Karlsruhe Institute of Technology

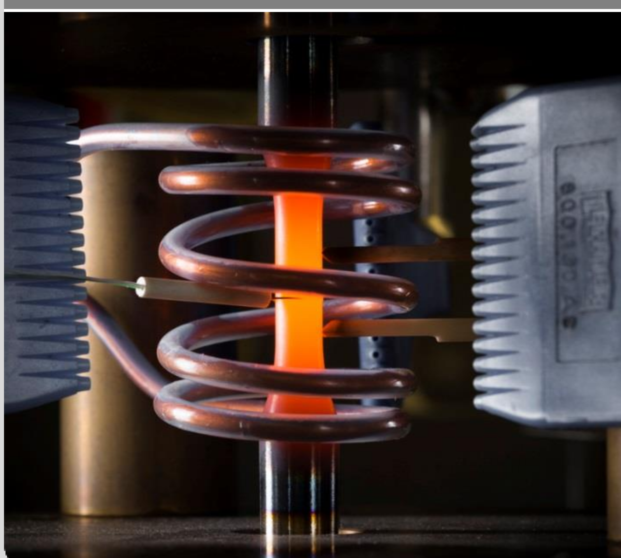
Institute for Applied Materials

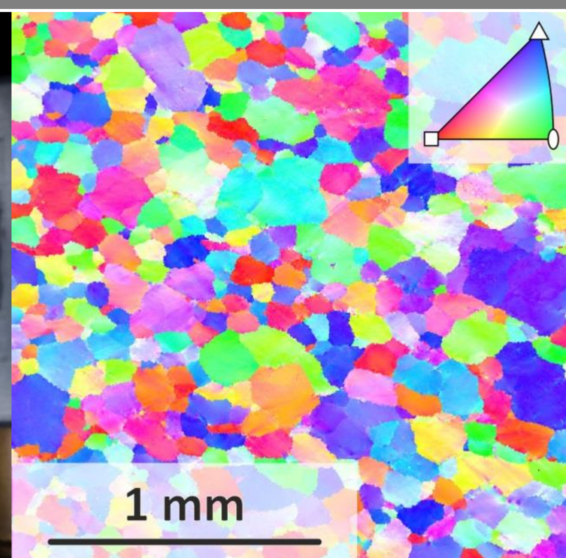
Plasticity

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 22-04-14

Institute for Applied Materials (IAM-WK)





Topics

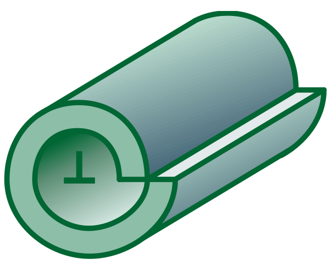
- Interaction of Straight Dislocations
  - Parallel Dislocations – Passing
    - Contribution to Dislocation Strengthening
    - Low Angle Grain Boundaries
    - Dipoles
    - Pile Ups and Their Contribution to Grain Boundary Strengthening
  - Non-Parallel Dislocations – Intersection
    - Contribution to Dislocation Strengthening
    - Vacancy Formation Due to Jogged Screw Dislocations

Parallel Dislocations

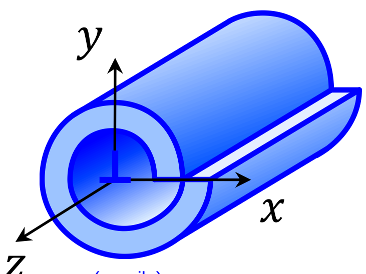
- In order to evaluate the interaction force between parallel dislocations, we can assume that **the stress field of one dislocation acts as external stress on the other**. Hence, Peach-Köhler force in conjunction with the stress fields are utilized.
- Important cases:
  - Parallel/anti-parallel edge dislocations
  - Parallel/anti-parallel screw dislocations

Parallel Dislocations

- Parallel/anti-parallel *edge* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm x$:



(passing)



(sessile)

$$\boldsymbol{b}_1 = \begin{pmatrix} b \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{b}_2 = \begin{pmatrix} \pm b \\ 0 \\ 0 \end{pmatrix}$$

+ parallel
– anti-parallel

$$\boldsymbol{s}_1 = \boldsymbol{s}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

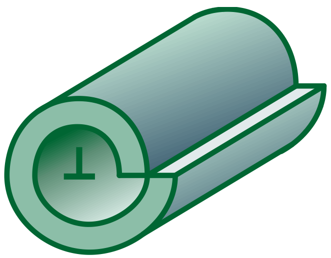
$$\boldsymbol{\sigma}_1 = \pm\boldsymbol{\sigma}_2 = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

$$\frac{\boldsymbol{F}}{L} = (\boldsymbol{b}_2 \cdot \boldsymbol{\sigma}_1) \times \boldsymbol{s}_2 = \begin{pmatrix} \pm b\,\tau_{xy} \\ \mp b\,\sigma_{xx} \\ 0 \end{pmatrix}$$

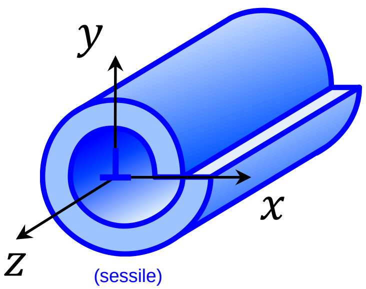
The force on dislocation (2) is a result of the stress field of dislocation (1).

