\frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

Simpler form in cylindrical coordinates:

Using $\sigma_{rz} = \sigma_{xz}\cos\theta + \sigma_{yz}\sin\theta$

$\sigma_{\theta z} = -\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta$

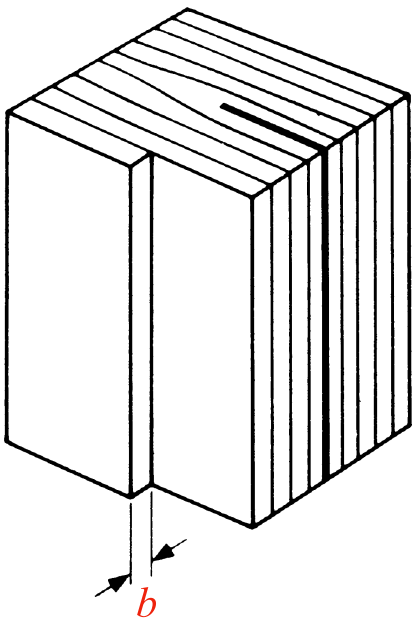
$$\boxed{\begin{aligned} \varepsilon_{\theta z} &= \varepsilon_{z\theta} = \frac{b}{4\pi r} \\ \sigma_{\theta z} &= \sigma_{z\theta} = \frac{Gb}{2\pi r} \end{aligned}}$$

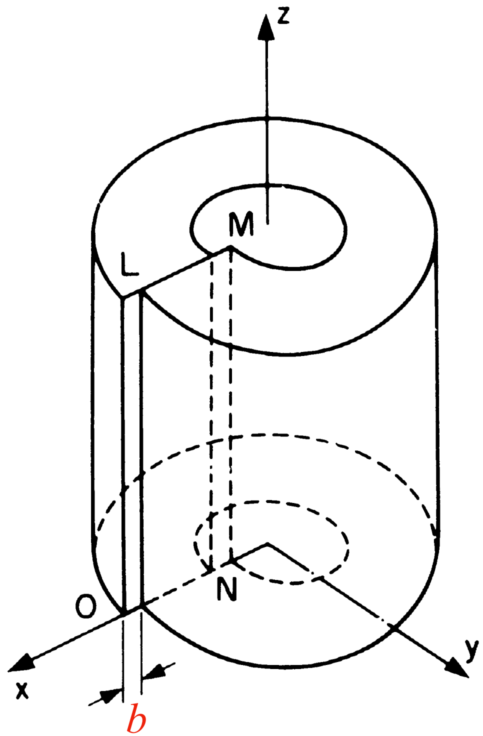
(the only non-zero components)

Discussion of the strain and stress fields

- Strain and stress $\propto 1/r$, diverge with $r \longrightarrow 0$
- Linear elasticity approach not valid at the center of the dislocation
- **Dislocation core** with atomistic model
- Theoretical stress limit reached at $r \approx b$
- Reasonable core radius ≤ 1 nm

