Plasticity

Lecture for "Mechanical Engineering" and "Materials Science and Engineering"
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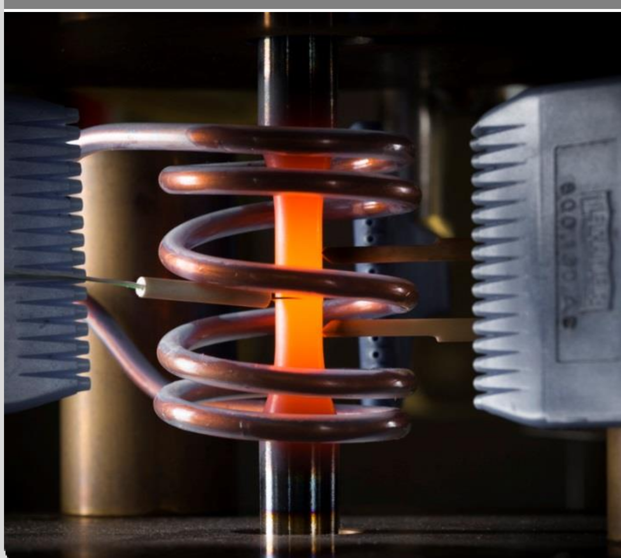
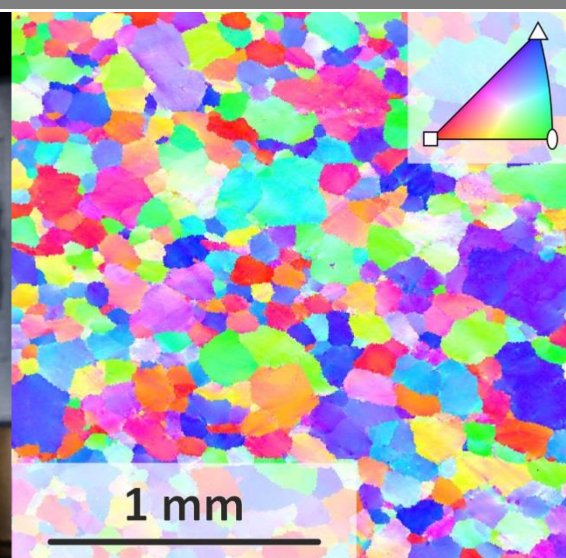
Institute for Applied Materials (IAM-WK)

Topics

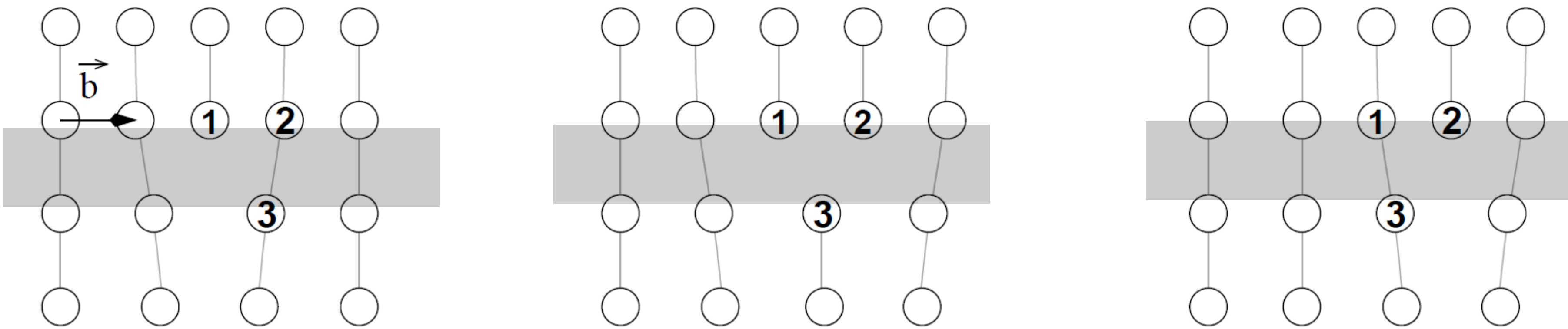
- Movement of dislocations
  - Peierls Potential
  - Peierls-Nabarro Equation
  - Velocity of Dislocations
  - Considerations on High-Speed Motion

Peierls Potential

- Without external load, **dislocations are in mechanical equilibrium with local minimum potential energy**.
- Due to the **periodicity of the crystal**, **similar situations of minimum potential energy are achieved at periodic distances**. The **movement of a dislocation line requests overcoming the energy barrier** between the local minima.
- **External mechanical load can provide sufficient work to overcome the barrier. At finite temperature, overcoming the barrier is assisted by thermal fluctuation.**
- Without external load, thermal fluctuations don’t lead to a net motion of the dislocation line but a constant swapping of the dislocation line between adjacent minima.
- The **periodic potential** the dislocation is experienced to is called **Peierls potential**.

Peierls Potential

glide ↔



relaxed situation
(low energy)

as obtained without
external stress

transition state
(high energy)

only obtained by applying
an external stress
or
by thermal fluctuation
or both

relaxed situation
(low energy)

as obtained without
external stress

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

Peierls Potential

- Note that **between two relaxed, low energy configurations** of the dislocation, **exactly one Burgers vector displacement** of the dislocation is obtained. The Peierls potential exhibits a periodicity of $\boldsymbol{b}$.
- From mathematical point of view, two approximations might be performed:
  - The **displacement field of a dislocation** (for example Ch. 4c) **is assumed constant** during its motion. This problem can be solved analytically, as done by Peierls (with the later correction by Nabarro) for example.
  - The other, more realistic option is to obtain the relaxed configuration of the moving dislocation at all positions even under applied stress. This can only be done numerically.

Peierls-Nabarro Equation

- The analytical treatment of Peierls is based on the treatment of Frenkel (see Ch. 4a, interaction of two complete half crystals) but considering the atoms immediately above and below the slip plane in a crystal containing a dislocation.
- The Peierls equation is obtained by:
  - Assuming a dislocation moving in x direction. Above the slip plane, atoms at x' are displaced by $u(x')$ against the atoms below the slip plane. The Burgers vector must be distributed along x' with small portions of $\frac{\mathrm{d}u}{\mathrm{d}x'}\mathrm{d}x'$ that integrate to $u(x' \rightarrow -\infty) = b$ and $u(x' \rightarrow +\infty) = 0$.
  - The shear stress introduced by such dislocations of strength $\frac{\mathrm{d}u}{\mathrm{d}x'}\mathrm{d}x'$ is (obtained using τ_{xy} for an edge dislocation in Ch. 4c with $b = \frac{\mathrm{d}u}{\mathrm{d}x'}\mathrm{d}x'$ and $x = x', y = 0$):
$$\tau_{xy} = \frac{G}{\pi(1-\nu)} \frac{\mathrm{d}u}{\mathrm{d}x'} \frac{\mathrm{d}x'}{x - x'}$$
  - This needs to be equilibrated by the stress across the planes separating the upper and the lower half crystal as obtained from the Frenkel model:
$$\tau_{xy} = \frac{G\,b}{2\pi\,d} \sin\frac{2\pi\,u}{b}$$
  - d denotes the distance between the atoms above and below the slip plane.
  - The equilibrium is obtained by the following conditions (Peierls equation):
$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}u}{\mathrm{d}x'} \frac{\mathrm{d}x'}{x - x'} = \frac{(1-\nu)b}{2h} \sin\frac{2\pi\,u}{b}$$

F.R.N. Nabarro: “Fifty-year study of the Peierls-Nabarro stress”, Materials Science and Engineering A 234-236 (1997) 67-76

Peierls-Nabarro Equation

- The solution yields for a straight dislocation in a cubic crystal at $0\ \mathrm{K}$ exhibits a Peierls potential with following amplitude:

$$E_{\mathrm{PN}} = \frac{G\ b^2}{\pi(1-\nu)} e^{-\frac{2\pi\, w}{b}}$$

- The external stress needed to overcome the barrier is given by the maximum derivative of the Peierls potential:

$$\tau_{\mathrm{PN}} = \frac{2\pi}{b^2} E_{\mathrm{PN}} = \frac{2G}{1-\nu} e^{-\frac{2\pi\, w}{b}}$$

Peierls-Nabarro Equation

- The derivation requires a flat core of a single dislocation (**no spread out of the slip plane, no dissociation of the dislocation**):
  - w denotes the width of the dislocation (characteristic distance of fade out of the disregistry Δu by the dislocation).
  - The width w correlates with the lattice spacing of the lattice plane $w \approx \frac{d}{1-\nu}$ and $w \approx d$ for the edge and screw dislocation, respectively. In the simple cubic crystal: $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$.
  - b denotes the Burgers vector. In the simple cubic crystal $b = a$.

