Karlsruhe Institute of Technology

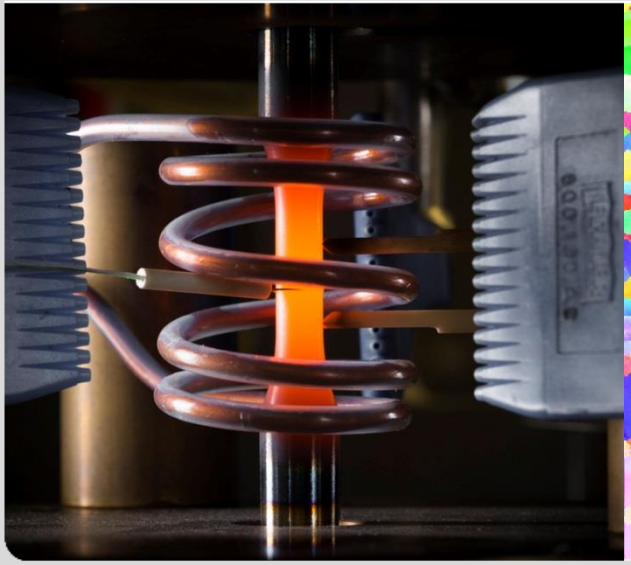
Institute for Applied Materials

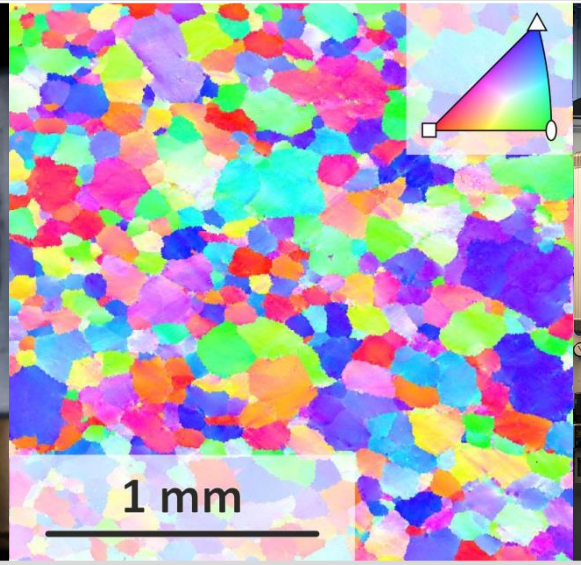
Plasticity

Lecture for “Mechanical Engineering” and “Materials Science and Engineering”
Dr.-Ing. Alexander Kauffmann (Bldg. 10.91, R. 375)
Prof. Martin Heilmaier (Bldg. 10.91, R. 036)

Version 22-04-27

Institute for Applied Materials (IAM-WK)



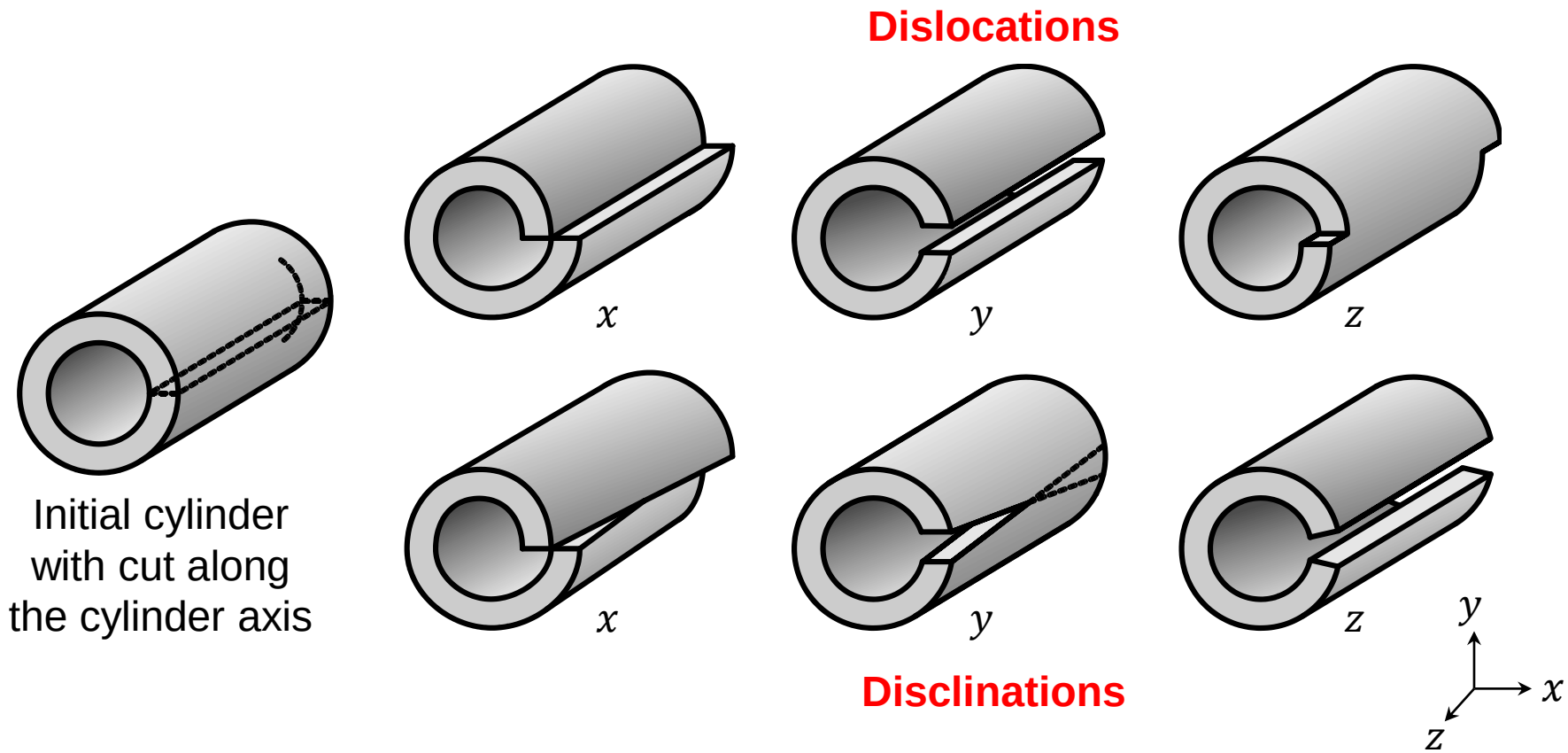


Topics

- Elastic Theory of Dislocations
  - Brief Introduction
  - Stress Fields (of Straight Dislocations)
  - Line Energy (of Straight Dislocations)
  - Peach-Köhler Force
  - Line Tension

Elastic Theory of Dislocations

- … traces back to V. Volterra and general consideration of cuts in conjunction with displacements (dislocations) or inclinations (disclinations):



Brief Introduction

- In general, the equilibrium condition must be fulfilled:

$$\partial/_{\partial x_i}\,\sigma_{ik} = 0$$

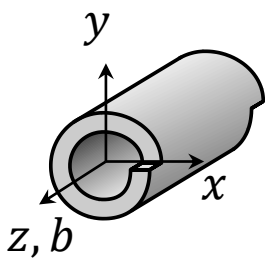
$$\sigma_{ik} = C_{iklm}\,\varepsilon_{lm}$$

$$\varepsilon_{ik} = \frac{1}{2}\left(\partial u_j/_{\partial x_i} + \partial u_i/_{\partial x_j}\right)$$

Stress Fields of Straight Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$:

Ansatz: $u_x = u_y = 0, u_z = \frac{b}{2\pi}\tan^{-1}(y, x)$



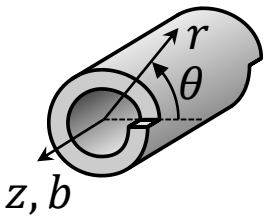
$$(\sigma_{ik}) = \begin{pmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & 0 \end{pmatrix} = \frac{G \cdot b}{2\pi} \begin{pmatrix} 0 & 0 & -\frac{y}{x^2 + y^2} \\ 0 & 0 & \frac{x}{x^2 + y^2} \\ -\frac{y}{x^2 + y^2} & \frac{x}{x^2 + y^2} & 0 \end{pmatrix}$$

In case of a finite cylinder, torque equilibrium is not fulfilled. There is an additional (constant) shear stress necessary in order to avoid spinning of the arrangement.