Stress field of a straight edge dislocation





$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

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

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

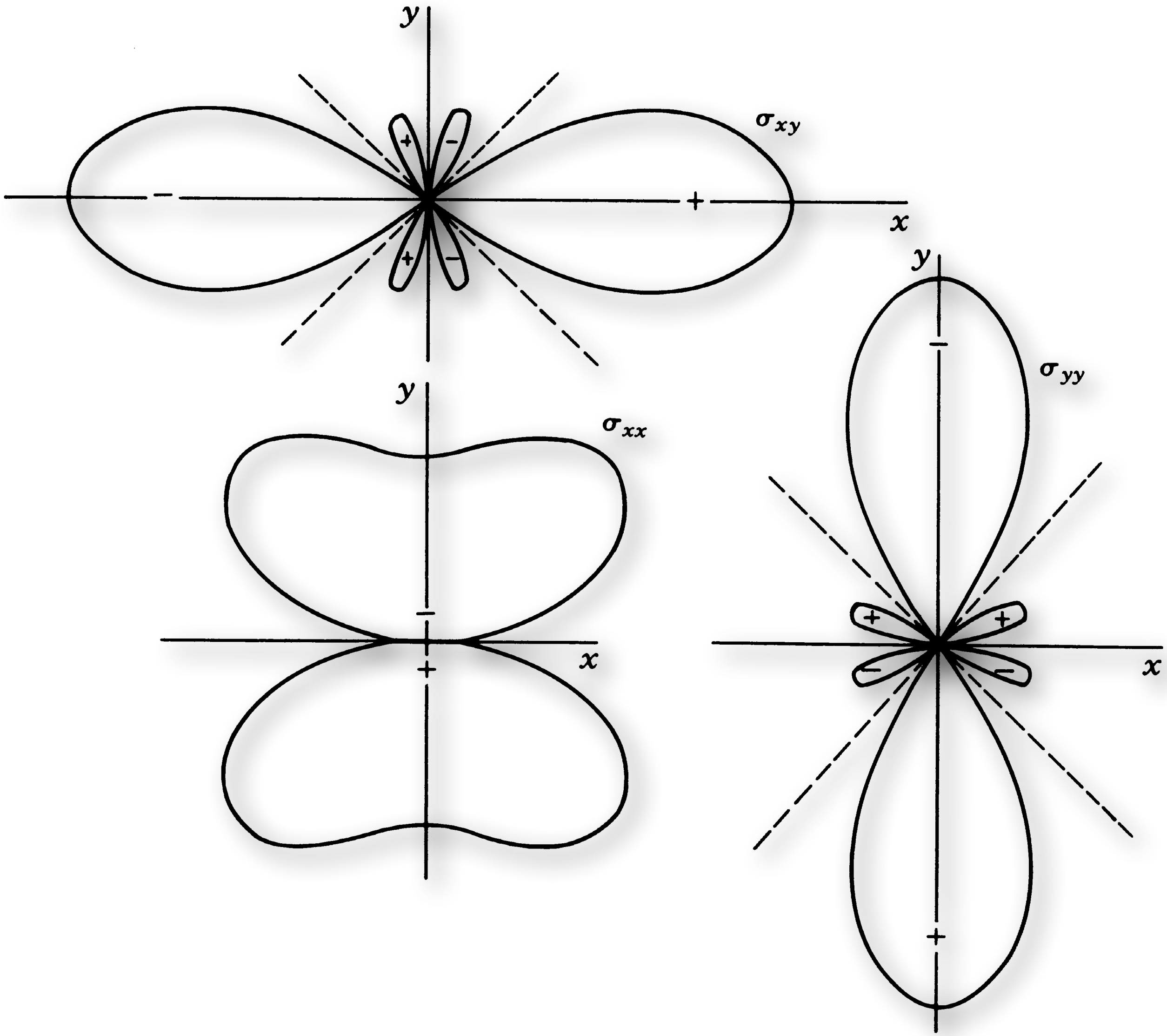
$$\sigma_{xy} = \sigma_{yx} = \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

Volterra edge dislocation

[Hull, Bacon 1992]

Stress field contours of an edge dislocation



Contours of equal stress about an edge dislocation
[Hirth, Lothe 1992]

Stress field of an edge dislocation

- Deformation is basically a plane strain.
- Both dilatational and shear components exist.
- Largest normal stress σ_{xx} || Burgers vector
- Max. compressive stress immediately above $y = 0$ (slip plane)
  max. tensile stress immediately below $y = 0$

- Pressure on a volume element

$$p = \frac{2}{3}\frac{Gb(1+\nu)}{1-\nu}\frac{y}{x^2+y^2}$$

Strain energy of a dislocation

- Elastic strain energy in theory of elasticity: $\mathrm{d}E = \frac{1}{2}\mathrm{d}V \sum_i \sum_j \sigma_{ij}\varepsilon_{ij}$

- Two parts of the total strain energy of a body containing a dislocation:

  $E = E_{\text{core}} + E_{\text{el}}$

- Elastic energy *per unit length* of a screw:

$$\mathrm{d}E_{\text{el}} = \frac{1}{2} 2\pi r\,\mathrm{d}r\,(\sigma_{\theta z}\varepsilon_{\theta z} + \sigma_{z\theta}\varepsilon_{z\theta})$$

$$= \frac{Gb^2}{4\pi}\frac{\mathrm{d}r}{r}$$

$$E_{\text{el}} = \frac{Gb^2}{4\pi}\int_{r_0}^{R}\frac{\mathrm{d}r}{r} = \frac{Gb^2}{4\pi}\ln\frac{R}{r_0}$$ (Total elastic energy per unit length)

Discussion of the strain energy

- Strain energy of an edge more complicated to calculate (lower symmetry)