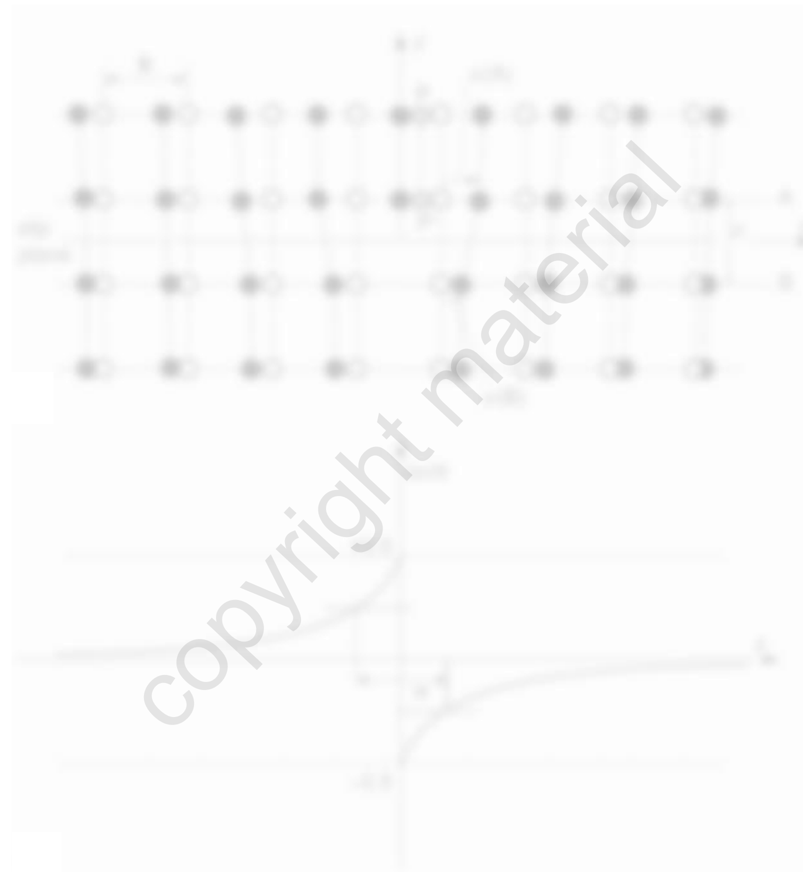


Illustration of the physical meaning of w for an edge dislocation: the displacement difference $\Delta u = u(\mathrm{A}) - u(\mathrm{B})$ describes the disregistry by the introduction of the dislocation.

D. Hull, D. J. Bacon: “Introduction to Dislocations”, Amsterdam, etc.: Elsevier (2011)

Peierls and Nabarro

- R. Peierls was a Jewish, German scientist significantly involved in the work on the newly introduced quantum mechanics together with the other German scientists back at the time: Sommerfeld, Heisenberg (PhD supervisor), Bloch, etc. During Hitler's rise to power, he spent time in Cambridge and decided not to come back to Germany. He stayed in Great Britain, e.g. Manchester, Cambridge, Birmingham and Oxford and became British citizen during World War Second.
- F.R.N. Nabarro was born in England and was appointed professor in Johannesburg in 1953. Based on work by Zener, he proposed the impact of grain boundaries to plastic deformation and, of course, made important contributions to the description of creep.

https://en.wikipedia.org/wiki/File:Sir_Rudolf_Ernst_Peierls.jpg
https://en.wikipedia.org/wiki/File:Frank_Nabarro00.jpg

Peierls-Nabarro Equation

- **The result is much smaller than the stress needed for the slip process of two half crystals**:

  $b \approx 2.5$ Å, $d \approx 2.1$ Å:

$$\tau_{\mathrm{PN}} = \frac{2G}{1-\nu} e^{-\frac{2\pi\, d}{b}} \approx 0.02\, G \ll \frac{G}{2\pi} = 0.16\, G$$

Peierls-Nabarro Equation

- **Low critical stresses** are achieved **on low indexed lattice planes in low indexed directions**.
- **Low indexed lattice planes exhibit high atomic packing factor.**
- Even though the derivation of the equation is limited, **these considerations turned out to be valid for many crystal structures**. The statement regarding low indexed lattice planes and directions remains also valid; just use the primitive unit cell of a structure.

Peierls-Nabarro Equation

- Based on the considerations by the Peierls-Nabarro equation, **screw dislocations exhibit a higher critical stress then edge dislocations**:

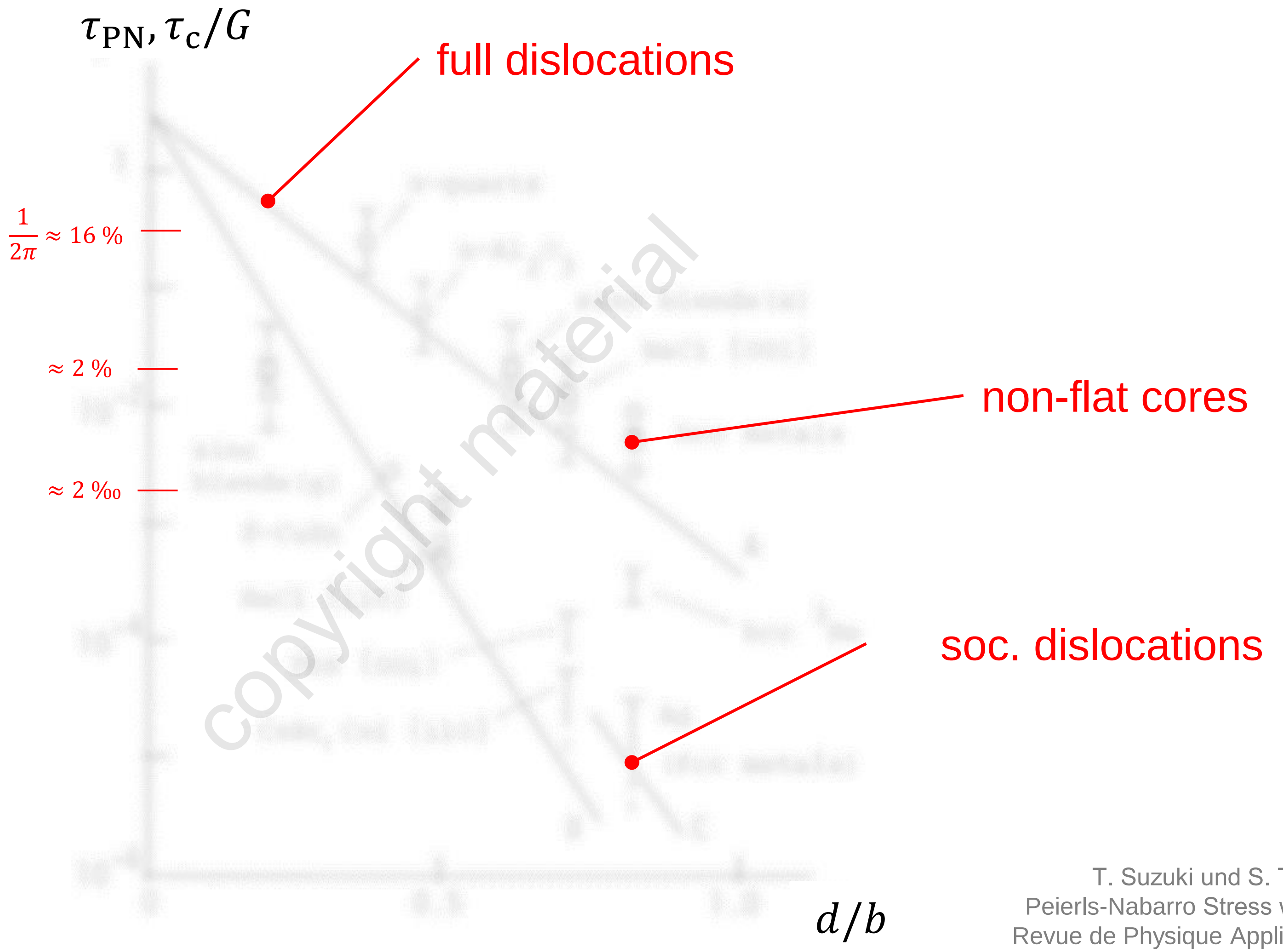
$b \approx 2.5\ \text{Å},\ d \approx 2.1\ \text{Å}$:

$$\tau_{PN} = \frac{2G}{1-\nu} e^{-\frac{2\pi \frac{d}{1-\nu}}{b}} \approx 0.002\ G < 0.02\ G$$

Peierls-Nabarro Equation

- Important discrepancies are found by:
  - **Extended core configurations** > A2 metals and alloys (bcc)
  - **Non-straight dislocations** > kink pair formation and propagation in A2 metals and alloys (bcc)
  - **Dissociation** (not in the direction of Burgers vector of the full dislocation) > A1 metals and alloys (fcc) and most intermetallic materials

Comparison with extrapolated yield strength



T. Suzuki und S. Takeuchi: “Correlation of Peierls-Nabarro Stress with Crystal Structure” in Revue de Physique Appliquee 23 (1988) 685-685

Dislocation Velocity

- The dislocation can move once the critical stress is applied.
- The velocity typically scales with the applied stress by a power law:

$$v \propto \left(\frac{\tau}{\tau_0}\right)^n$$

- n is usually large.

Velocity determination by pit etching in LiF before and after plastic deformation (no scale bar).

J. P. Hirth und J. Lothe: „Theory of dislocations“, Malabar: Krieger Publishing Company (1982)

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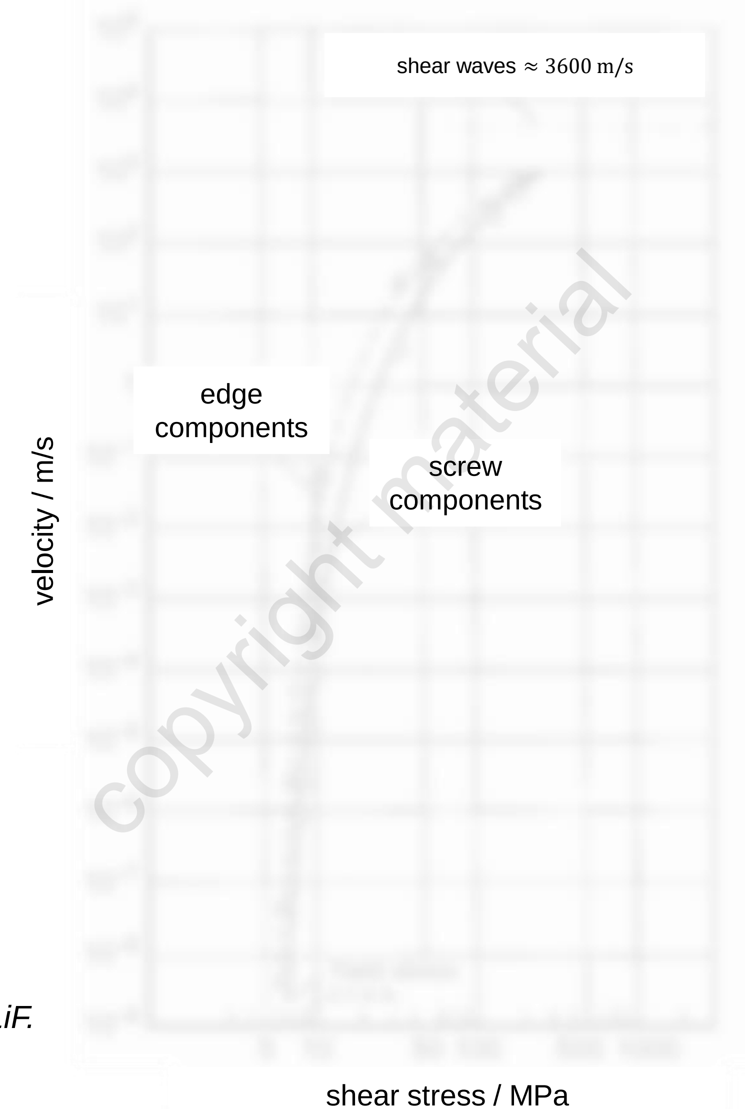

Dislocation velocity in LiF.

D. Hull, D. J. Bacon: “Introduction to Dislocations”, Amsterdam, etc.: Elsevier (2011)

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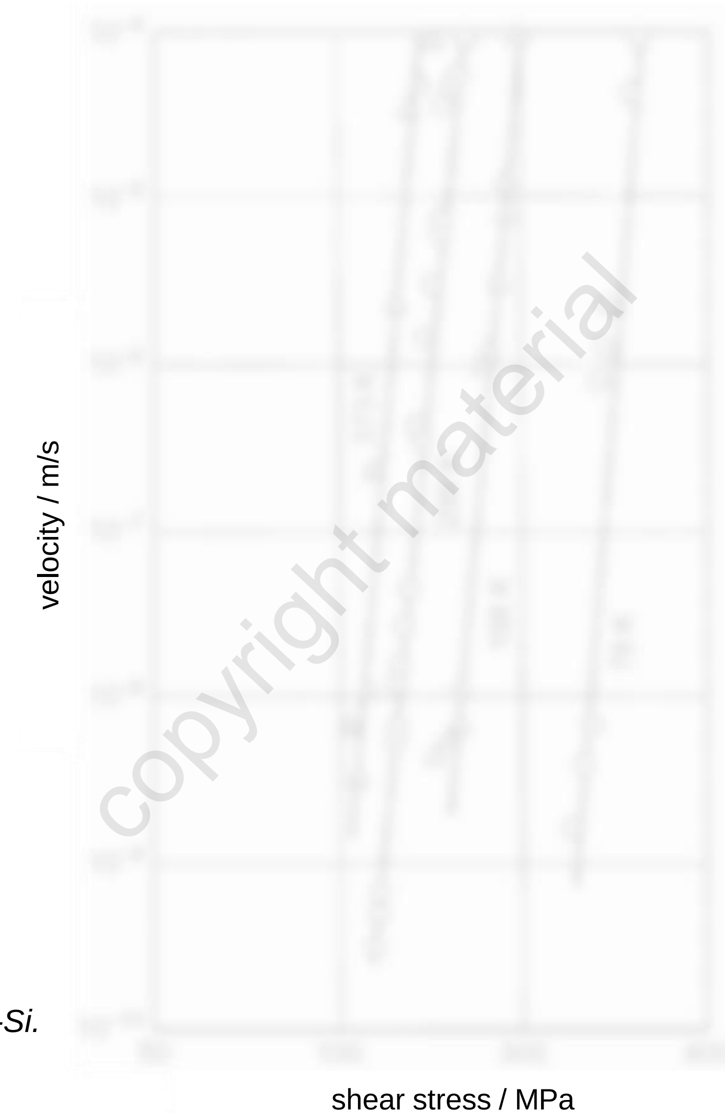


Dislocation velocity in Fe-Si.