. P. Hirth, J. Lothe: “Theory of Dislocations”, Malabar, USA: Krieger Publishing Company (1982, reprint 1992)

Stress Fields of Straight Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$:



$$\sigma_{\theta z} = \frac{G \cdot b}{2\pi \cdot r}$$

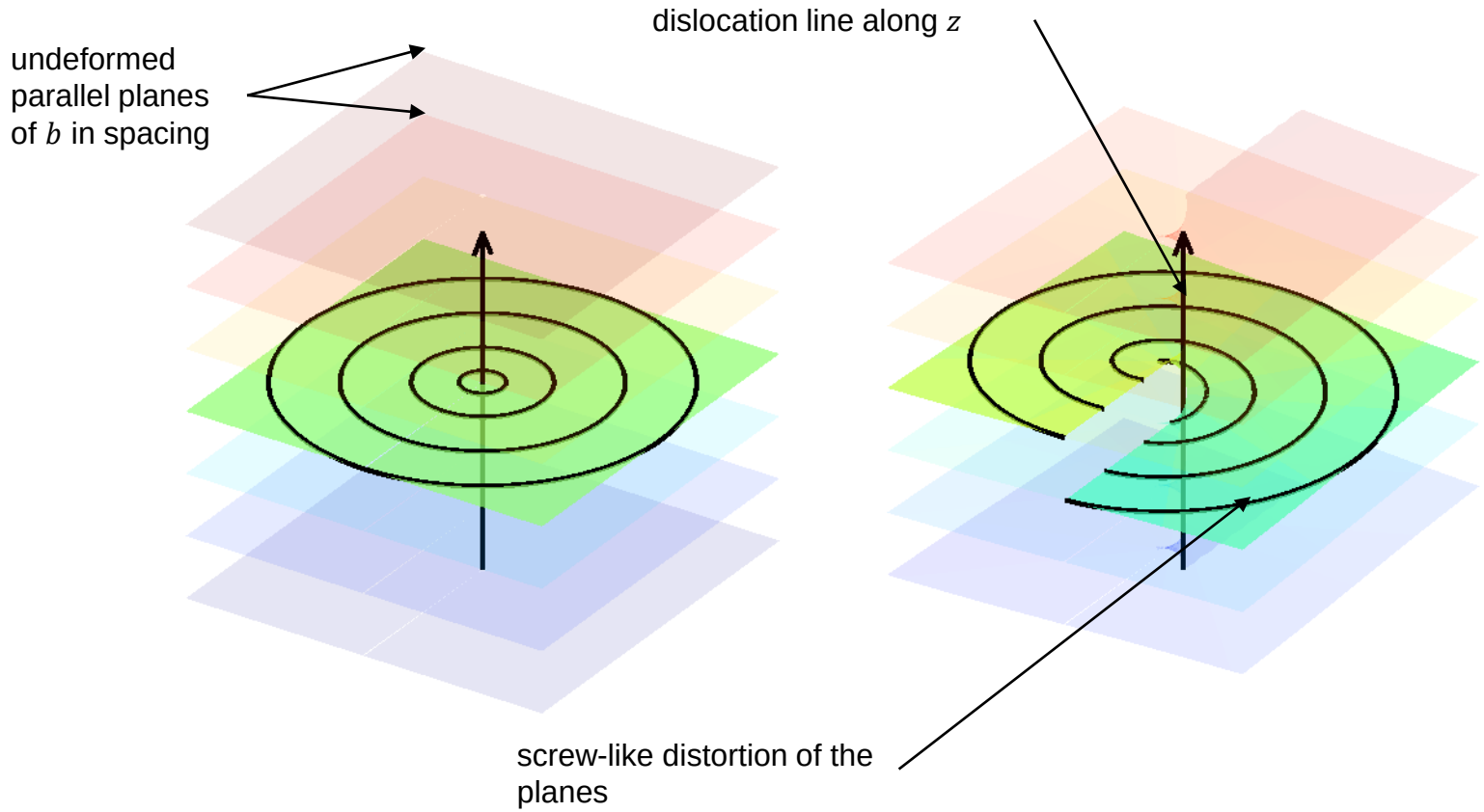
$$\sigma_{rz} = \sigma_{r\theta} = \sigma_{rr} = \sigma_{\theta\theta} = \sigma_{zz} = 0$$

If you want to do it your own, you also have to convert the divergence to cylinder coordinates ${}^{\partial}/_{\partial x_i}\,\sigma_{ik} = 0$.

P. Hirth, J. Lothe: “Theory of Dislocations”, Malabar, USA: Krieger Publishing Company (1982, reprint 1992)

Stress Fields of Straight Dislocations

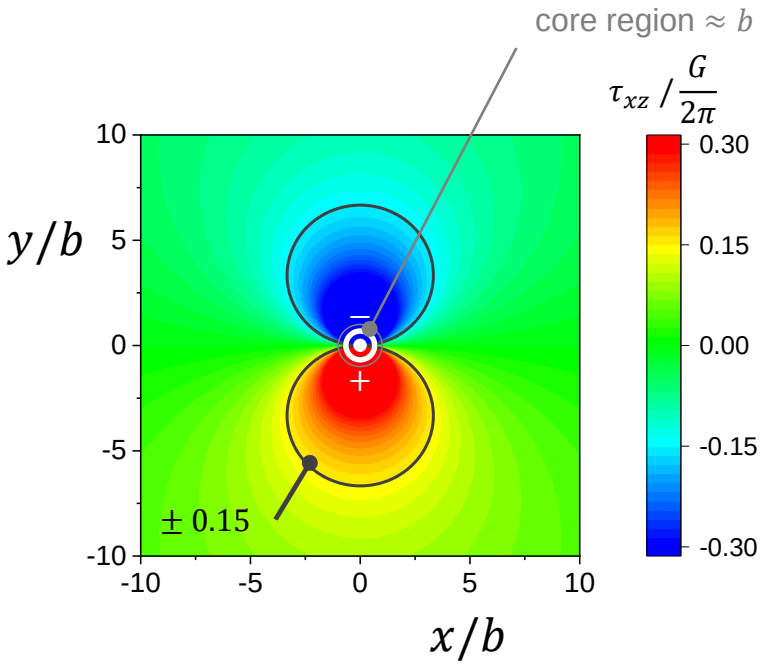
- Screw dislocation with dislocation line along z and plane of displacement within $x - z$:

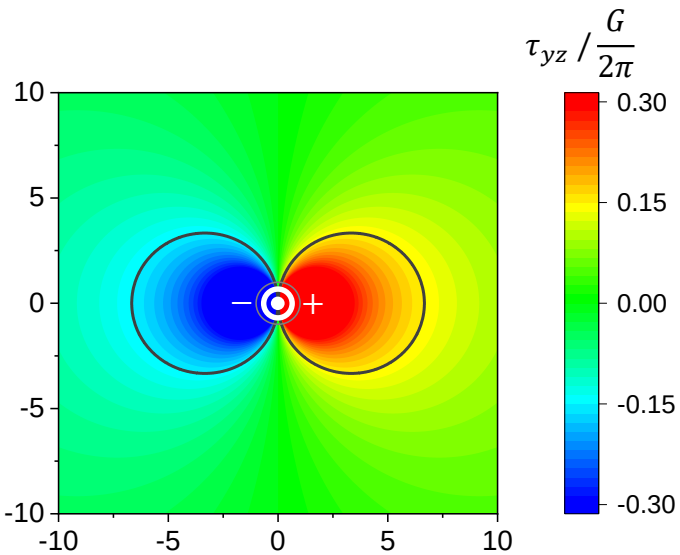


$$u_z = \frac{b}{2\pi}\tan^{-1}(y, x)$$

Stress Fields of Straight Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$:





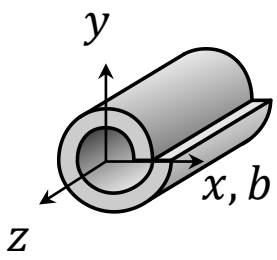
$0.15 \frac{G}{2\pi}$ is in the order of $1.2\ \mathrm{GPa}$ for Cu!

Stress Fields of Straight Dislocations

- Edge dislocation with dislocation line along z and Burgers vector along x:

Ansatz: $u_x = \frac{b}{2\pi}\left(\tan^{-1}(y,x) + \frac{xy}{2\,(1-\nu)(x^2+y^2)}\right)$,

$u_y = -\frac{b}{8\pi\,(1-\nu)}\left((1-2\nu)\ln(x^2+y^2) + \frac{x^2-y^2}{x^2+y^2}\right), u_z = 0$

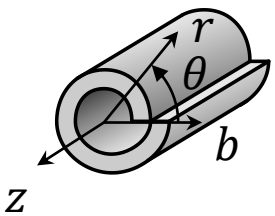


$$(\sigma_{ik}) = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix} = \frac{G\cdot b}{2\pi\cdot(1-\nu)}\begin{pmatrix} -\frac{y\cdot(3x^2+y^2)}{(x^2+y^2)^2} & \frac{x\cdot(x^2-y^2)}{(x^2+y^2)^2} & 0 \\ \frac{x\cdot(x^2-y^2)}{(x^2+y^2)^2} & \frac{y\cdot(x^2-y^2)}{(x^2+y^2)^2} & 0 \\ 0 & 0 & \frac{-2\nu\,y}{x^2+y^2} \end{pmatrix}$$