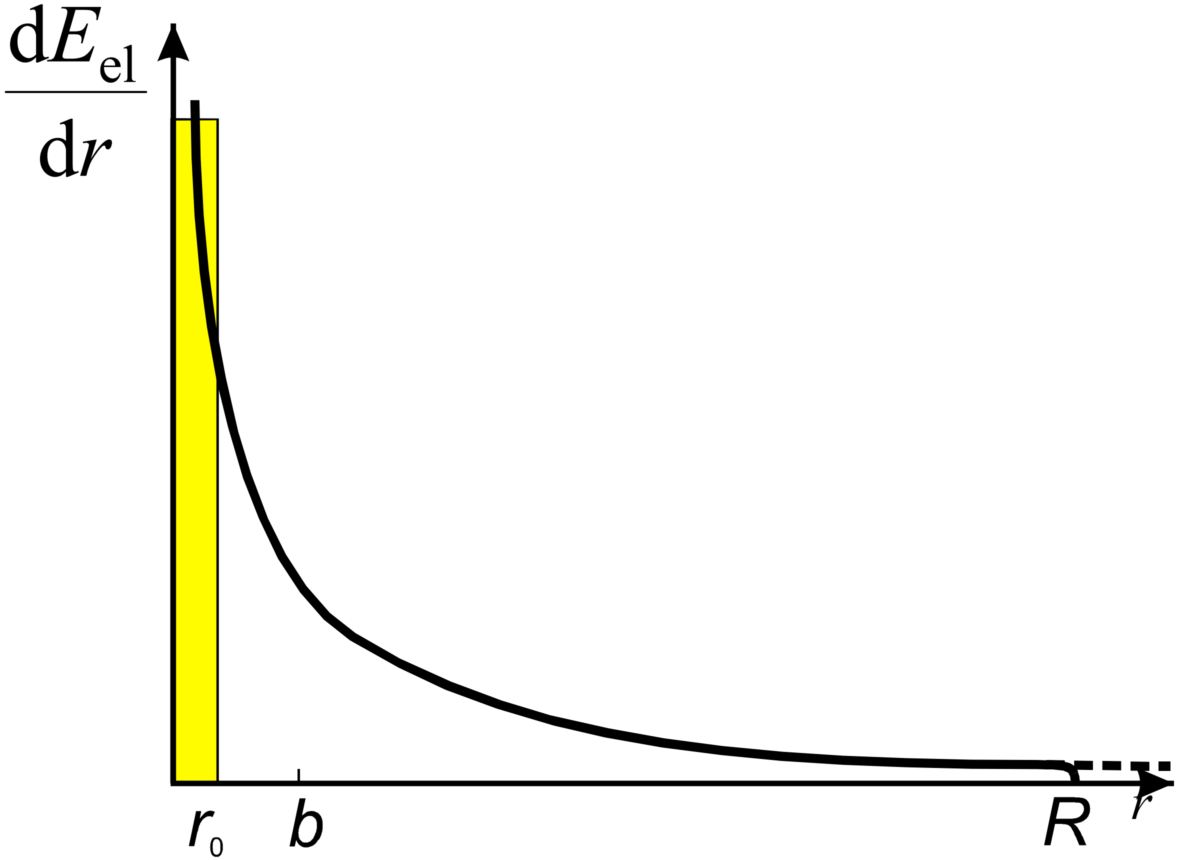
$$E_{el} = \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{R}{r_0}$$

- Elastic energy of an edge dislocation higher by about 3/2 than that of a screw

- E_{el} depends on r_0 and R (core radius and cut-off radius).
- Example: $G = 4 \cdot 10^{10}$ Nm^{-2}, $r_0 = 1$ nm, $R = 1$ mm, $b = 0.25$ nm
  $E_{el} \approx 6$ eV per unit length of a dislocation

- R corresponds to crystal dimensions. $R = \dfrac{1}{2\sqrt{\rho}}$
- For many dislocations in a crystal, superposition of the long-range strain fields

Elastic energy of dislocations



$$E_{el} = \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{R}{r_0}$$

Elastic energy in a ring cylinder of the thickness dr

Energy of mixed dislocations

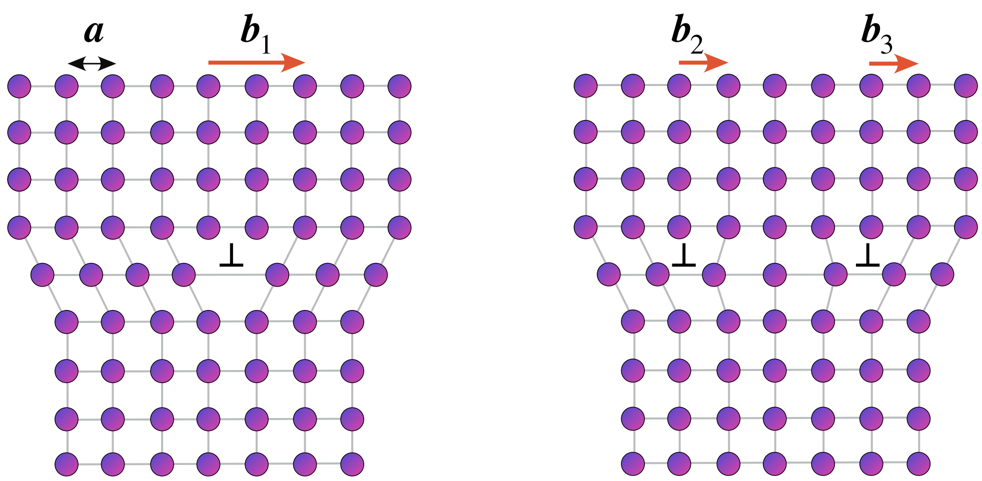
- Superposition of edge and screw parts E_{el}