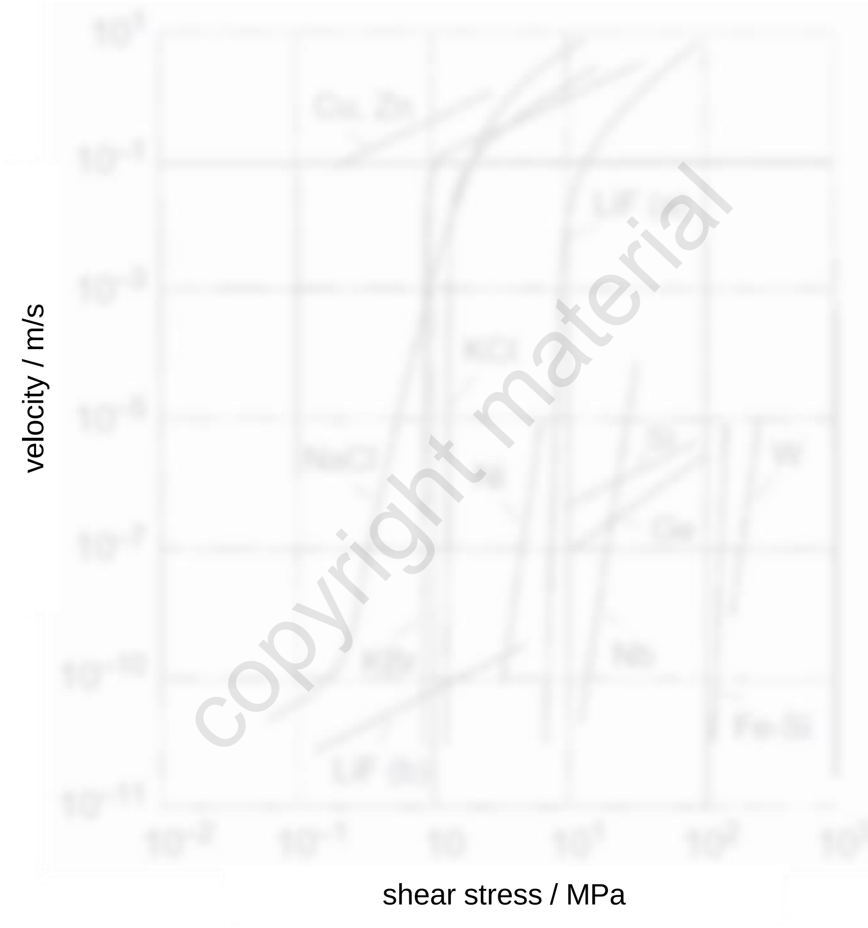
D. Hull, D. J. Bacon: “Introduction to Dislocations”, Amsterdam, etc.: Elsevier (2011)

Dislocation Velocity

- Slightly above on-set stress, the equation is usually used in the following form:

$$v \approx \frac{b}{B}\,\tau^m$$

- The velocity is in the order of $1\ \mathrm{m}/s$ at $m = 1$ in metals at room temperature and $m = 2 \dots 5$ in alloys. At low temperatures, $m = 4 \dots\ 12$ is found.
- Using a Newton equation of motion, this can be used to describe dislocation motion in dislocation dynamics simulations.
- B is typically dominated by phonon damping.



Comparison of various materials.

D. Hull, D. J. Bacon: “Introduction to Dislocations”, Amsterdam, etc.: Elsevier (2011)

High-Speed Motion

- When strain rate becomes very high, e.g. impact experiments or localized plastic deformation at crack tips, dislocations can be accelerated significantly.
- **Dislocations are displacement field moving through their own displacement field.**

High-Speed Motion

- Analogous to theory of relativity, there are special velocities observed for the motion of a dislocation as moving displacement field. **Different speeds depending on the type of the propagating wave need to be considered.**
- In solids, following speeds of propagating elastic waves are important in the following:
  - Shear/transverse waves with c_T
    (amplitude perpendicular to the propagation direction)
  - Pressure/longitudinal waves with $c_\mathrm{L} \approx 2\ c_\mathrm{T}$
    (volumetric density changes, amplitude in the propagation direction)
  - Rayleigh waves with $c_\mathrm{R} \approx 0.87 \ldots 0.95\ c_\mathrm{T}$
    (surface acoustic wave)

Stress Fields of Moving Dislocations

- For the moving dislocation, the equilibrium condition changes by the inertia term to:

$$\frac{\partial \sigma_{ik}}{\partial {x'}_k} - \rho \frac{\partial^2 u_i}{\partial t^2} = 0$$

- For a straight dislocation along z and a movement perpendicular to it in x direction (simple glide only), the following transform to a moving coordinate system simplifies the equation:

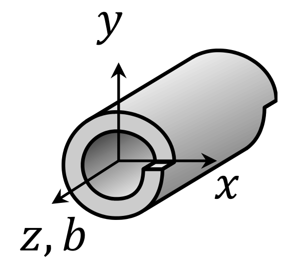
$$x = x' - v\,t$$
$$\partial/\partial x' = \partial/\partial x$$
$$\partial/\partial t = -v\,\partial/\partial x$$

- For the screw dislocation with $u_x = u_y = 0$, the differential equation $\left(1 - {}^{v^2}\!/_{c_\mathrm{T}^2}\right)\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} = 0$ with $c_\mathrm{T} = \sqrt{{}^{G}\!/_{\rho}}$ follows.

Stress Fields of 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. The is an additional (constant) shear stress necessary in order to avoid spinning of the arrangement.

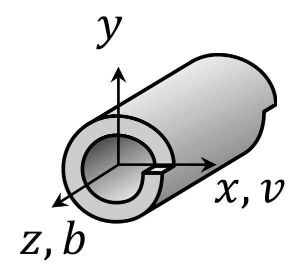
J. P. Hirth und J. Lothe: „Theory of dislocations“ (1982)

Remember Ch. 4c

Stress Fields of Moving Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$ and moving in x direction (glide):

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



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

J. Weertman und J. R. Weertman: „Moving dislocations“ in „Dislocations in Solids“ by F. R. N. Nabarro (Ed.), North-Holland Publ. Company, Amsterdam, New York, Oxford (1980)

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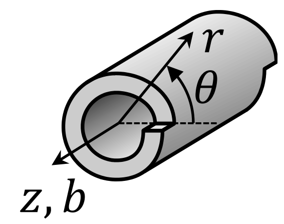
Stress Fields of Dislocations

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



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

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

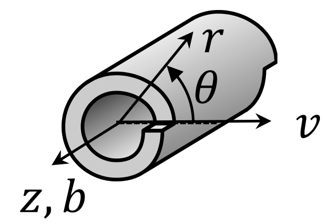
If you want to do it your own, you also have to convert the divergence to cylinder coordinates ${}^{\partial}/_{\partial x_i}\, \sigma_{ik} = 0$!