Parallel Dislocations

- Parallel/anti-parallel *edge* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm x$:



(passing)



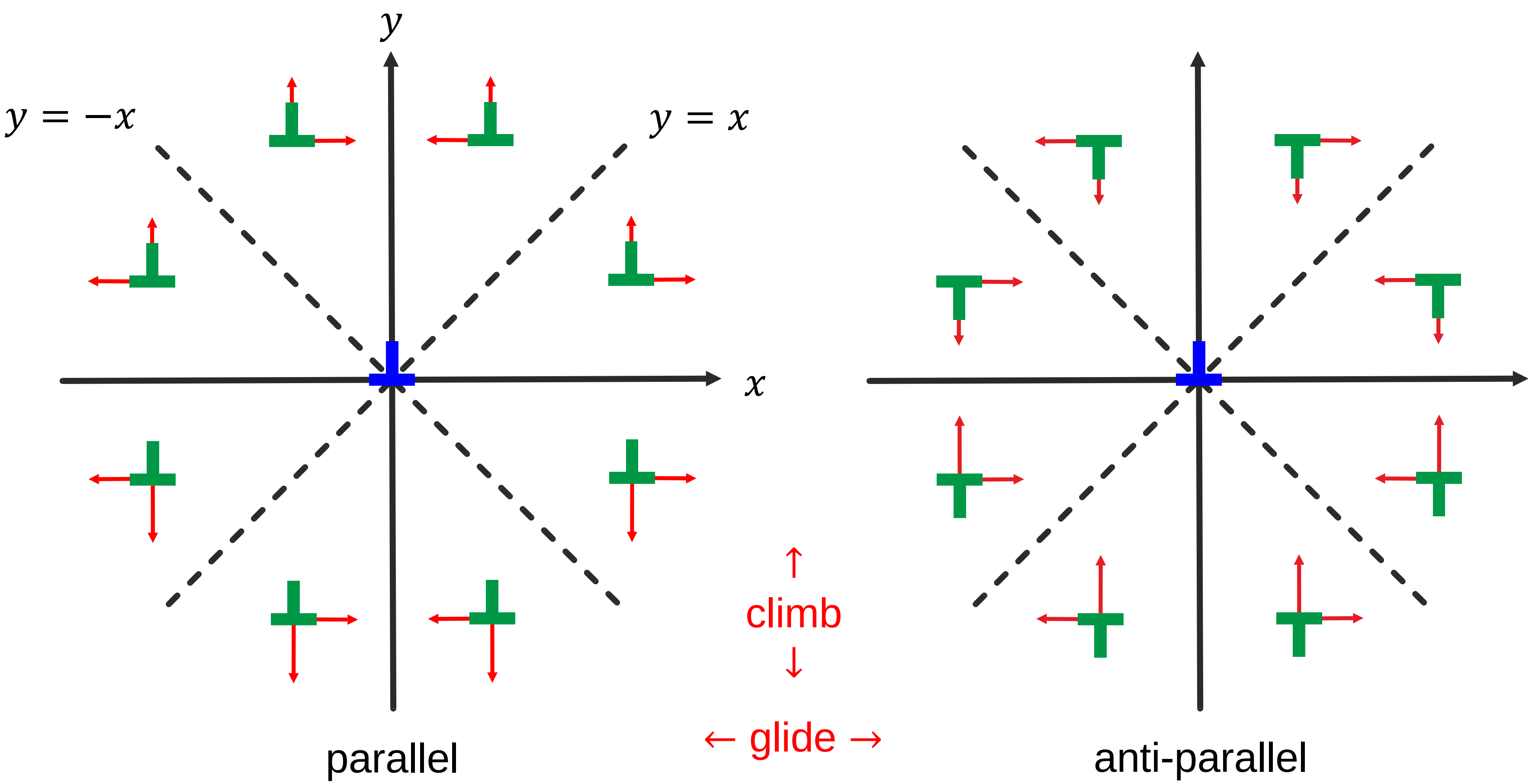
(sessile)

$$\frac{\boldsymbol{F}}{L} = (\boldsymbol{b}_2 \cdot \boldsymbol{\sigma}_1) \times \boldsymbol{s}_2 = \begin{pmatrix} \pm\, b\, \tau_{xy} \\ \mp\, b\, \sigma_{xx} \\ 0 \end{pmatrix}$$

$$\frac{\boldsymbol{F}}{L} = \frac{G \cdot b^2}{2\pi \cdot (1-\nu)} \begin{pmatrix} \pm \dfrac{x \cdot (x^2 - y^2)}{(x^2+y^2)^2} \\ \pm \dfrac{y \cdot (3x^2 + y^2)}{(x^2+y^2)^2} \\ 0 \end{pmatrix}$$

Parallel Dislocations

- Parallel/anti-parallel *edge* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm x$:



Parallel Dislocations

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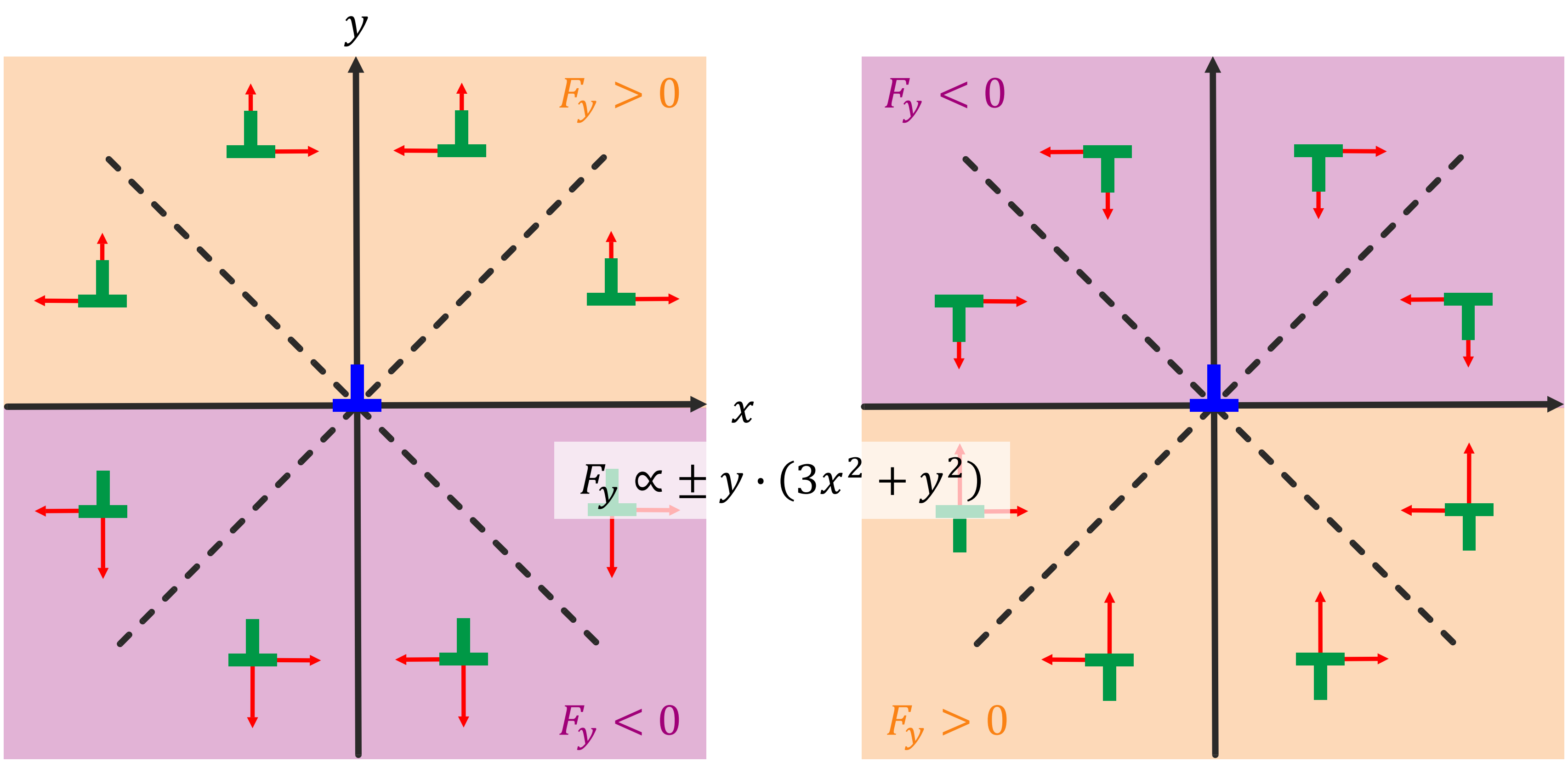

parallel

anti-parallel

Parallel Dislocations

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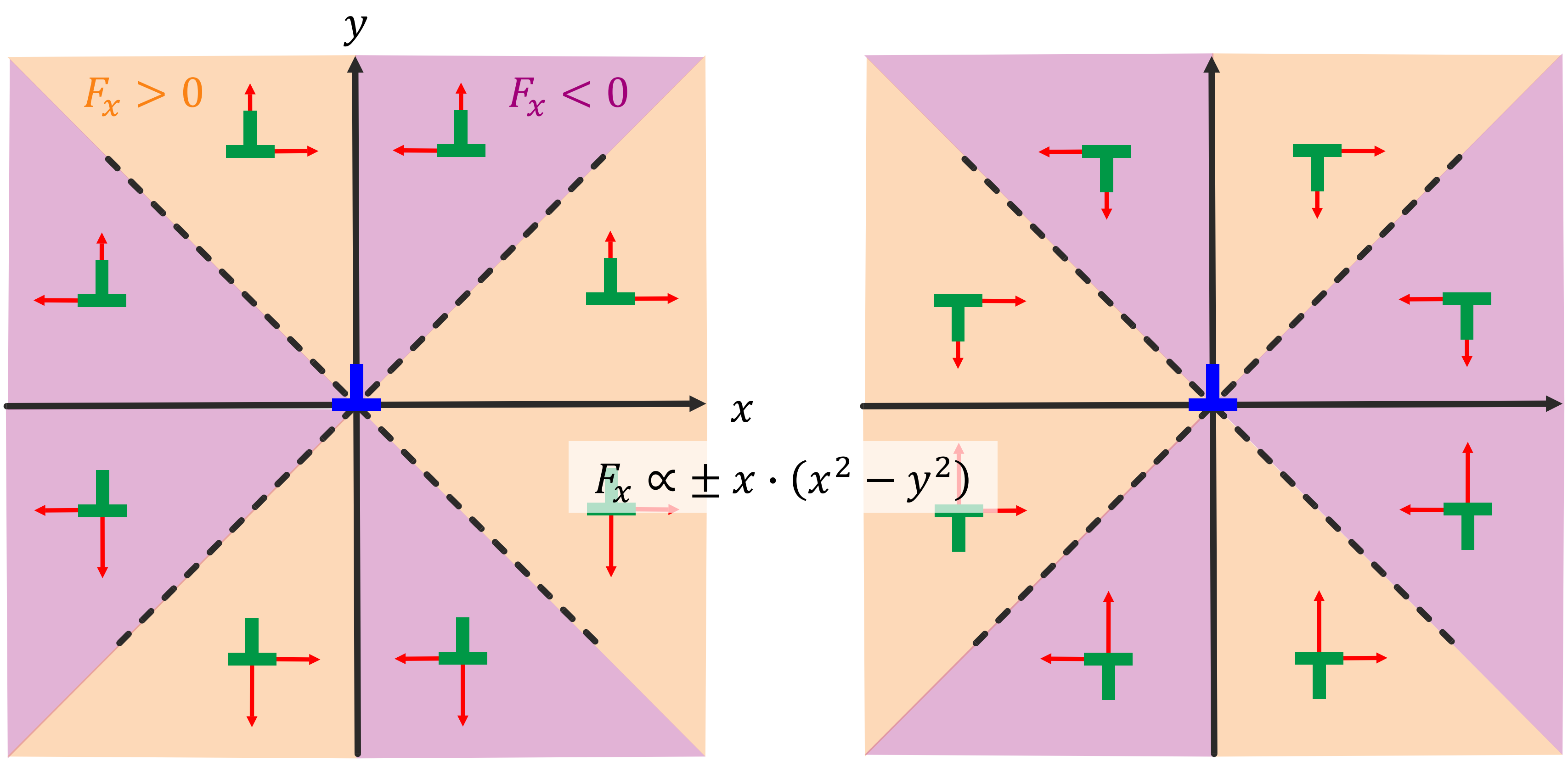
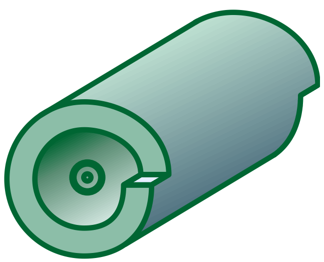