$$= \left[\frac{Gb_e^2}{4\pi(1-\nu)} + \frac{Gb_s^2}{4\pi}\right] \ln \frac{R}{r_0}$$

$$= \left[\frac{Gb^2 \sin^2\vartheta}{4\pi(1-\nu)} + \frac{Gb^2\cos^2\vartheta}{4\pi}\right] \ln \frac{R}{r_0}$$

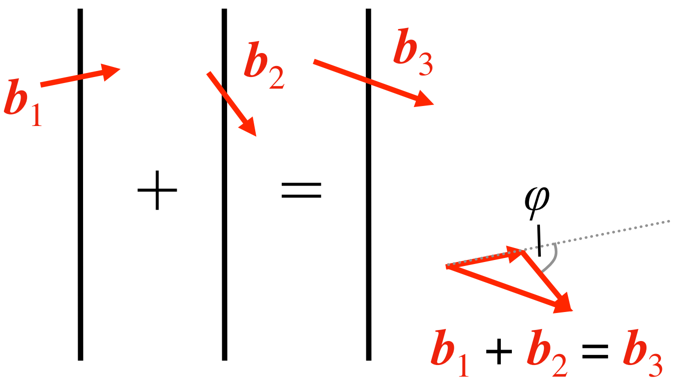
$$= \frac{Gb^2(1-\nu\cos^2\vartheta)}{4\pi(1-\nu)} \ln \frac{R}{r_0}$$

- $E_{el} \approx \alpha G b^2$, with $\alpha \approx 0.5 \ldots 1.0$
- Shortest lattice translation vectors preferred as E_{el} is at min.



Splitting of a dislocation with $\boldsymbol{b}_1 = 2\boldsymbol{a}$ into two dislocations with $\boldsymbol{b}_2 = \boldsymbol{b}_3 = \boldsymbol{a}$, $E_1 \propto 4a^2$, $E_2 = E_3 \propto 2a^2$

Frank's rule



- Energy criterion for dislocation reaction

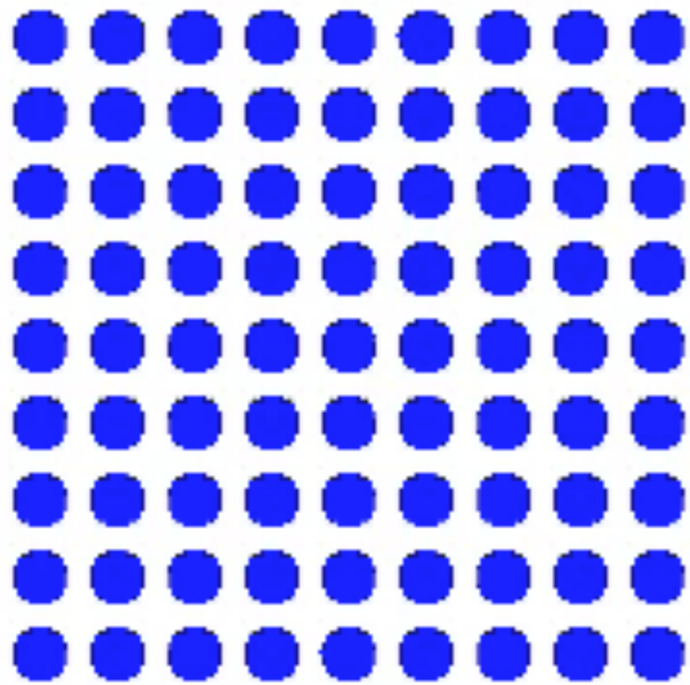
$$b_1^2 + b_2^2 > b_3^2 \quad \text{Reaction favorable}$$

- Condition with angle φ:

$\pi/2 < \varphi \leq \pi$ Reaction preferred

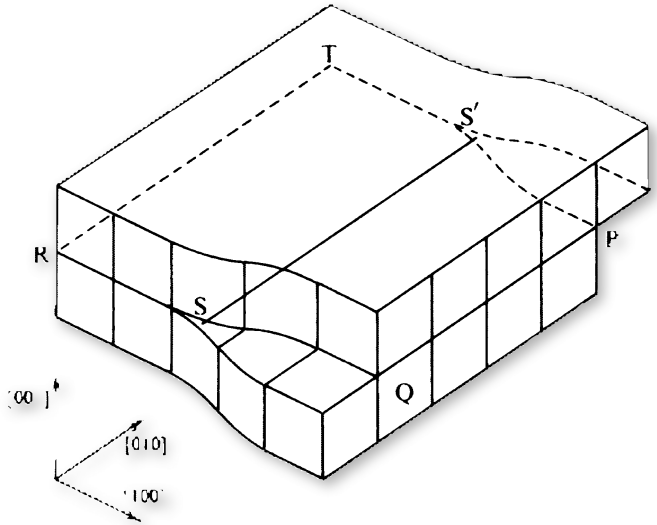
$0 \leq \varphi < \pi/2$ Dissociation preferred

Elementary process of plastic deformation

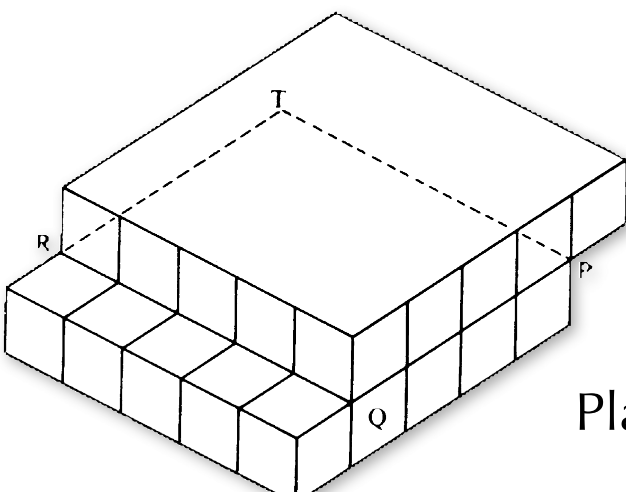


The motion of dislocations is the elementary process of the plastic deformation of crystals.

External forces on dislocations



- Dislocation separates slipped region from unslipped one
- Deformation work may be done by external force ⇒ shift of the dislocation

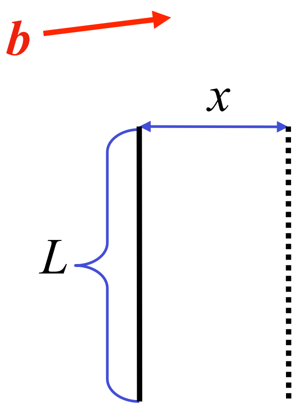


Plastic deformation by motion of a dislocation

[Kelly:2000]