J. P. Hirth und J. Lothe: „Theory of dislocations“ (1982)

Remember Ch. 4c

Stress Fields of Moving Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$ and moving in x direction (glide):



$$\sigma_{\theta z} = \frac{G \cdot b \cdot \beta}{2\pi \cdot r \cdot (\cos^2 \theta + \beta^2 \sin^2 \theta)}$$

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

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

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Stress Fields of Dislocations

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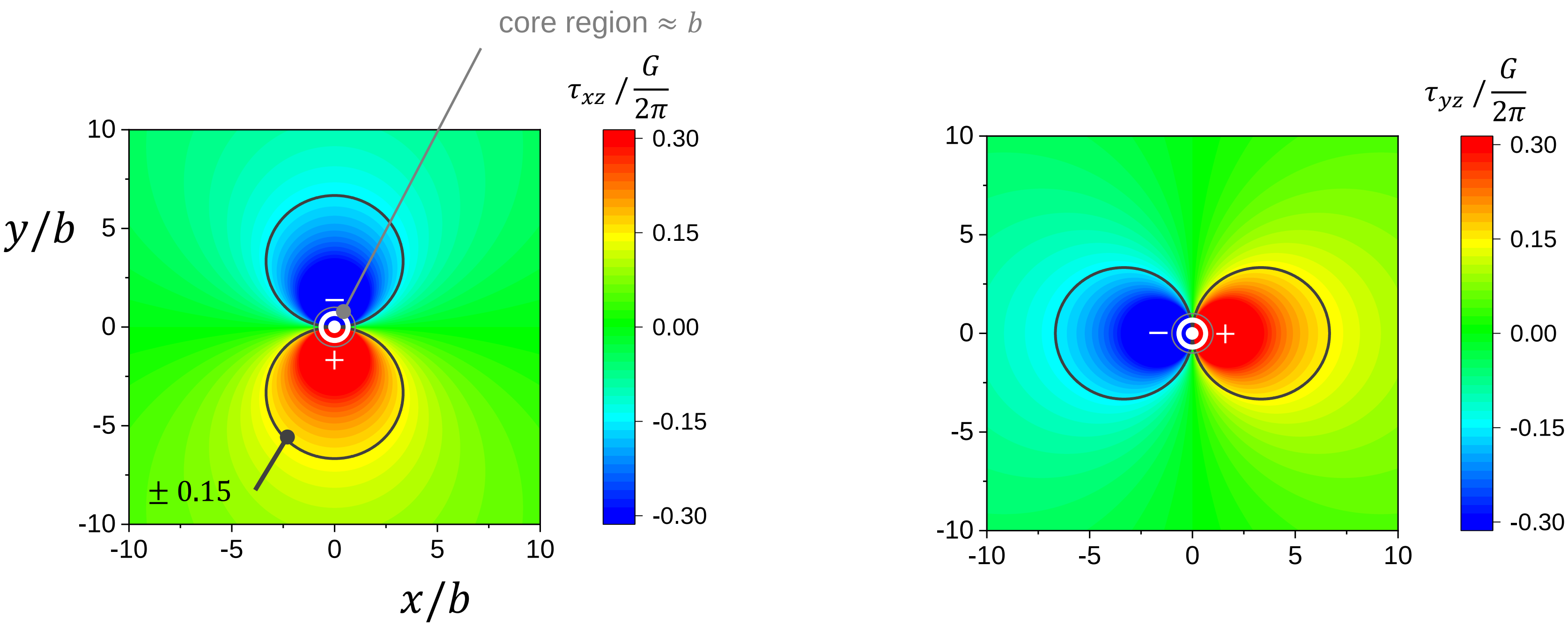
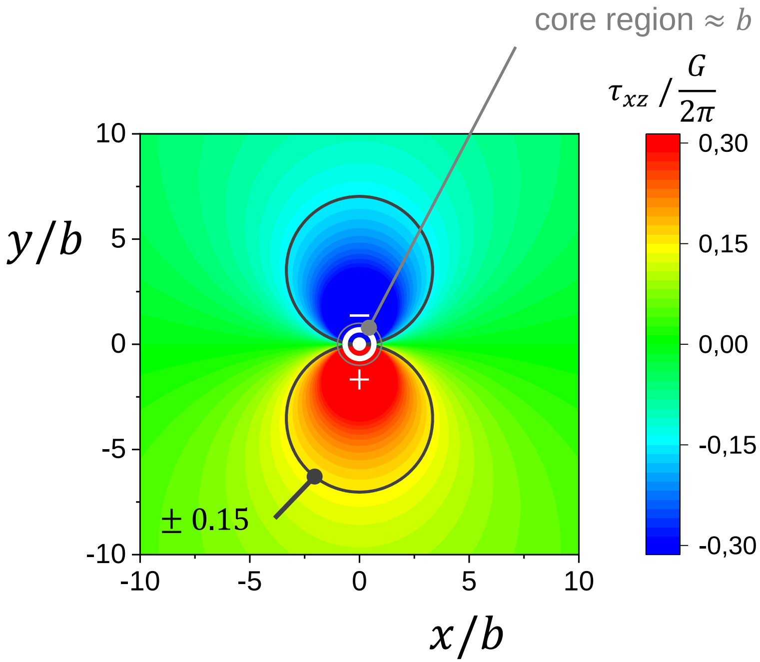


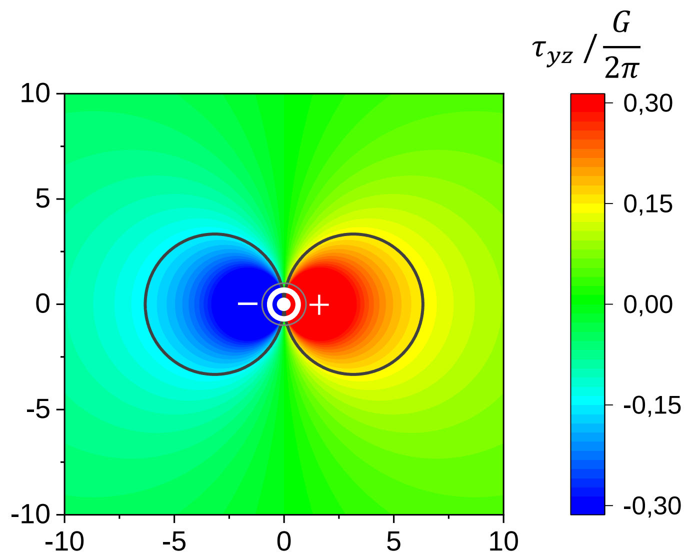
$$v = 0,\ 1 - {}^{v^2}/_{c_T^2} = 1$$

$0.15\ \frac{G}{2\pi}$ is in the order of $1.2\ \mathrm{GPa}$ for Cu. c_T is in the about $2300\ \mathrm{m/s}$.