P. Hirth, J. Lothe: “Theory of Dislocations”, Malabar, USA: Krieger Publishing Company (1982, reprint 1992)

Stress Fields of Straight Dislocations

- Edge dislocation with dislocation line along z and Burgers vector along x:



$$\sigma_{rr} = \sigma_{\theta\theta} = -\frac{G\ b \sin\theta}{2\pi \cdot (1-\nu) \cdot r}$$

$$\sigma_{r\theta} = \frac{G\ b \cos\theta}{2\pi \cdot (1-\nu) \cdot r}$$

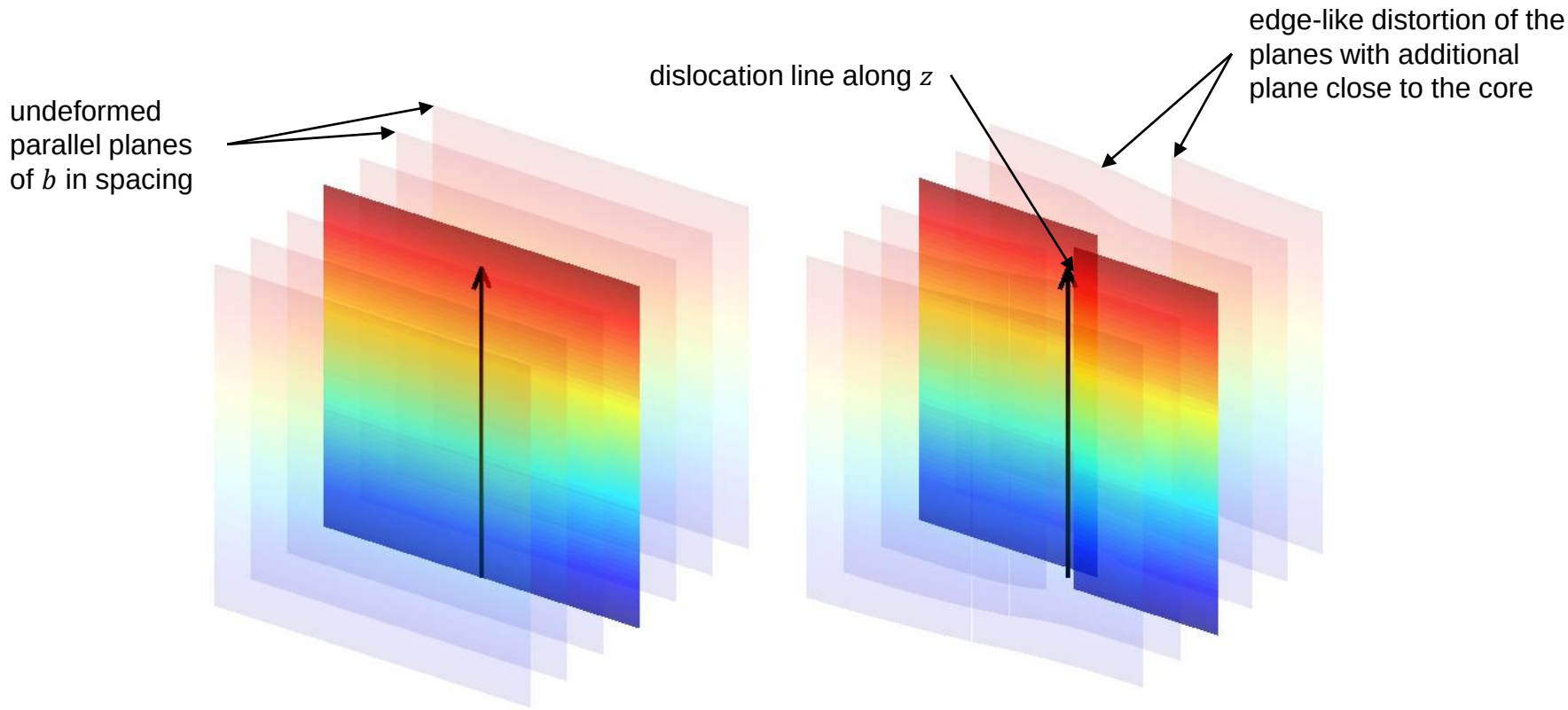
$$\sigma_{zz} = \nu\,(\sigma_{rr} + \sigma_{\theta\theta}) = \frac{G\ b\ \nu \sin\theta}{\pi \cdot (1-\nu) \cdot r}$$

$$\sigma_{rz} = \sigma_{\theta z} = 0$$

P. Hirth, J. Lothe: “Theory of Dislocations”, Malabar, USA: Krieger Publishing Company (1982, reprint 1992)

Stress Fields of Straight Dislocations

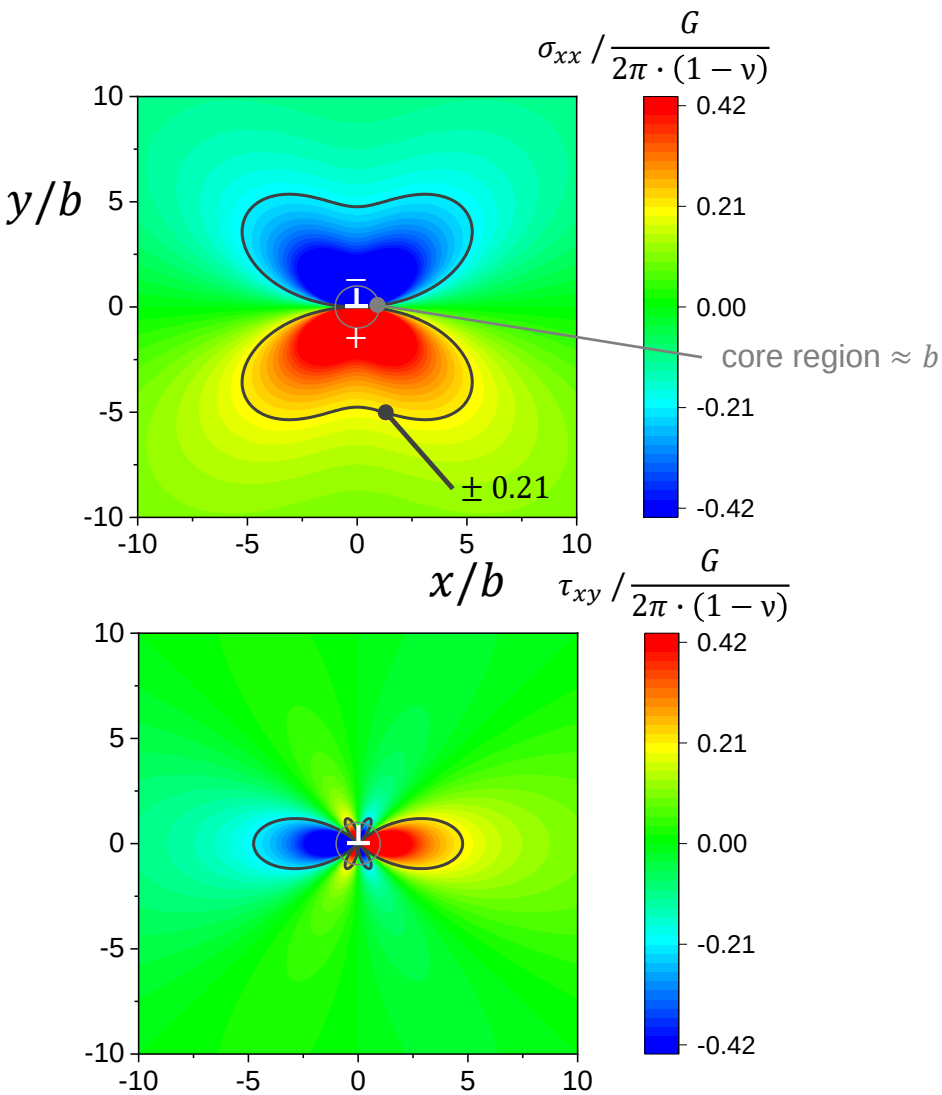
- Edge dislocation with dislocation line along z and Burgers vector along x:

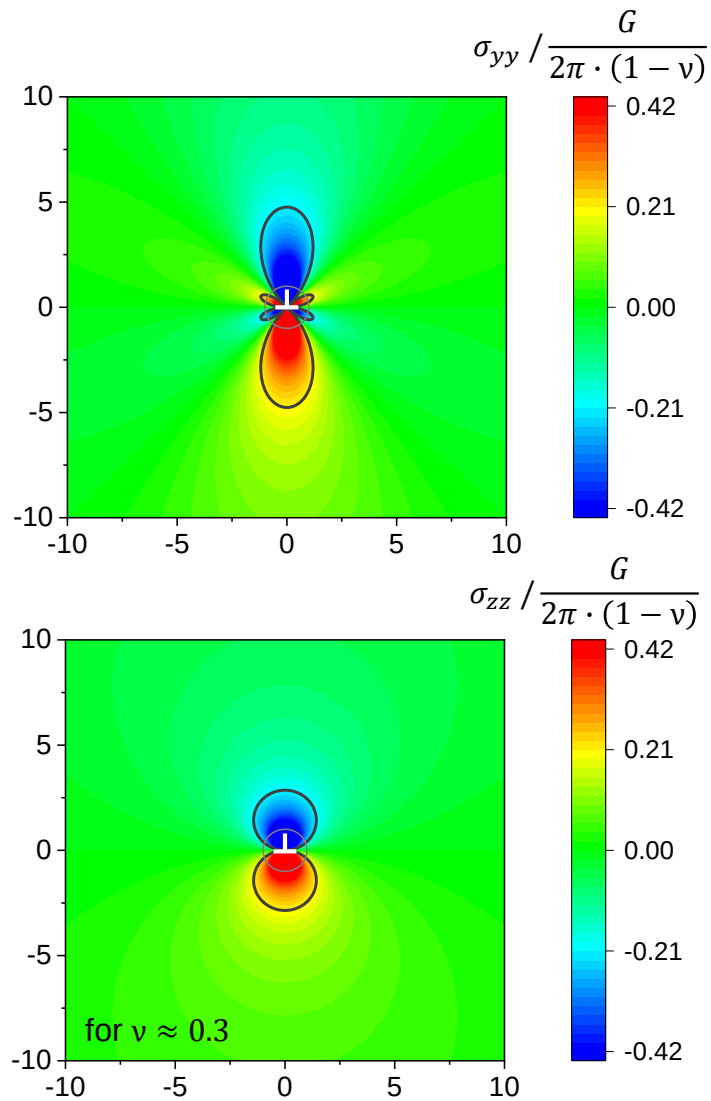


$$u_x = \frac{b}{2\pi}\left(\tan^{-1}(y,x) + \frac{xy}{2\,(1-\nu)(x^2+y^2)}\right),$$

$$u_y = -\frac{b}{8\pi\,(1-\nu)}\left((1-2\nu)\ln(x^2+y^2) + \frac{x^2-y^2}{x^2+y^2}\right)$$

Stress Fields of Straight Dislocations





$0.21 \frac{G}{2\pi \cdot (1-\nu)}$ is in the order of 1.2 GPa for Cu!

Stress Fields of Straight Dislocations

- The stress fields of **general dislocations** are obtained by **linear superposition**.
- The stress fields can be used to **determine the interactions of dislocations and other defects** being itself associated with stress fields.
- In case of **dislocation-dislocation interactions**, we will utilize the **stress field in conjunction with Peach-Köhler force** to calculate the interaction force between parallel dislocations.
- In the case of **solute-dislocation interactions**, the dominant part of the interaction stems from **hydrostatic distortion of the lattice by solute atoms and the pressure associated with it** (generally valid for substitutional solutes in most metallic materials due to symmetric coordination and interstitials in Cu-type metals; not valid for interstitials in W-type metals): $p = -{}^{1}/_{3}\left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right)$.
- It is possible (not done here since very lengthy) to show that **external forces do *not* alter the stress fields**.

Stress Fields of Straight Dislocations

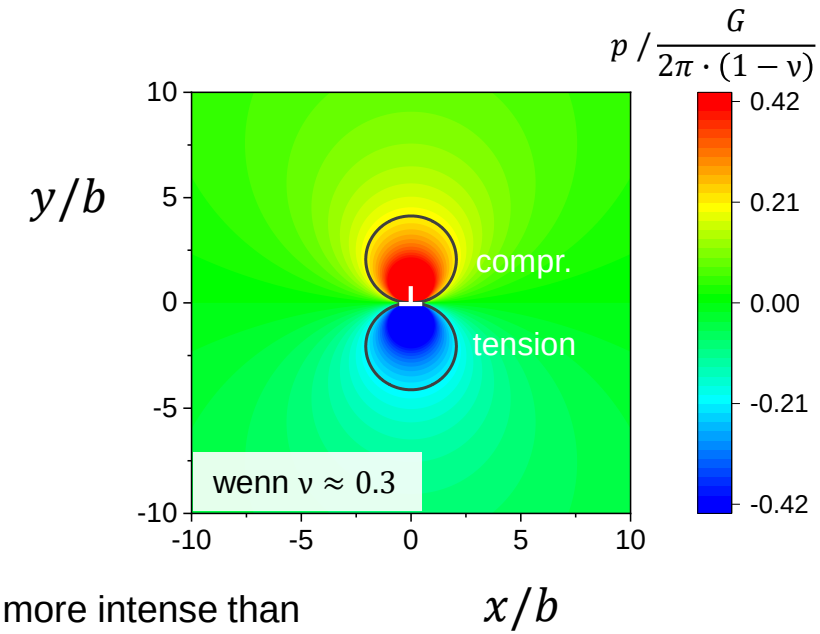
- Hydrostatic contribution: $p = -{}^{1}/_{3}\left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right)$

  $p > 0$ is compression and $p < 0$ hydrostatic tension load

screw

$p = 0$

edge



$0.21 \frac{G}{2\pi \cdot (1-\nu)}$ is in the order of 1.2 GPa for Cu!

The interaction of edge dislocations with solutes is more intense than the interactions of screw dislocations. Solutes with deviatoric stress fields can interact with both types of dislocations.

Line Energy by Elastic Distortion

- The elastic distortion needs certain work/energy which can be obtained by integration over the distorted volume:

$$\frac{W_\odot}{L} = \int_{r_0}^{R} \frac{{\sigma_{\theta z}}^2}{2G}\, 2\pi r\, dr = \frac{G\, b^2}{4\pi} \ln \frac{R}{r_0}$$

$$\frac{W_\perp}{L} = \int_{r_0}^{R} r\, dr \int_0^{2\pi} d\theta \left(\frac{1}{2G} {\tau_{xy}}^2 + \frac{1}{2E} \left({\sigma_{xx}}^2 + {\sigma_{yy}}^2 - 2\nu\, \sigma_{xx}\sigma_{yy} - {\sigma_{zz}}^2 \right) \right)$$

$$= \frac{G\, b^2}{4\pi \cdot (1-\nu)} \ln \frac{R}{r_0} = \frac{1}{1-\nu} \frac{W_\odot}{L}$$

- **Both solutions diverge** for $r_0 \to 0$ and $R \to \infty$. The dislocation has, therefore, only under certain circumstances a finite energy in terms of linear elastic theory. The cut-offs are typically set by physically relevant bounds: $R \propto l/2$ for the average distance between the dislocation and $r_0 \propto b$ as the typical size of the core of a dislocation:
  - Note the considerations from Ch. 4a: $\tau_c \approx \frac{G}{2\pi}$
  - For the screw dislocation, cut-off of the stress field might be determined by $\sigma_{\theta z}|_{r_0} = \tau_c$ with $r_0 \approx b$.
  - For the edge dislocation, cut-off of the stress field might be determined by $\sigma_{r\theta}|_{r_0,\theta=0} = \tau_c$ with $r_0 \approx \frac{b}{1-\nu} \approx 1.5b$.
  - The upper limit for estimates is typically set at $4b$ since the solutions from the present Chapter need to be corrected for the cut-off.

Line Energy by Elastic Distortion

- The core energy is in the order of **0.05 ... 0.2** Gb^2 (various approaches needed; lower bound in closed placked metals, upper bound in ionic crystals). This corresponds to $2 \ \ldots \ 10\ \mathrm{eV/nm}$ (keep in mind approx. 1/40 eV of thermal energy $k_B T$ at room temperature):

$$G \approx 50\ \mathrm{GPa},\ b \approx 2.5\ \text{Å}:$$
$$0.1\ Gb^2 \approx 1.5\ \mathrm{nJ/m} \approx 2\ \mathrm{eV/nm}$$

- This is much smaller compared to the line energy by the elastic distortion which is in the order of **several** $10\ \mathrm{eV/nm}$:

$$G \approx 50\ \mathrm{GPa},\ b \approx 2.5\ \text{Å},\ \mathrm{R} \approx 500\ \mu\mathrm{m},\ r_0 \approx b,\ \nu \approx 0.3:$$
$$\frac{Gb^2}{4\pi \cdot (1-\nu)} \ln \frac{R}{r_0} \approx 5.2\ \mathrm{nJ/m} \approx 32\ \mathrm{eV/nm}$$

- Anyhow, the energy of the core changes periodically (due to the discrete, periodic nature of the crystal) with the position of the dislocation line; this is not the case for the elastic energy. Even though being smaller in magnitude, the periodic change of the core energy is the reason for the appearance of the **Peierls potential (later in this Chapter)**.

Line Energy by Elastic Distortion

- For the further course of the lecture, we roughly sum up in the following way:

$$\frac{W_\perp}{L} = \frac{1}{1-\nu}\frac{W_\odot}{L} \approx \frac{4}{3}\frac{W_\odot}{L}$$

- Glissile (mixed) dislocation loops, therefore, have an oval shape (remember: always draw the arrow of the Burgers vector in the exam first and then the oval around it). The screw portions are typically of larger length in comparison to other segments. Even when anisotropy of the crystal structure and elastic constants are considered.