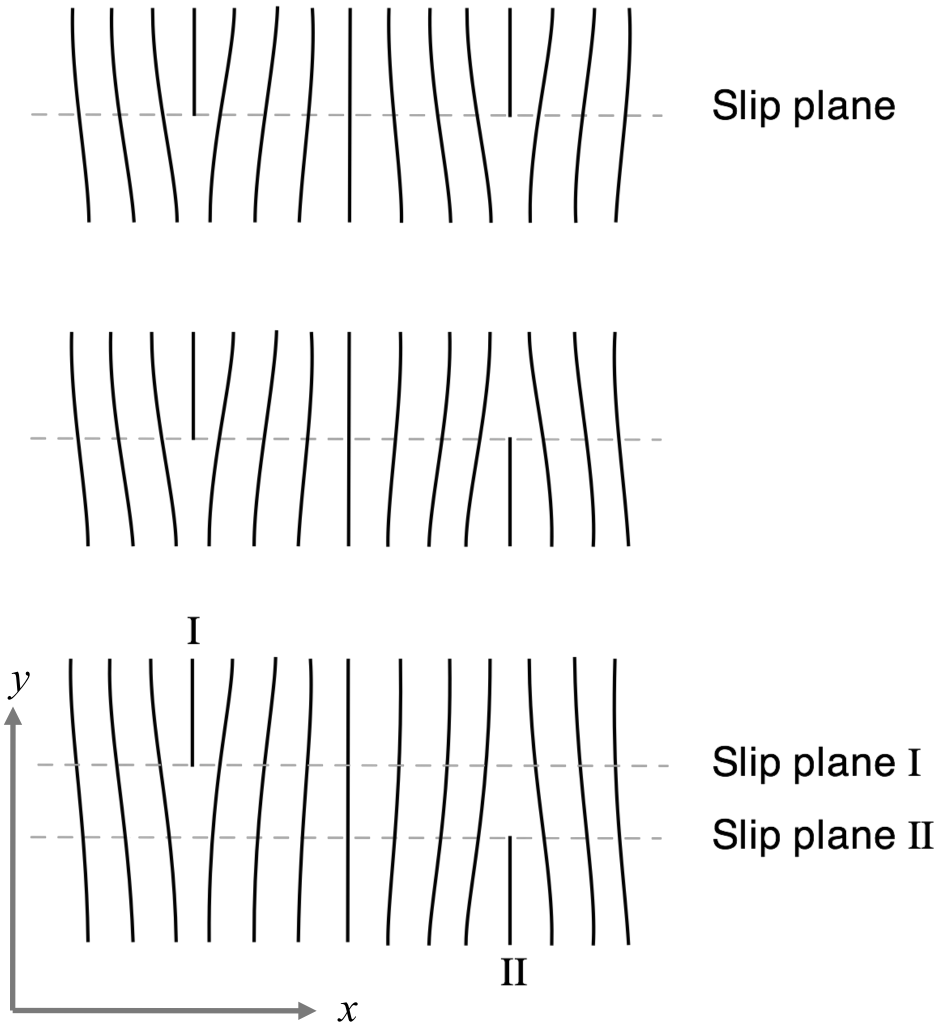
Definition of force

- Dislocation of length L, swept distance on the slip plane x
- Applied shear force on the crystal (per length L): $F = \sigma x$
- Work done by the crystal (per length L): $W = \sigma x b$



- Definition of a force (per length L) to move the dislocation in x-direction: work W = force on dislocation $\times\, x$
- $F_d = \sigma b$

Forces between dislocations



- Edge dislocations with the same slip plane
  repulsive force if ***b*** has the same sign, attractive if opposite sign
- More complicated, if slip planes different
- Displacement in dislocation I is Burgers vector ***b*** of dislocation II

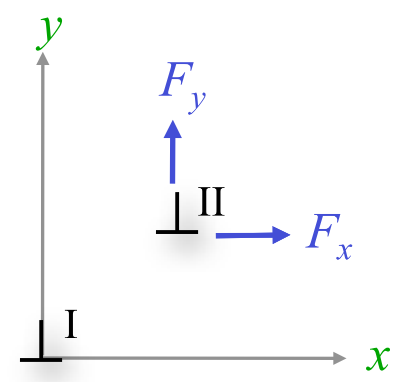
Calculation of the force

Components of the force on dislocation II per unit length
($b_x = b$, $b_y = b_z = 0$):