Stress Fields of Moving Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$ and moving in x direction (glide):



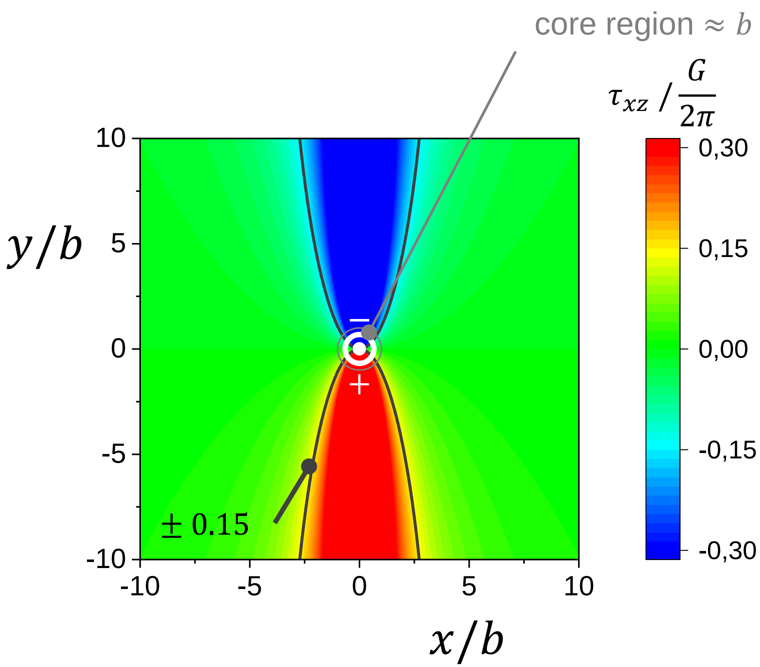


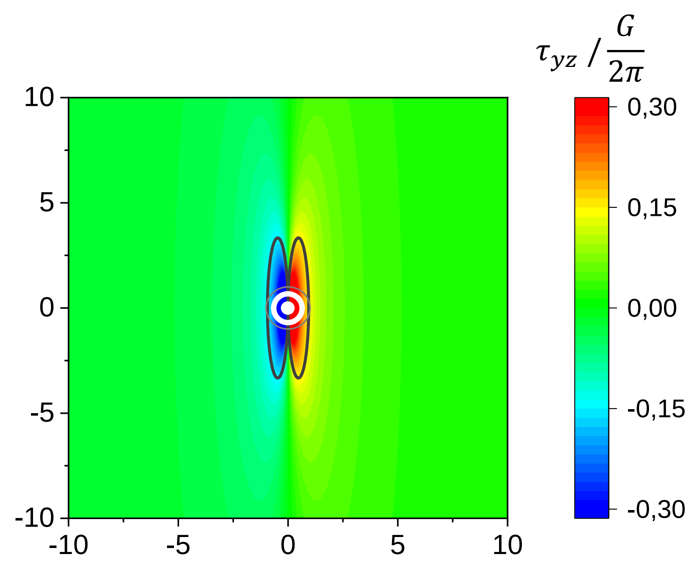
$v = 0.9\, c_T,\ 1 - v^2/c_T^2 = 0.19$

$0.15 \frac{G}{2\pi}$ is in the order of 1.2 GPa for Cu. c_T is in the about 2300 m/s.

Stress Fields of Moving Dislocations

- Screw dislocation with dislocation line along z and plane of displacement within $x - z$ and moving in x direction (glide):





$v = 0.99\, c_\mathrm{T}$, $1 - {}^{v^2}/_{c_\mathrm{T}^2} = 0.0199$

$0.15\, \frac{G}{2\pi}$ is in the order of $1.2\ \mathrm{GPa}$ for Cu. c_T is in the about $2300\ \mathrm{m/s}$.

High-Speed Motion

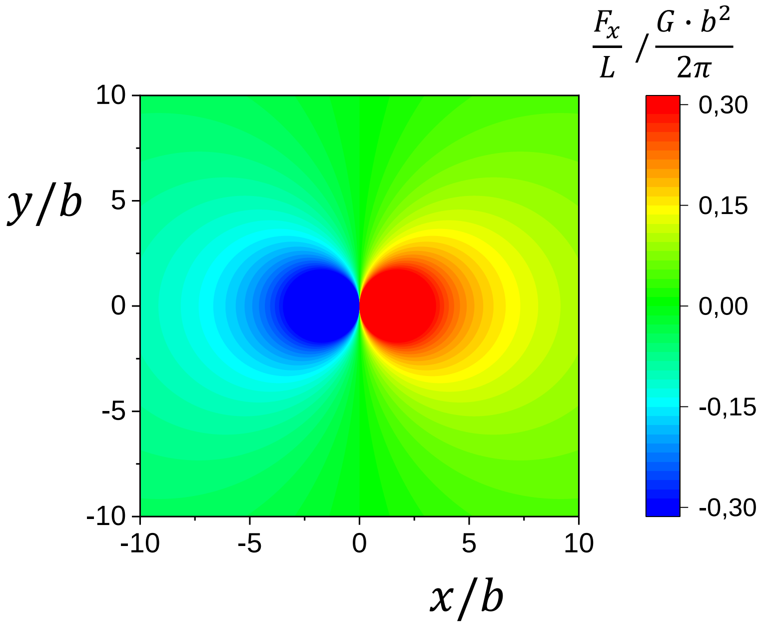
- **The stress field of screw dislocations contracts by the movement of the dislocation.**
- The changing stress field causes a change in line energy of the dislocation (kinetic energy contribution in addition to only elastic contribution). **The energy diverges when approaching c_T:**

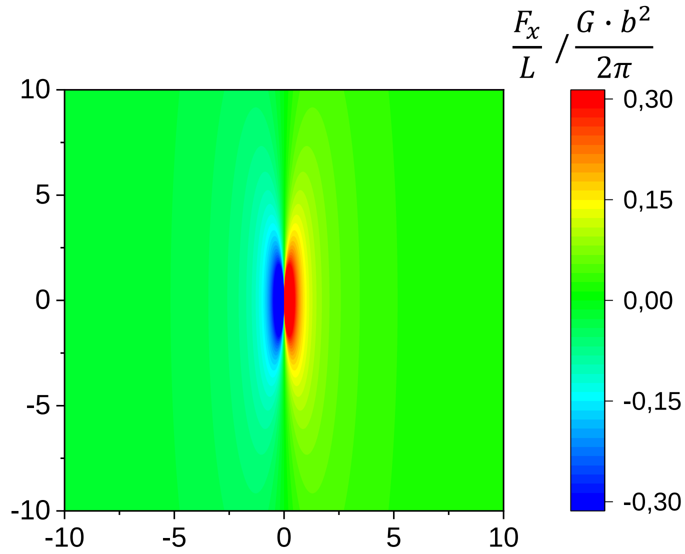
$$\frac{W_\odot}{L} = \frac{1}{\beta}\frac{G\,b^2}{4\pi}\ln\frac{R}{r_0}$$

- **The dislocation-dislocation interaction changes due to the changing stress field.**

Interaction of Moving Dislocations

Example: *glide* component of the interaction force between parallel moving screw dislocations $\frac{F_x}{L} = \frac{G \cdot b^2}{2\pi} \frac{\beta\, x}{x^2 + \beta^2\, y^2}$