- A significant energy reduction occurs when short Burgers vectors can be established (dislocation dissociation, dislocation reactions, etc.):

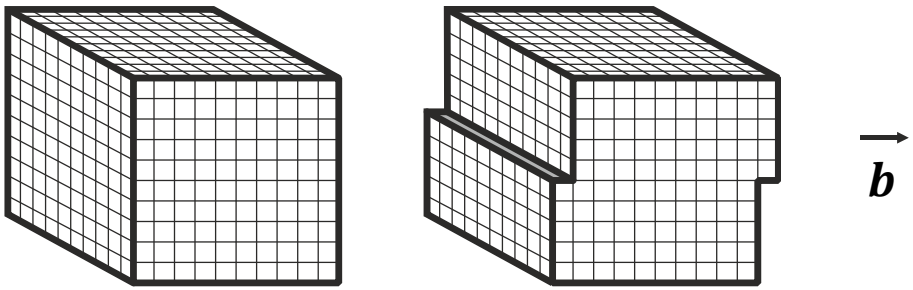
$$\frac{W}{L} \propto Gb^2$$

Forces Acting on Dislocations

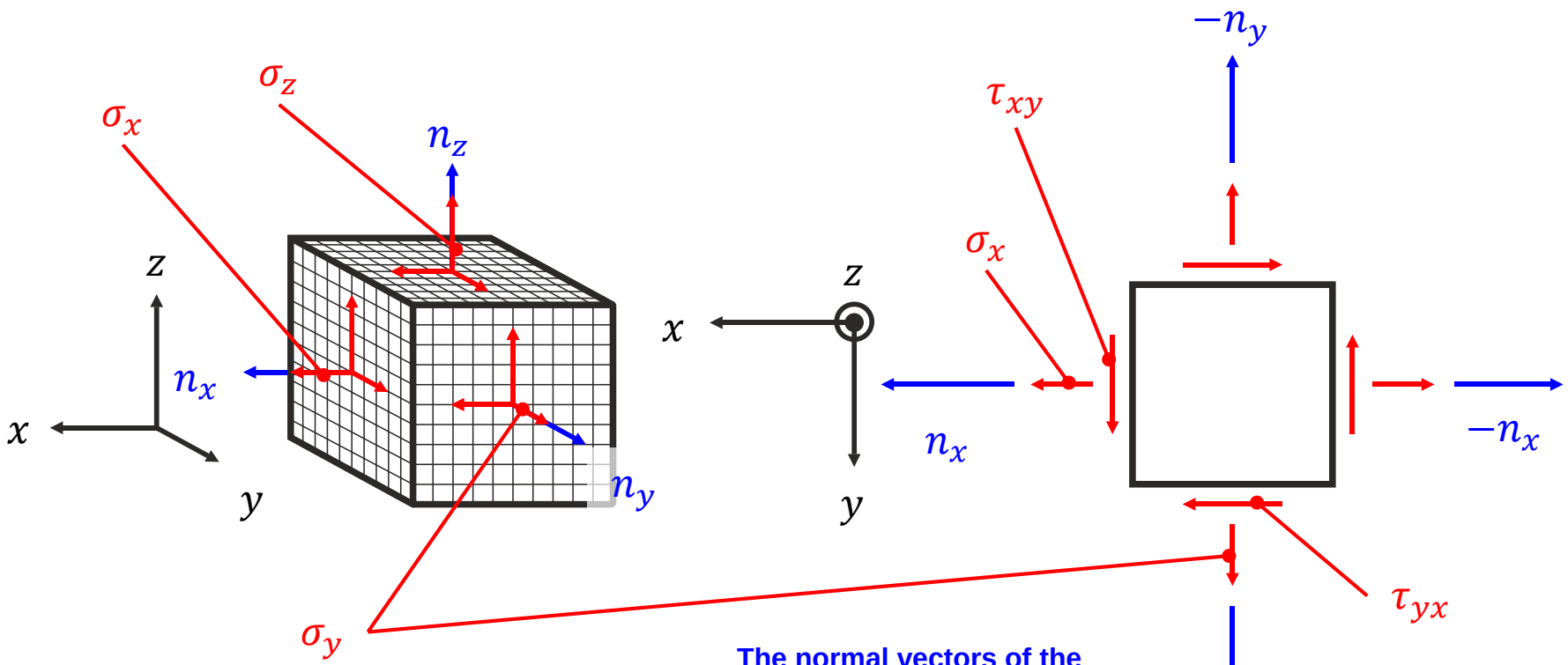
- In general, dislocations are „just“ displacement fields. These are no physical objects in the classical sense, a force can be applied to.
- However, as we have seen there is work associated with the application of the slip operation to the body. This work is independent of the actual type of the dislocation since the slip operation is the same for the screw, edge or mixed dislocation as we have seen in the introduction slides.
- From the work done on the body, can be transformed into a virtual force acting on the dislocation line:

$$\boldsymbol{F}/_{L} = (\boldsymbol{b} \cdot \boldsymbol{\sigma}) \times \boldsymbol{s}$$

(Peach-Köhler force)



Reference Frame



The normal vectors of the surfaces point out of the solid. The direction of the acting force automatically follows from the equation on the slide before.

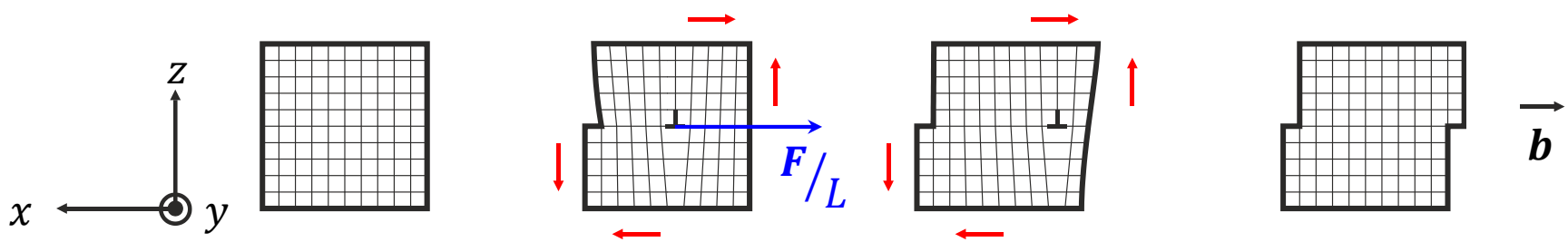
Forces Acting on Dislocations

- Forces on the dislocation lines of initial examples (Ch. 4a):

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & -\tau \\ 0 & 0 & 0 \\ -\tau & 0 & 0 \end{pmatrix}, \boldsymbol{F}/_L = \begin{pmatrix} -b\,\tau \\ 0 \\ 0 \end{pmatrix}$$

$$\boldsymbol{b} \cdot \boldsymbol{\sigma} = \begin{pmatrix} 0 \\ 0 \\ b\,\tau \end{pmatrix}$$

initial state | mechanical loading under shear stress | one full slip process

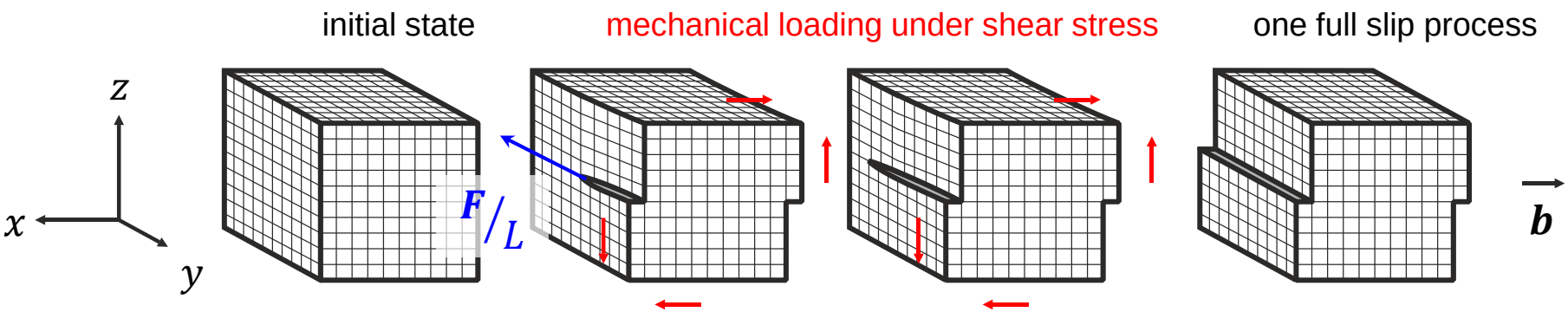


Forces Acting on Dislocations

- Forces on the dislocation lines of initial examples (Ch. 4a):

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s} = \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & -\tau \\ 0 & 0 & 0 \\ -\tau & 0 & 0 \end{pmatrix}, \boldsymbol{F}/_L = \begin{pmatrix} 0 \\ -b\,\tau \\ 0 \end{pmatrix}$$

$$\boldsymbol{b} \cdot \boldsymbol{\sigma} = \begin{pmatrix} 0 \\ 0 \\ b\,\tau \end{pmatrix}$$