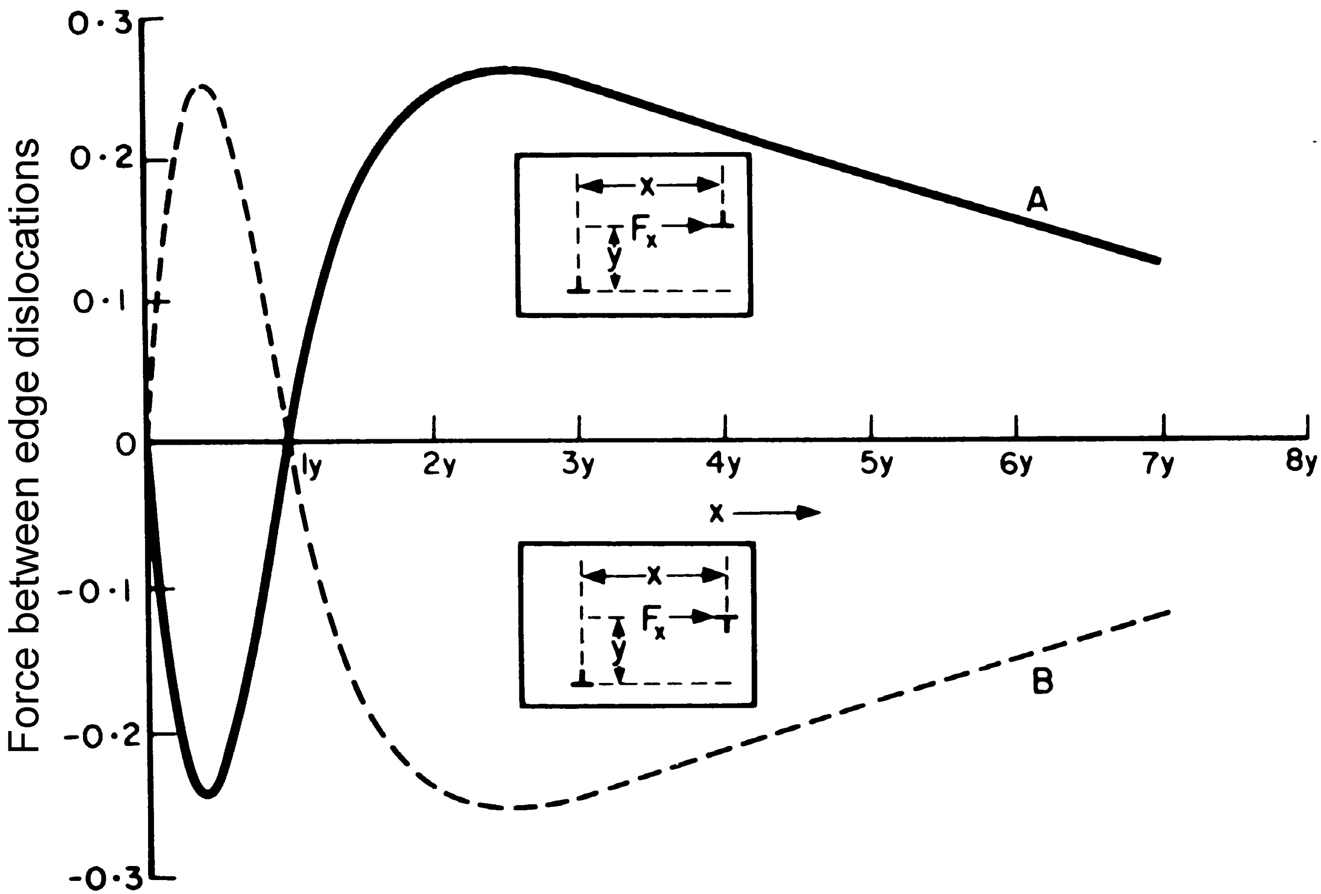
$$F_x = \sigma_{xy} b, \quad F_y = \sigma_{xx} b$$

$$F_x = \frac{Gb^2}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$F_y = \frac{Gb^2}{2\pi(1-\nu)} \frac{y(3x^2 - y^2)}{(x^2 + y^2)^2}$$



Force between parallel edge dislocations

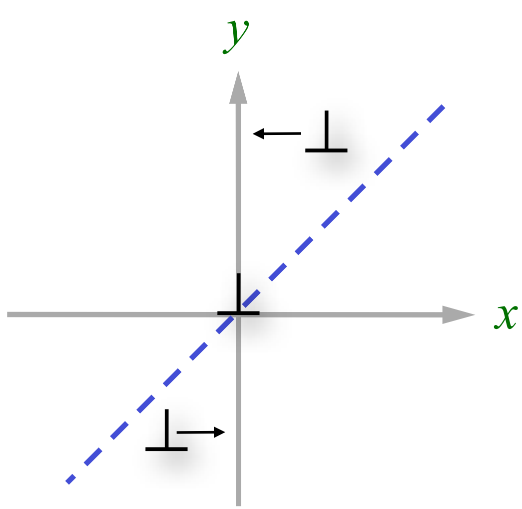


Force between parallel edge dislocations. Unit of force F_x is $Gb^2y/[2\pi(1-v)]$. Curve A for like dislocations, curve B for unlike dislocations.

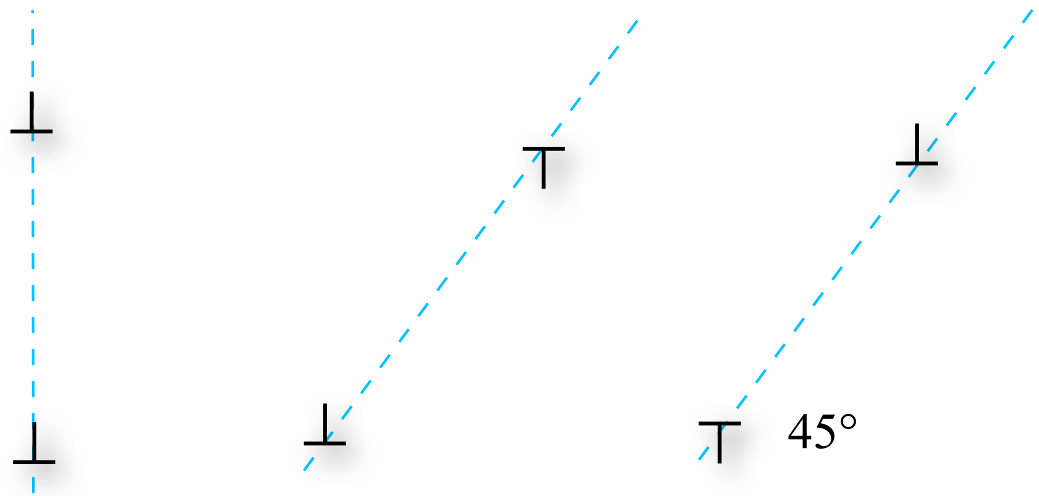
[Hull, Bacon 1993/Cottrell 1953]