$v = 0,\ 1 - {}^{v^2}\!/_{c_\mathrm{T}^2} = 1$

$v = 0.99\, c_\mathrm{T},\ 1 - {}^{v^2}\!/_{c_\mathrm{T}^2} = 0.0199$

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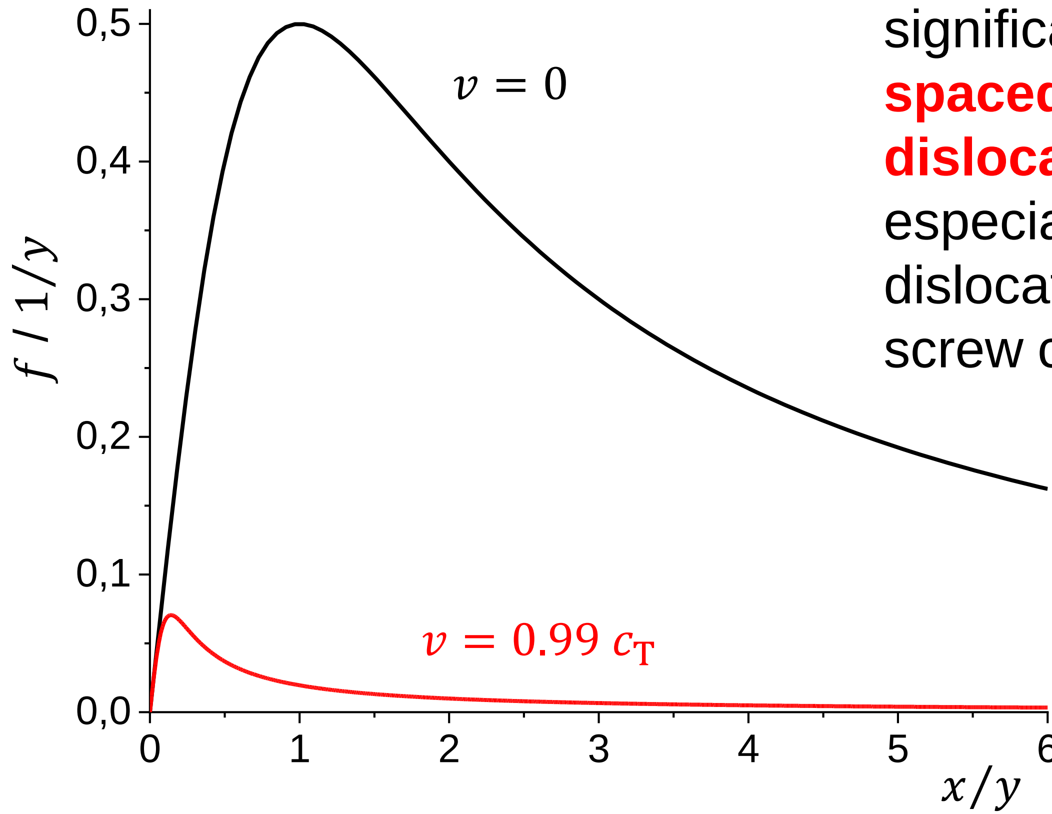
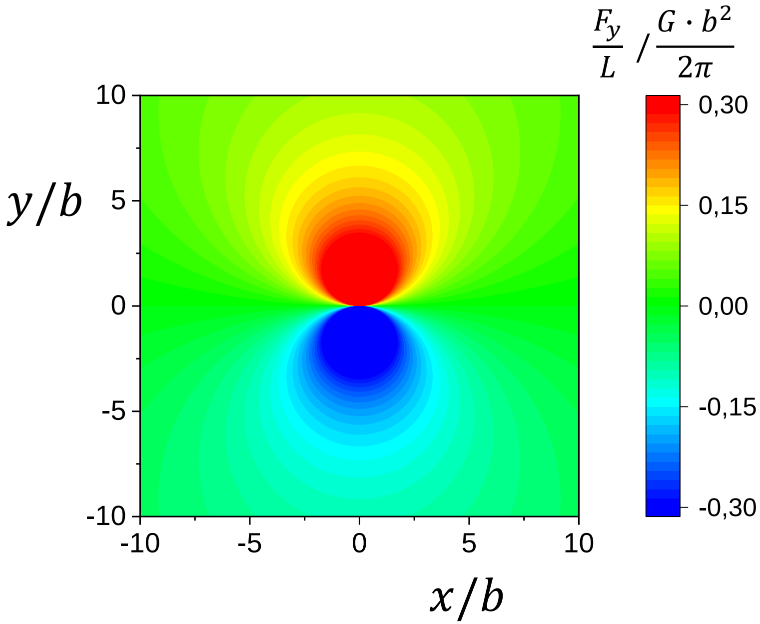


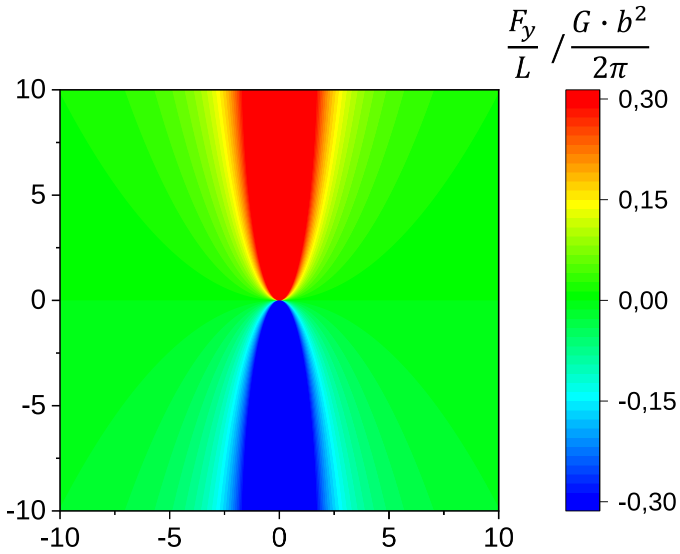
The stress for passing by significantly decreases. **Closely spaced *parallel* screw dislocations can collapse.** This is especially important for dissociated dislocation with otherwise repelling screw components.

$$f = \frac{\beta\, x}{x^2 + \beta^2\, y^2}$$

Interaction of Moving Dislocations

Example: *cross-slip* component of the interaction force between parallel moving screw dislocations $\frac{F_y}{L} = \frac{G \cdot b^2}{2\pi} \frac{\beta\, y}{x^2 + \beta^2\, y^2}$