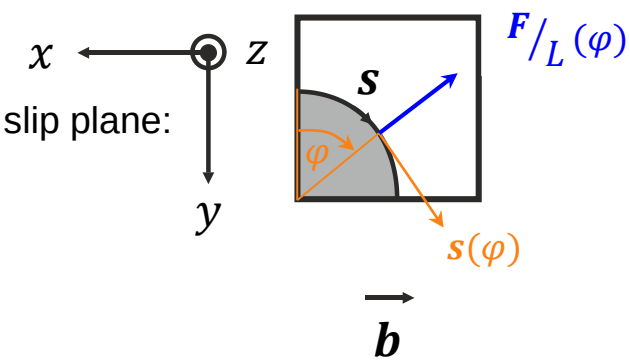
Forces Acting on Dislocations

- Forces on the dislocation lines of initial examples (Ch. 4a):

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s} = \begin{pmatrix} -\cos\varphi \\ \sin\varphi \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & -\tau \\ 0 & 0 & 0 \\ -\tau & 0 & 0 \end{pmatrix}, \boldsymbol{F}/_L = \begin{pmatrix} -b\,\tau\sin\varphi \\ -b\,\tau\cos\varphi \\ 0 \end{pmatrix}$$

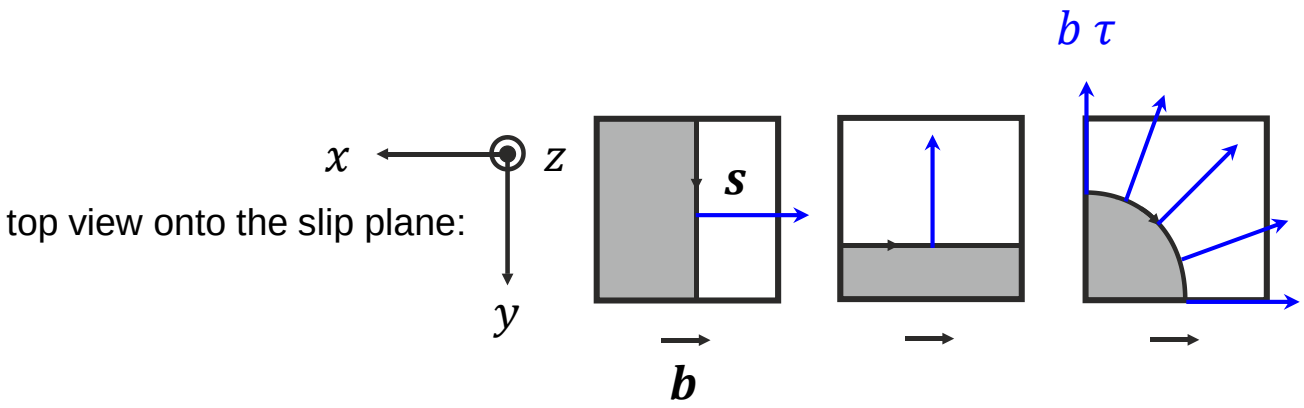
$$\boldsymbol{b} \cdot \boldsymbol{\sigma} = \begin{pmatrix} 0 \\ 0 \\ b\,\tau \end{pmatrix}$$

top view onto the slip plane:



Forces Acting on Dislocations

- As known from the introduction slides, shear stress within the slip plane and along the slip direction leads to glide motion of the dislocation. The virtual glide (line) force on the dislocation line is $b\,\tau$. The magnitude of the glide force only depends on the shear stress within the slip system. It is independent of the character of the dislocation (since the same deformation is performed)!

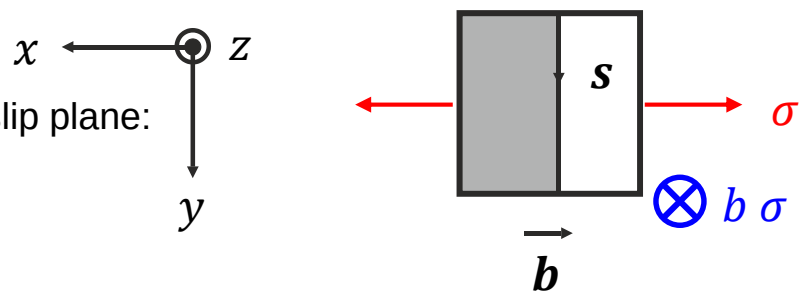


Forces Acting on Dislocations

- Normal loading of the edge dislocation (σ along x) leads to a climb (line) force of $b\,\sigma$ along z:

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} \sigma & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \boldsymbol{F}/_L = \begin{pmatrix} 0 \\ 0 \\ -b\,\sigma \end{pmatrix}$$

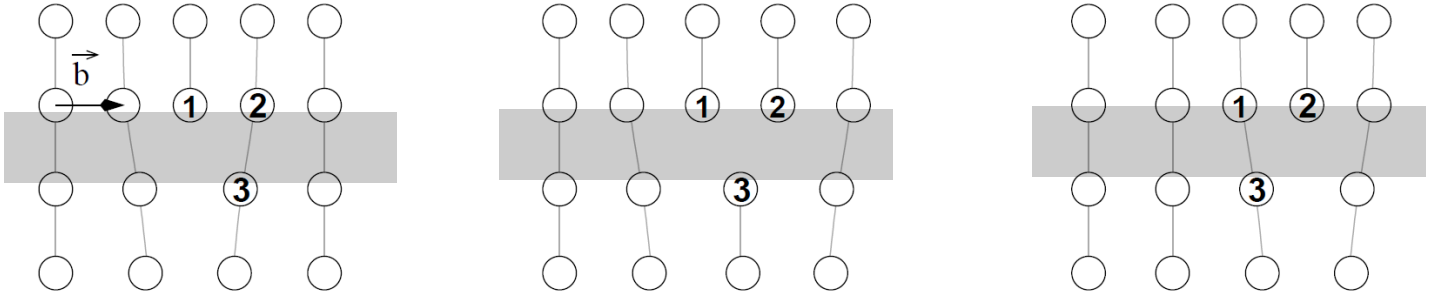
top view onto the slip plane:



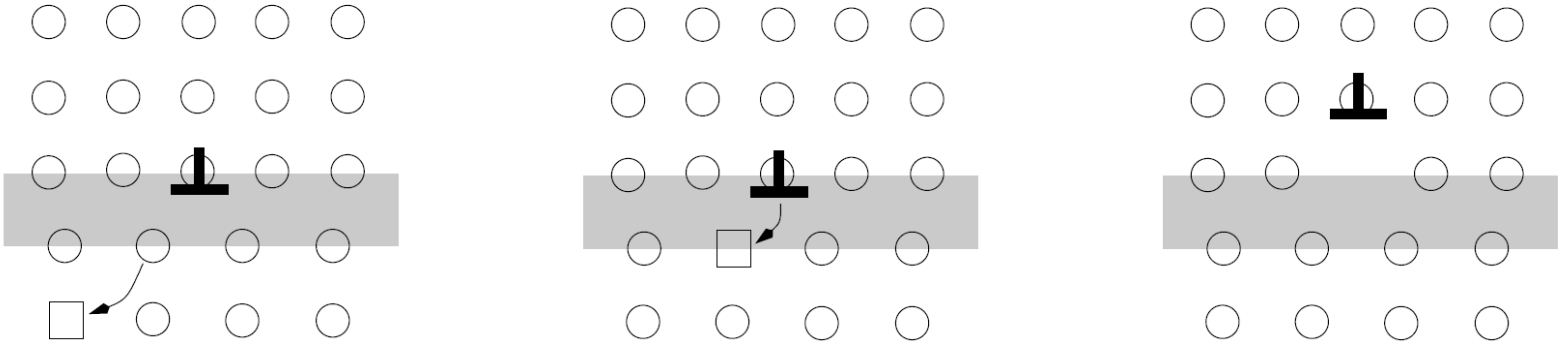
In order to achieve the elongation of the sample along the normal load, atoms have to diffuse from the surfaces of the body to the extra half-plane in order to enlarge this extra half-plane.