Interaction force between edge dislocations

- Dislocations motion only in the slip plane
  most important F_x
- For $x > 0$, $F_x < 0$ (attractive) if $x < y$
- For $x < 0$, $F_x > 0$ (attractive) if $x < -y$
  (dislocations of the same sign)



Stable positions of edge dislocations

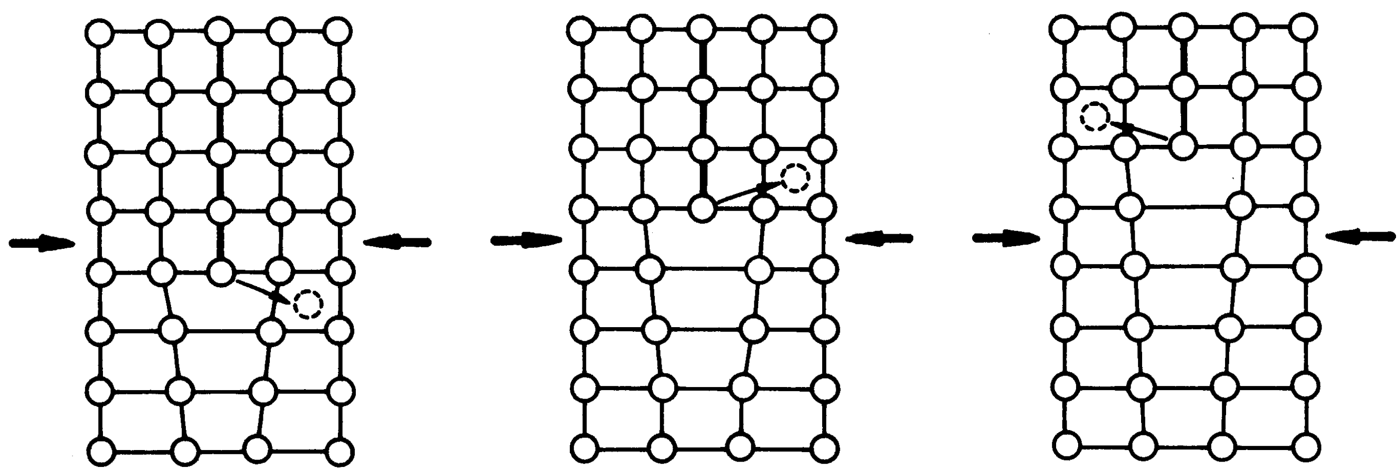


Interaction force between screws

- Screws much easier: attractive for opposite sign, repulsive for the same sign
- No forces between parallel screw and edge dislocations, as the stress fields are not mixing

Climb force

- Force F_y not in glide plane, no *conservative* motion of dislocation possible
- Motion only possible, if intrinsic point defects can be emitted or absorbed
- Vacancy or interstitial mechanism



Emission of interstitials by dislocation climb

Chemical force

- No. of vacancies absorbed: bls/Ω

  (l length of dislocation segment, s climb distance, Ω atomic volume)

- Change in the vacancy concentration ⬄ change in the chemical potential of vacancies

$$c = \exp\left(-\frac{E_\mathrm{f} + F_y\Omega/b}{k_\mathrm{B}T}\right)$$

$$= c_0 \exp\left(-\frac{F_y\Omega}{bk_\mathrm{B}T}\right)$$

- *vice versa:* chemical force f by supersaturation of vacancies
- Dislocation climbs, until equilibrium between f and F_y

$$f = \frac{bk_\mathrm{B}T}{\Omega}\ln\frac{c}{c_0}$$

Summary

- Elastic energy of a dislocation $\propto Gb^2$
- Total energy $E_{\mathrm{el}} + E_{\mathrm{core}}$
- Frank's energy criterion for dislocation reaction:

$$b_1^2 + b_2^2 > b_3^2$$

- Glide force on dislocation σb (per unit length)
- Repulsive and attractive slip forces responsible for dislocation patterning
- Interaction between point defects and dislocations gives rise to climb

Literature

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