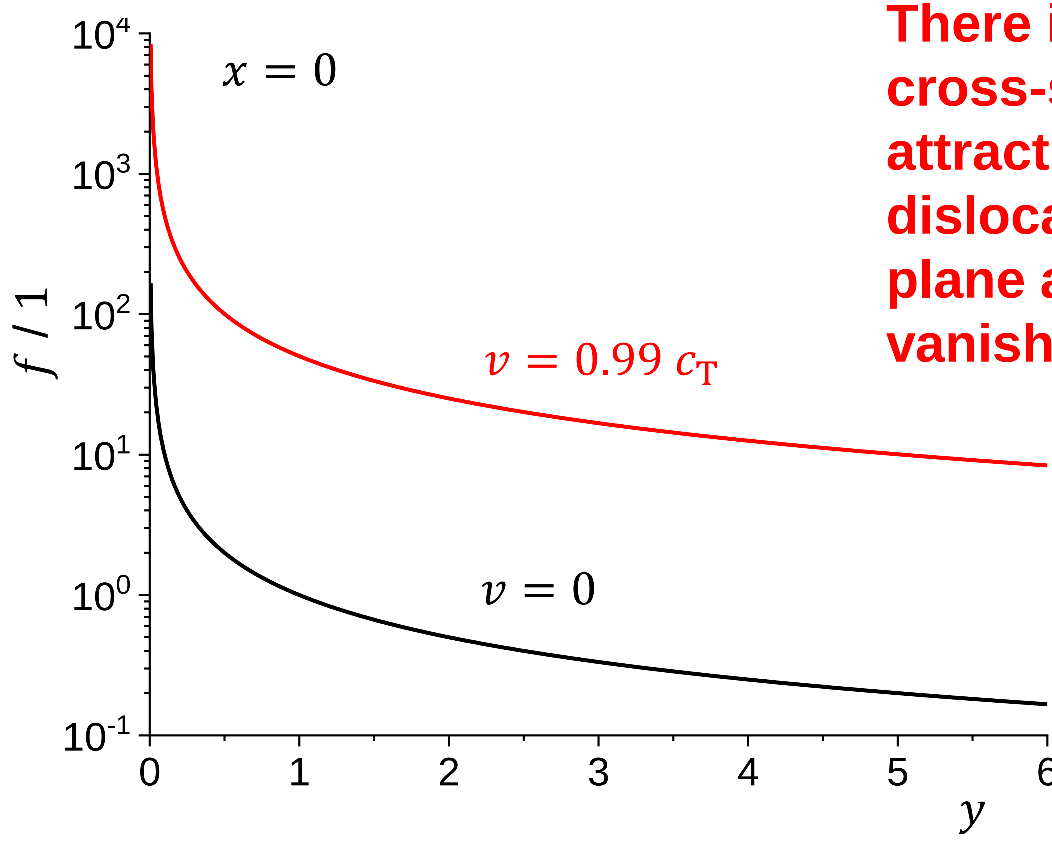


$v = 0,\ 1 - {v^2}/{c_T^2} = 1$

$v = 0.99\, c_T,\ 1 - {v^2}/{c_T^2} = 0.0199$

Interaction of Moving Dislocations

Example: *cross-slip* component of the interaction force between parallel moving screw dislocations $\frac{F_y}{L} = \frac{G \cdot b^2}{2\pi} \frac{\beta\, y}{x^2 + \beta^2\, y^2}$



There is a stronger tendency for cross-slip which can lead to attraction of the second dislocation into the same slip plane and collapse due to the vanishing glide interaction.

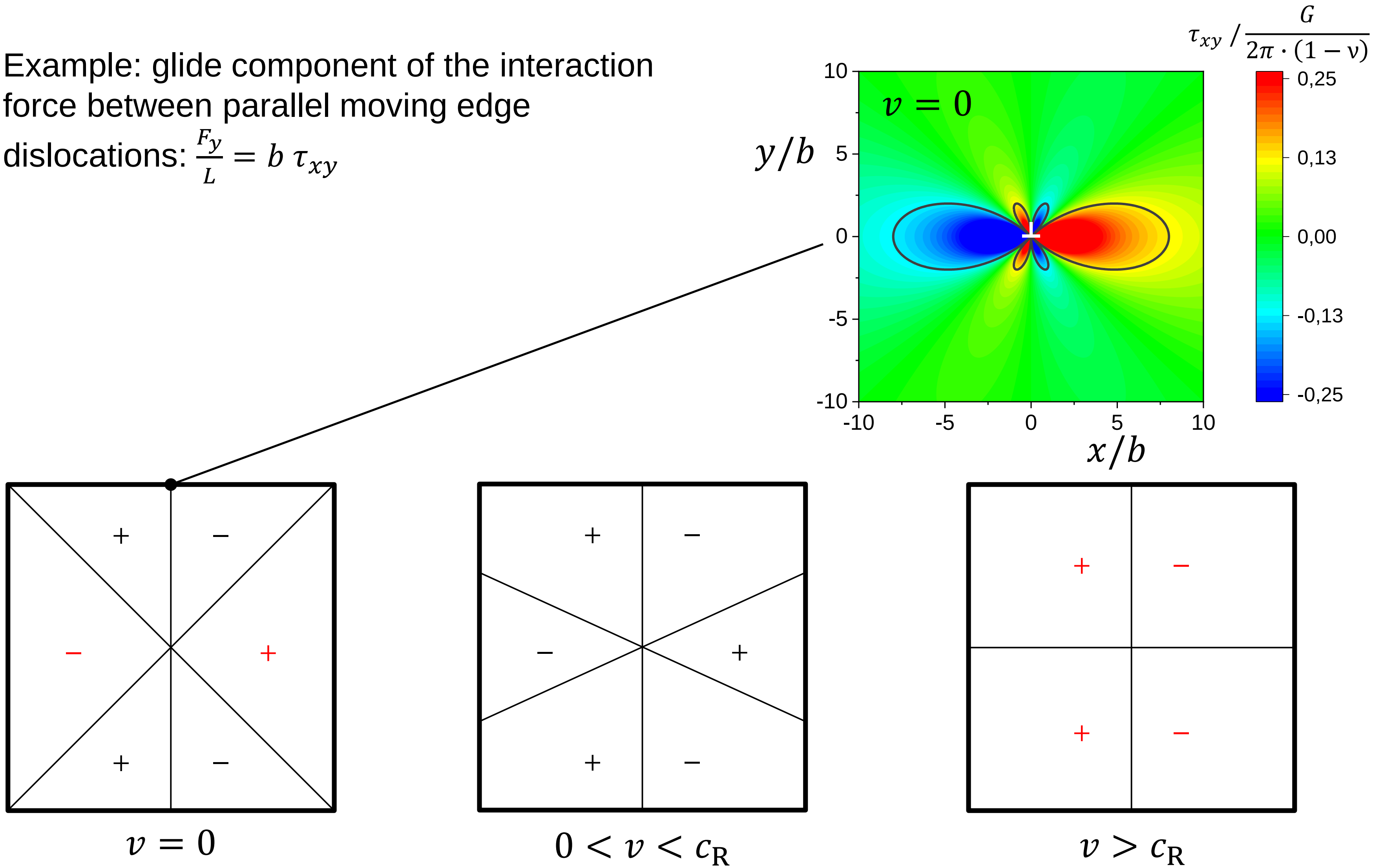
$$f = \frac{\beta\, y}{x^2 + \beta^2\, y^2}$$

High-Speed Motion

- The discussion of edge dislocations is more complex since both, c_{L} and c_{R} have to be considered.
- For $v < c_{\mathrm{R}}$ (sub-sonic), the **zero transitions of τ_{xy} shift from $x = y$ towards the slip plane.** Remember: the zero transitions of τ_{xy} are responsible for the metastable configurations of parallel edge dislocations (see Ch. 4d).
- For $c_{\mathrm{R}} < v < c_{\mathrm{T}}$ (trans-sonic), there is no τ_{xy} within the slip plane anymore and the signs of τ_{xy} are opposite to what is observed for the stationary dislocation. **Parallel edge dislocation attract each other, then!**
- **Also in the case of edge dislocations, the considerations on the interaction of stationary dislocations cannot be easily transferred to fast moving dislocations.**
- The **line energy of a moving edge dislocation also diverges** when $v \rightarrow c_{\mathrm{T}}$.

Interaction of Moving Dislocations

Example: glide component of the interaction force between parallel moving edge dislocations: $\frac{F_y}{L} = b\,\tau_{xy}$



High-Speed Motion

- The aforementioned considerations can also be done for climb processes.
- The aforementioned considerations are restricted to no dampening of the dislocation motion. **The interaction of dislocations with phonons gives rise to dampening.**
- In principle, **the slip plane can release energy to the dislocation** during motion! This allows for **supersonic motion** of dislocations. Especially in real crystals such energy transfer can be assume, e.g. by a removal of a stacking fault by a gliding partial dislocation.
- Advanced theories with no discontinuity in consideration also limit the energy required to move the dislocation at high speeds.

Summary

- **There is a critical stress needed to move a dislocation.**
- **The Peierls-Nabarro equation predicts densely packed planes and directions as slip planes and directions, respectively.**
- **The stress required to move the dislocation at $0\ \mathrm{K}$ is much smaller than $\frac{G}{2\pi}$. Thermal activation can assist dislocation motion.**
- Dislocation velocity as a function of applied stress follows a power-law.
- **At high velocities, the equation of motion has to be corrected** by relativistic terms. This has **significant impact on the stress fields and energy of the dislocations and**, therefore, on the **interaction of dislocations**. There are limiting speeds.