Dislocation Motion

- **Glide, slip** — **motion ↔**



- **Climb** — **motion ↕**



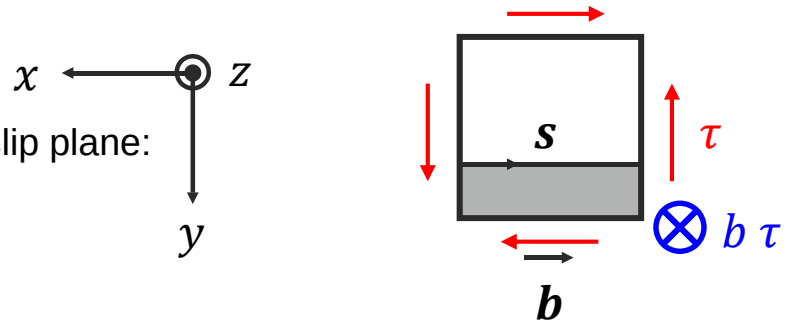
J. Freudenberger and L. Schultz: „Physikalische Werkstoffeigenschaften“ (2004)
https://www.ifw-dresden.de/ifw-institutes/ikm/lectures/vorlesungsskript-physikalische-werkstoffeigenschaften

Forces Acting on Dislocations

- Shear load of a screw dislocation in a slip plane other than the current slip might induce a change of the slip plane by cross-slip; the cross-slip (line) force amounts to $b\,\tau$:

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s} = \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} 0 & \tau & 0 \\ \tau & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \boldsymbol{F}/_L = \begin{pmatrix} 0 \\ 0 \\ -b\,\tau \end{pmatrix}$$

top view onto the slip plane:

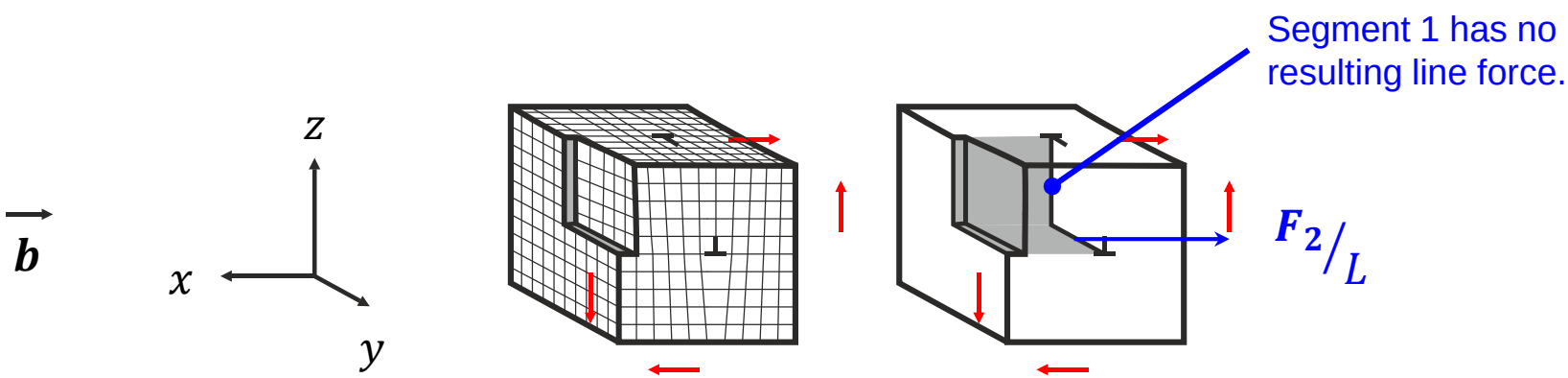


Forces Acting on Dislocations

- The following dislocation with Burgers vector along x is subdivided in two segments: (1) within x-z and (2) within x-y:

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s_1} = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \boldsymbol{s_2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & -\tau \\ 0 & 0 & 0 \\ -\tau & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{F_1}/_L = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \text{ und } \boldsymbol{F_2}/_L = \begin{pmatrix} -b\,\tau \\ 0 \\ 0 \end{pmatrix}$$



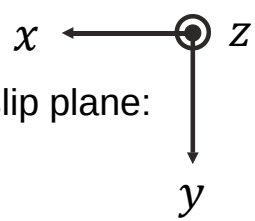
Forces Acting on Dislocations

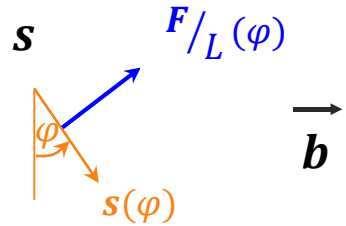
- The following dislocation with Burgers vector along x is subdivided in two segments: (1) within x-z and (2) within x-y:

$$\boldsymbol{b} = \begin{pmatrix} -b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{s}_2 = \begin{pmatrix} -\sin\varphi \\ \cos\varphi \\ 0 \end{pmatrix}, \boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & -\tau \\ 0 & 0 & 0 \\ -\tau & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{F}_2/_L = \begin{pmatrix} -b\,\tau\cos\varphi \\ -b\,\tau\sin\varphi \\ 0 \end{pmatrix}$$

top view onto the slip plane:

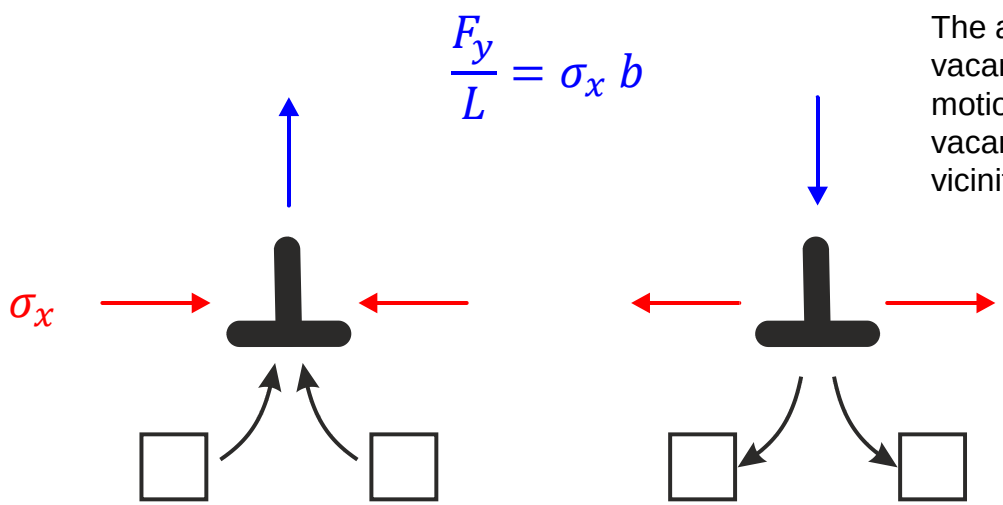




Since there is no force on segment 1, segment 2 starts to rotate around the segment 1 (pole). By every revolution, one slip operation is applied the body. By continuous rotation of the second dislocation segments, a displacement of the upper half of the crystal against the lower one of several Burgers vectors in length can be achieved with just one dislocation!

Chemical Force on Dislocations

- As we have seen, a proper external normal stress leads to a climb force on edge dislocations or on edge components of dislocations.
- Additionally, the climb process is non-conservative. The direction of movement, the Burgers vector and the dislocation line vector form a finite triple product. Hence, certain fluxes of atoms and vacancies are necessary to obtain the movement:



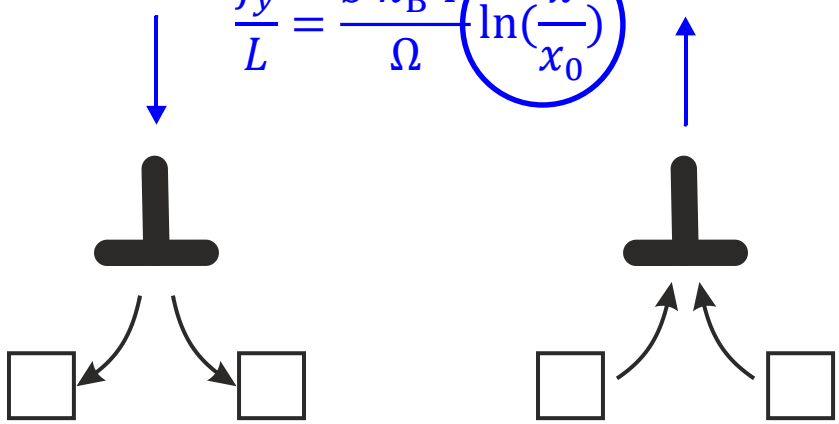
The absorption or emission of vacancies due to dislocation motion, reduces or increases the vacancy concentration in the vicinity of the dislocation!