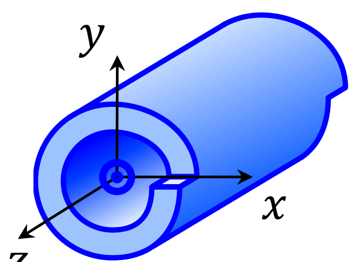
parallel　　　　　　　　anti-parallel

Parallel Dislocations

- Parallel/anti-parallel *screw* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm z$:



(passing)



(sessile)

$$\boldsymbol{b}_1 = \begin{pmatrix} 0 \\ 0 \\ b \end{pmatrix}, \boldsymbol{b}_2 = \begin{pmatrix} 0 \\ 0 \\ \pm b \end{pmatrix}$$

+ parallel
– anti-parallel

$$\boldsymbol{s}_1 = \boldsymbol{s}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\boldsymbol{\sigma}_1 = \pm \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & 0 \end{pmatrix}$$

$$\frac{\boldsymbol{F}}{L} = (\boldsymbol{b}_2 \cdot \boldsymbol{\sigma}_1) \times \boldsymbol{s}_2 = \begin{pmatrix} \pm b\, \tau_{yz} \\ \mp b\, \tau_{xz} \\ 0 \end{pmatrix}$$

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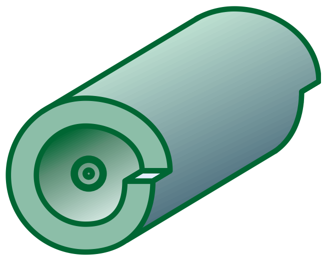
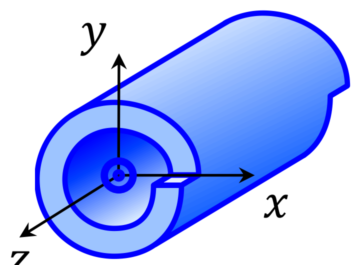
- Parallel/anti-parallel *screw* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm z$:



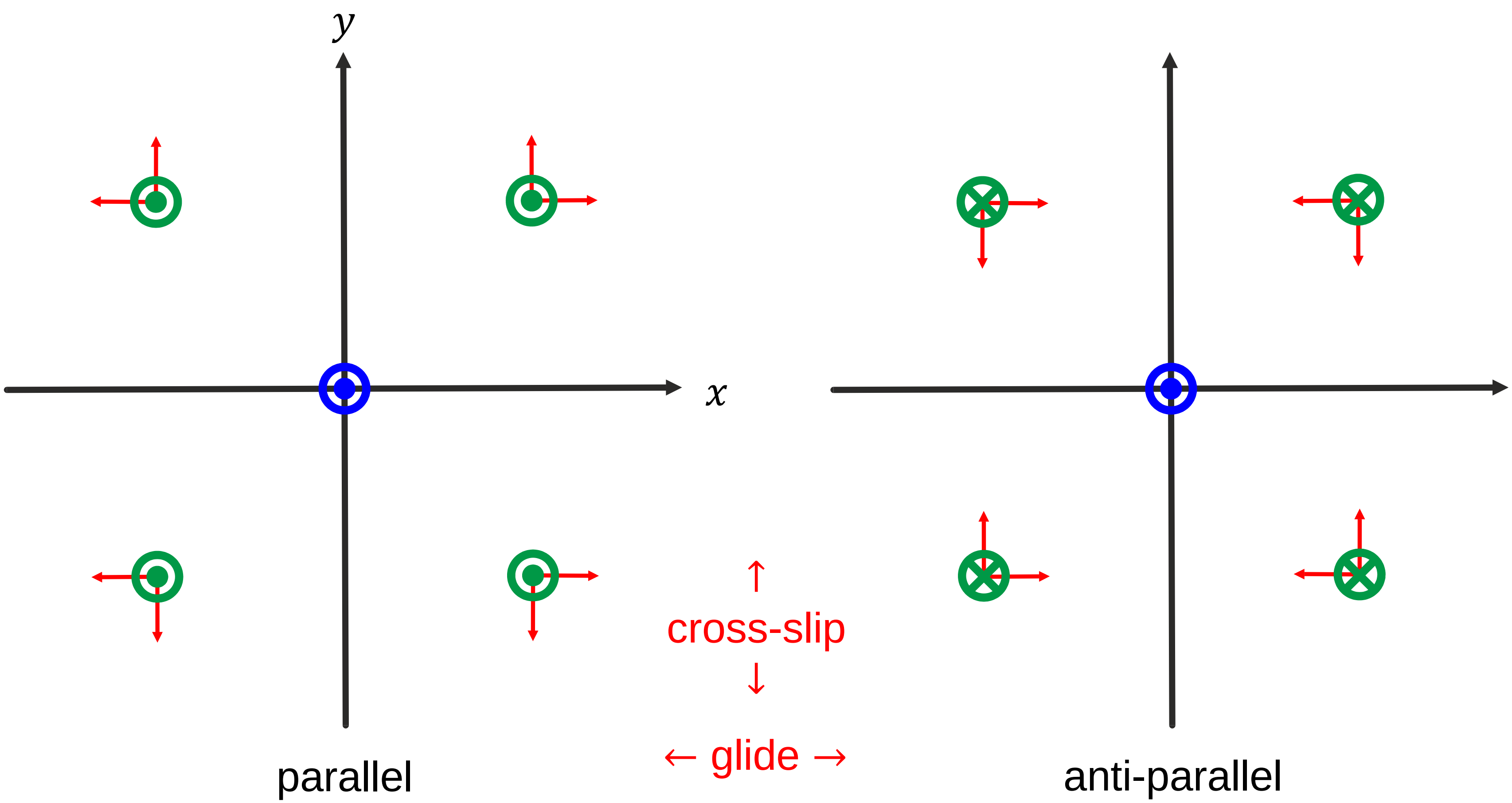
$$\frac{\boldsymbol{F}}{L} = (\boldsymbol{b_2} \cdot \boldsymbol{\sigma_1}) \times \boldsymbol{s_2} = \begin{pmatrix} \pm b\,\tau_{yz} \\ \mp b\,\tau_{xz} \\ 0 \end{pmatrix}$$



$$\frac{\boldsymbol{F}}{L} = \frac{G \cdot b^2}{2\pi} \begin{pmatrix} \pm \dfrac{x}{x^2 + y^2} \\ \pm \dfrac{y}{x^2 + y^2} \\ 0 \end{pmatrix}$$

Parallel Dislocations

- Parallel/anti-parallel *screw* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm z$:



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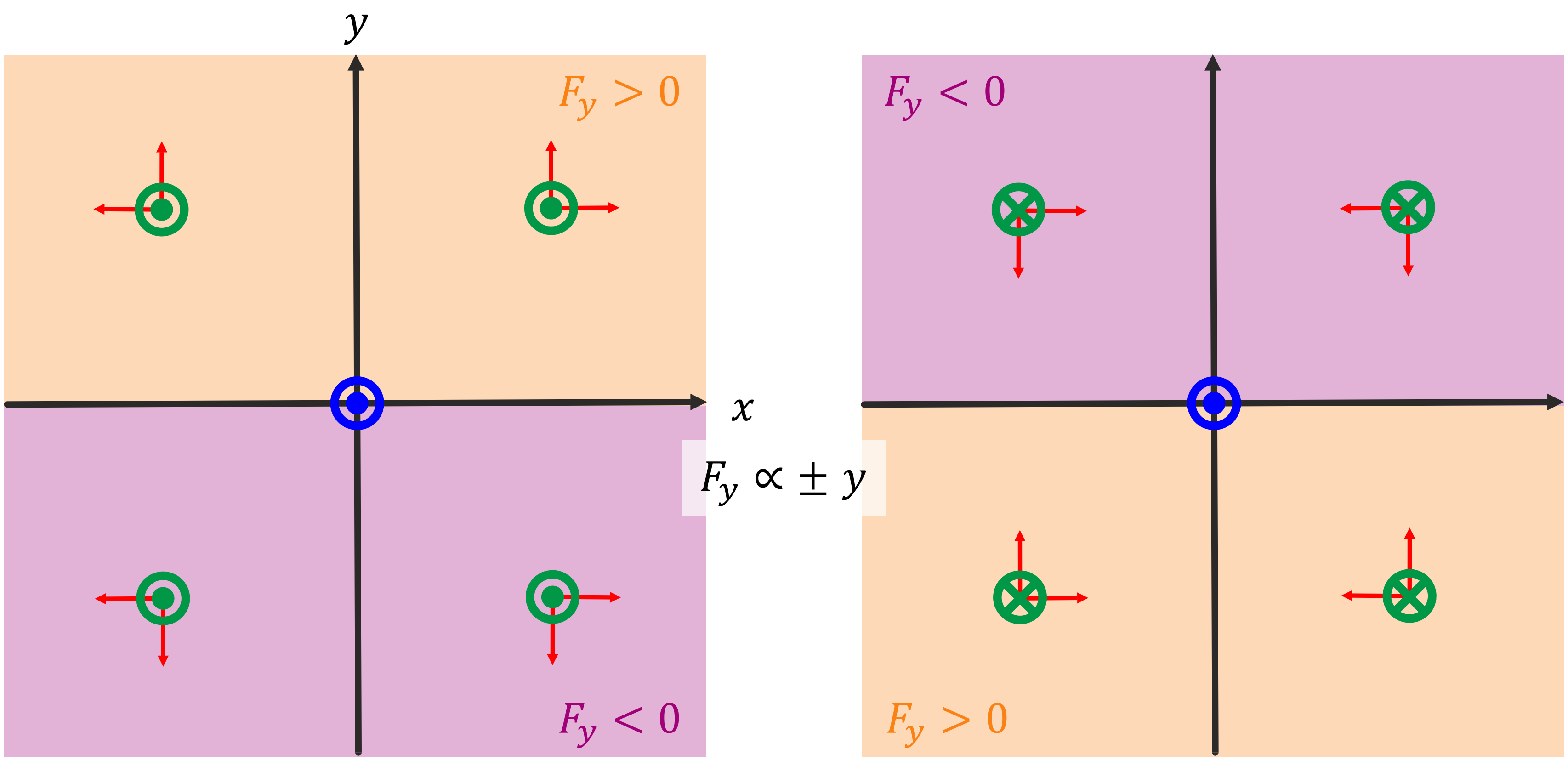
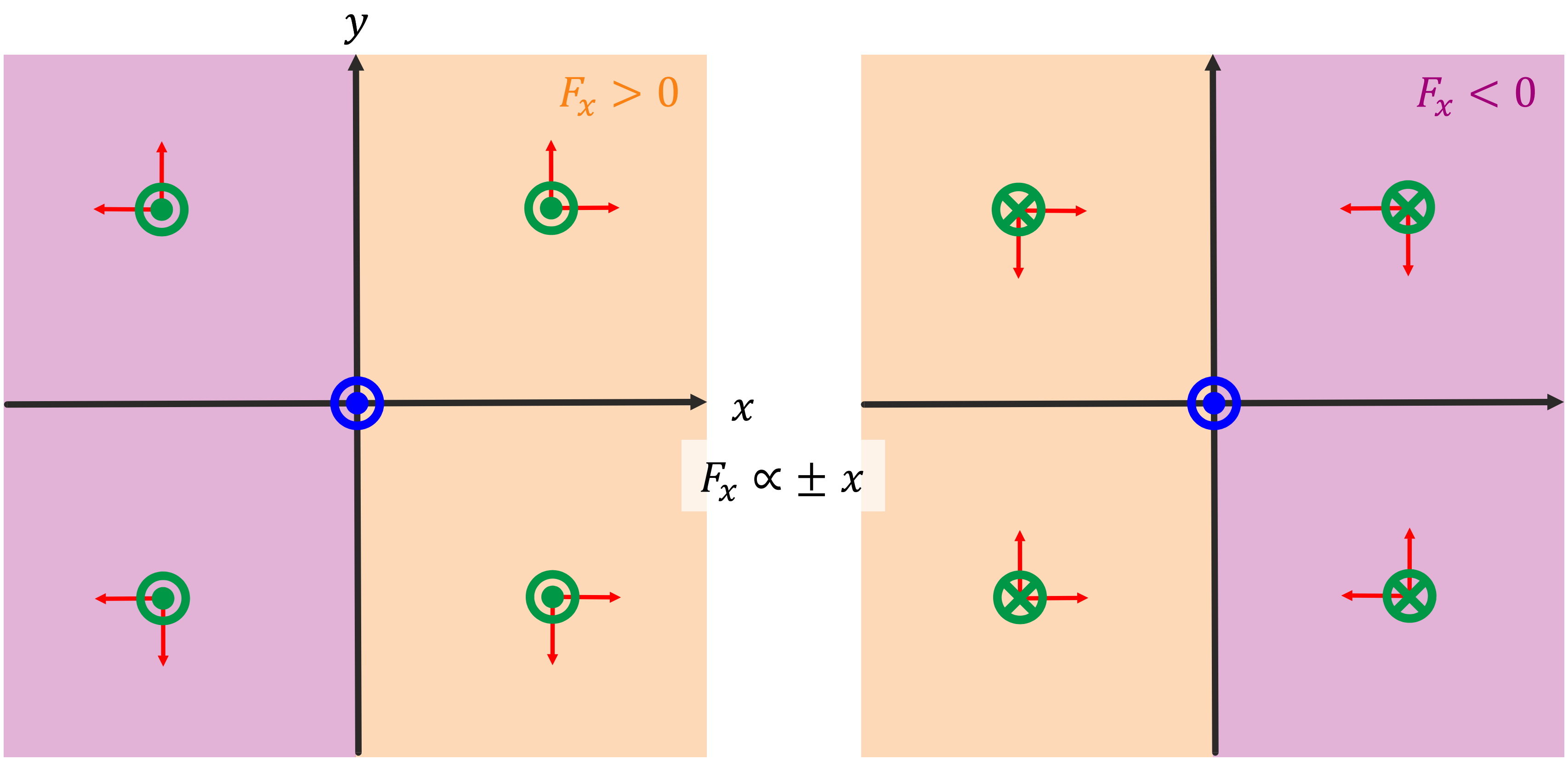


parallel

anti-parallel

Parallel Dislocations

- Parallel/anti-parallel *screw* dislocations with the dislocation line along z (positive sense) and Burgers vectors along $\pm z$:



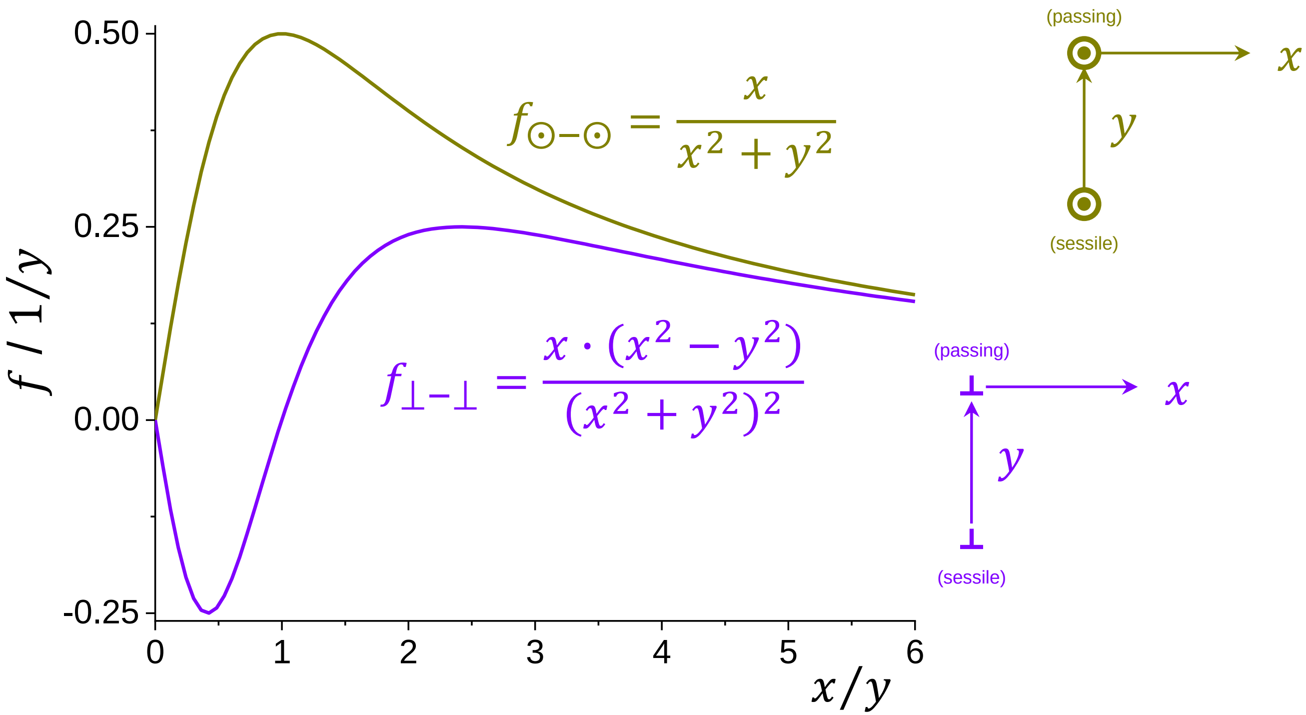
parallel

anti-parallel

Parallel Dislocations – Dislocation Strengthening

- **Parallel dislocations generally repel each other. Antiparallel dislocations attract each other.**
- In any case, **passing by requires overcoming a certain stress maximum**. **This stress is inversely proportional to the dislocation spacing** (equivalent to y). The by-pass stress is an **important contribution to dislocation strengthening**: $\Delta\tau \propto \frac{F^{\max}}{b} \propto \frac{1}{y} \propto \sqrt{\rho}$

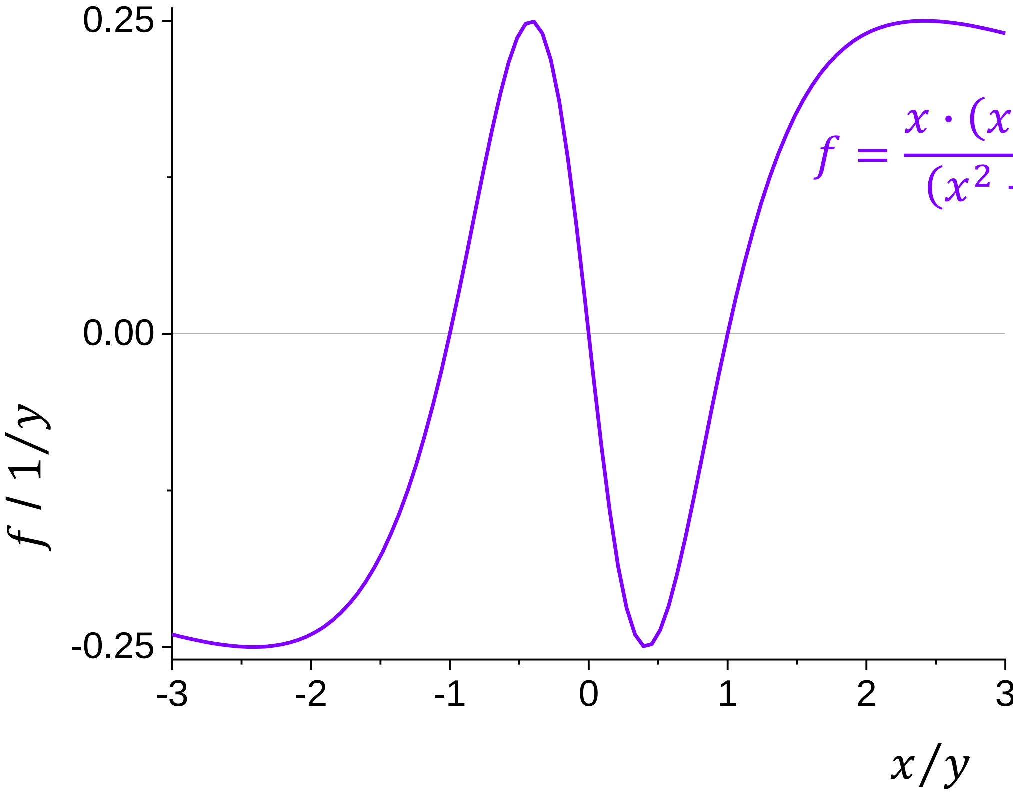
Lateral dependence of the interaction force between a passing and a sessile dislocation. Note that the force is normalized by the reciprocal distance of the dislocations.