Chemical Force on Dislocations

- In turn, this means that any vacancy concentration different from thermodynamic equilibrium leads to a climb force on the dislocation since it acts as vacancy source or sink:

This factor is intuitively underestimated! The quenched in vacancy concentration can be tremendous as we will see with the Bardeen-Herring source.

$$\frac{f_y}{L} = \frac{b\, k_\mathrm{B}\, T}{\Omega} \ln\left(\frac{x}{x_0}\right)$$



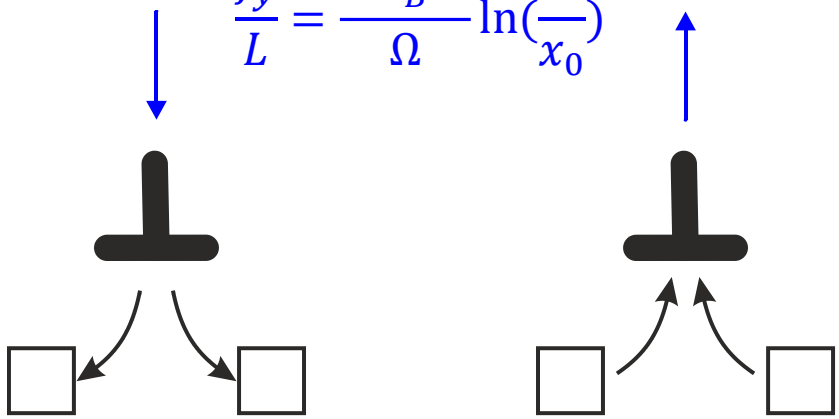
vacancy concentration away from the dislocation: $x < x_0$ $x > x_0$

using $x_0 = \exp\left(\frac{\Delta S_\mathrm{V}^\mathrm{P}}{k_\mathrm{B}}\right) \cdot \exp\left(-\frac{\Delta H_\mathrm{V}^\mathrm{F}}{k_\mathrm{B}\, T}\right)$ (see Ch. 3d) and $x = x_0\, e^{-\frac{F\Omega}{b\, k_\mathrm{B}\, T}}$ until F (Peach-Köhler) becomes compensated by f to achieve mechanical equilibrium.

Chemical Force on Dislocations

- The same principle can of course be transferred to solute atoms as well since solubility at the dislocation is altered by the distortion field. Hence, solute atoms cause forces on dislocations.

$$\frac{f_y}{L} = \frac{b\, k_B\, T}{\Omega} \ln\left(\frac{x}{x_0}\right)$$



vacancy concentration away from the dislocation: $x < x_0$ $x > x_0$

Line Tension

- We have seen that the total strain energy of a dislocation scales with $W \propto G\, b^2\, L$.
- If a straight dislocation gets longer by $\mathrm{d}L$, the total energy W increases. Hence, there is a back force restricting the extension of line length:

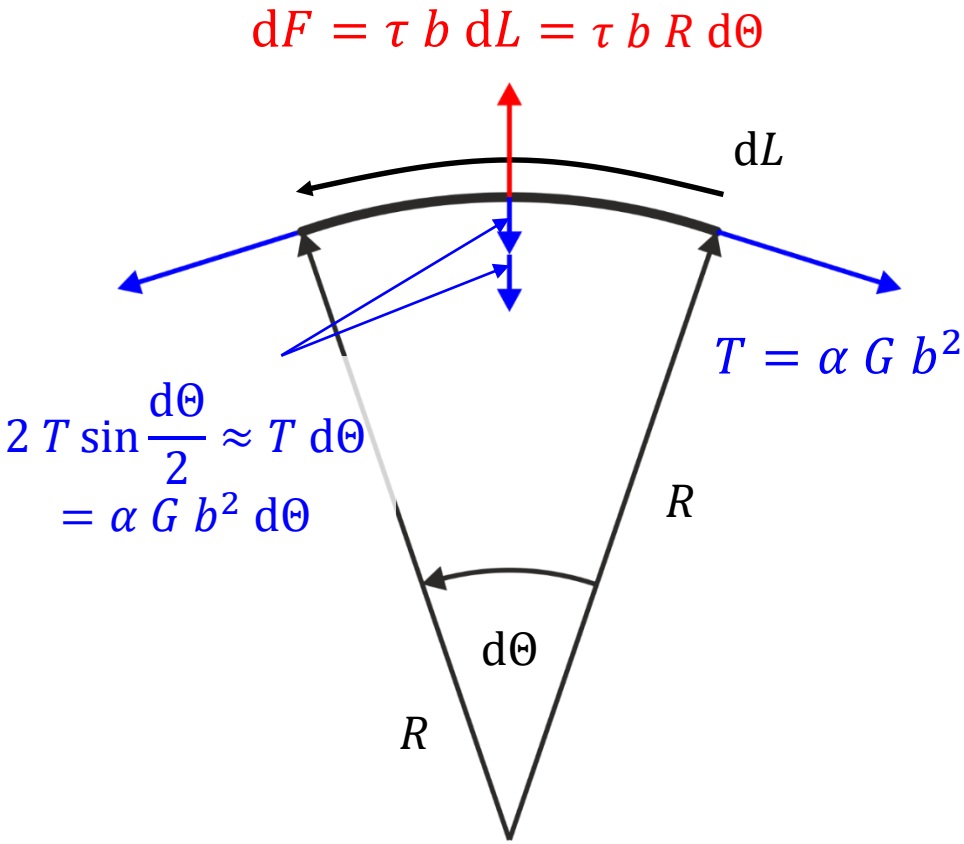
$$T = -\frac{\mathrm{d}W}{\mathrm{d}L} \propto G\, b^2$$

Line Tension

- Under external load τ, Peach-Köhler force may lead to bending of an incremental part $\mathrm{d}\Theta$ of the dislocation to a radius R.
- Assuming only glide forces, the Peach-Köhler force simplifies to $\mathrm{d}F = \alpha\,\tau\,b\,\mathrm{d}L$.
- Line tension $T\,\mathrm{d}\Theta = \alpha\,G\,b^2\,\mathrm{d}\Theta$ counteracts the bending processes.
- The shear stress needed to bend to a local *equilibrium* radius of R:

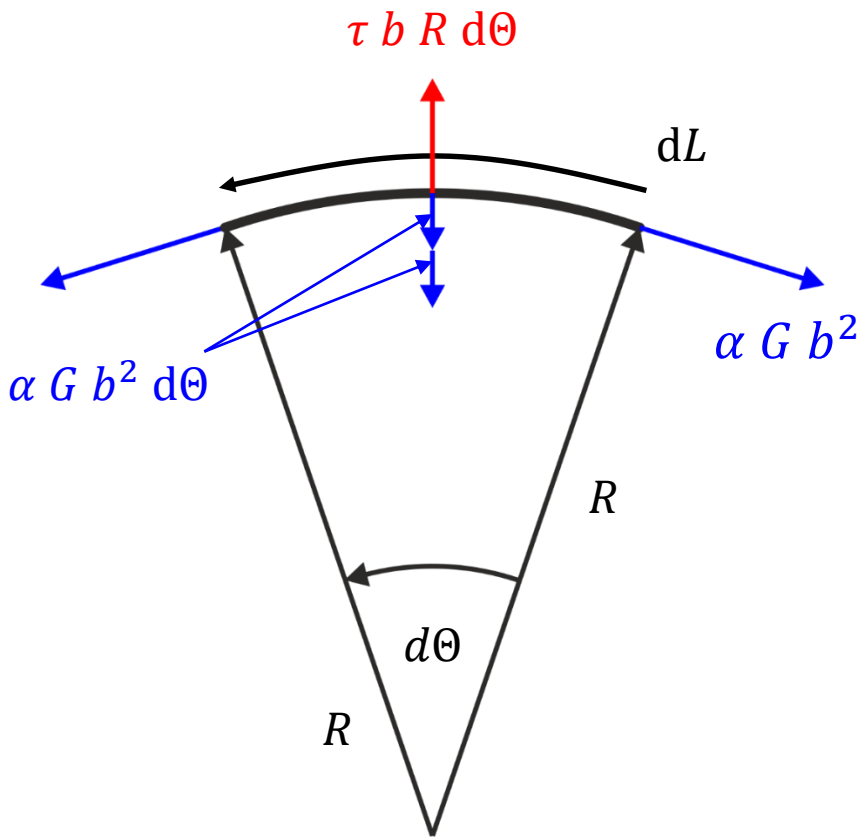
$$\tau\,b\,R\,\mathrm{d}\Theta = \alpha\,G\,b^2\,\mathrm{d}\Theta$$

$$\tau = \frac{\alpha\,G\,b}{R}$$



Line tension

- In order to achieve **high curvature** (= small radius of curvature R) in the dislocation line, **high stresses** are needed.
- **Below a critical curvature (above the equilibrium radius of curvature), the Peach-Köhler force leads to extension of the dislocation line because it surpasses the back stress by line tension.**



Line tension

- Of course, the major contribution arises from the length dependence of total energy of the dislocation. This gives rise to the line tension $T = -\frac{dW}{dL} \propto G\, b^2$ as shown on the slides before. Anyhow, the concept differs significantly from lines as known from mechanical engineering due to the following aspects:
  - The line energy depends on the character of the dislocation β, e.g. $W = W(\beta)$ with much lower line energy for screw over edge dislocation segments. During bending of the dislocation line, the character changes along the line length $\mathrm{d}L$. **There should be a strong tendency to preferably form screw segments. E.g. the line tension T of a screw segment is approx. 4 times larger than for edge segments at a Poisson's ratio of ~ 0.3.**
  - Dislocation segments interact with each other! The interaction of the individual segments is usually not considered at all.

Summary

- The **energy of a dislocation** has contributions **by** the **dislocation core** and by the **elastic displacement field**. The latter **scales with** the **stiffness** and the **square of the length of the Burgers vector**.
- **External stresses lead to virtual forces on the dislocation lines.** The stresses can lead to **glide/slip**, **climb**, **cross-slip** or **rotation motion** of dislocations.