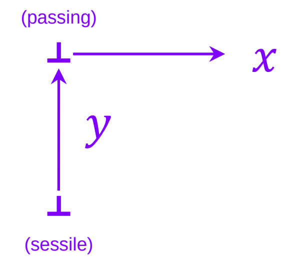
Parallel Dislocations – Low Angle Grain Boundaries

- The glide component of the interaction of two edge dislocations exhibits **roots** with one of them being associated with a **minimum in the interaction energy**. **The stacked configuration of the edge dislocations is metastable.**

Lateral dependence of the interaction force between a passing and a sessile dislocation. Note that the force is normalized by the reciprocal distance of the dislocations.



$$f = \frac{x \cdot (x^2 - y^2)}{(x^2 + y^2)^2}$$



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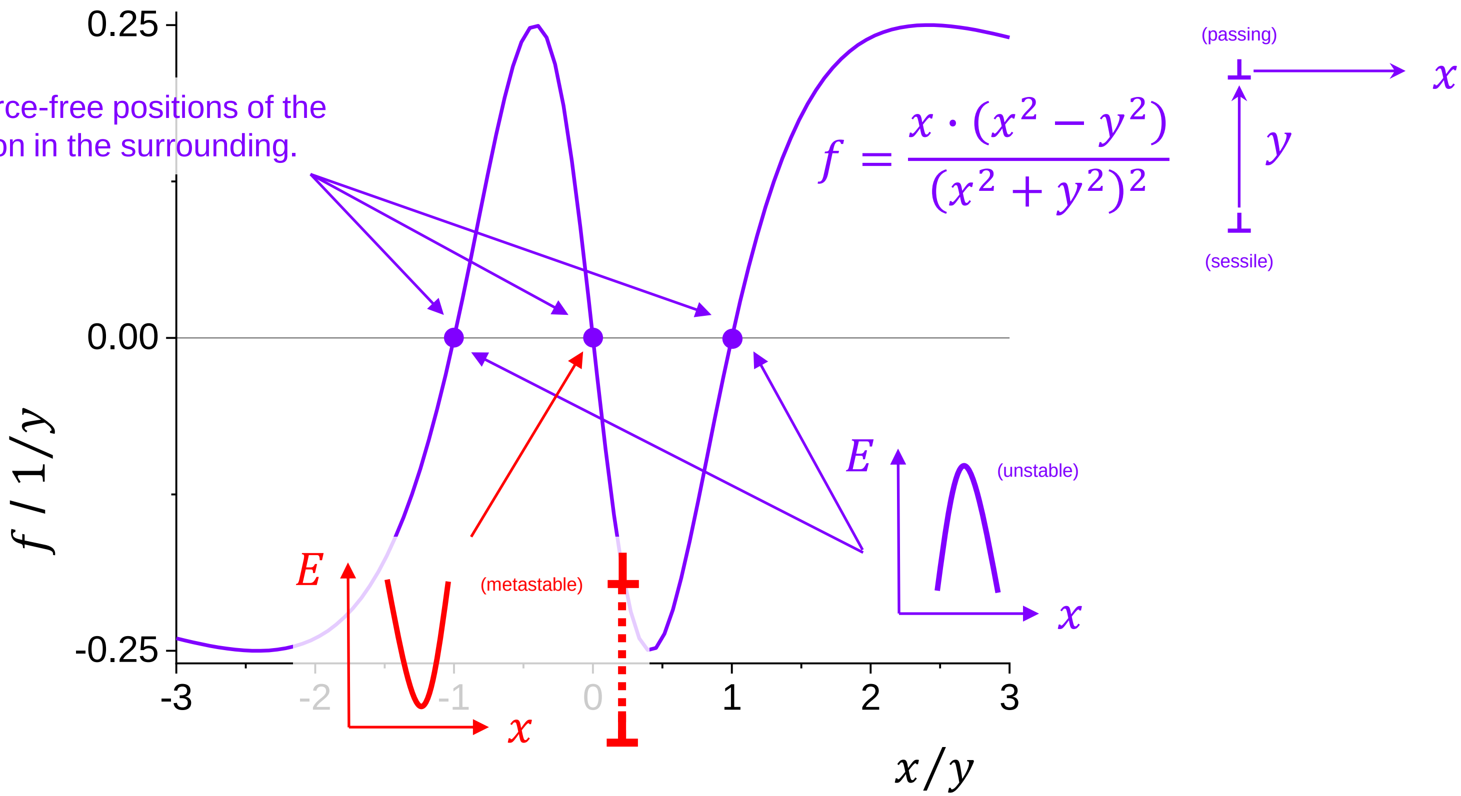
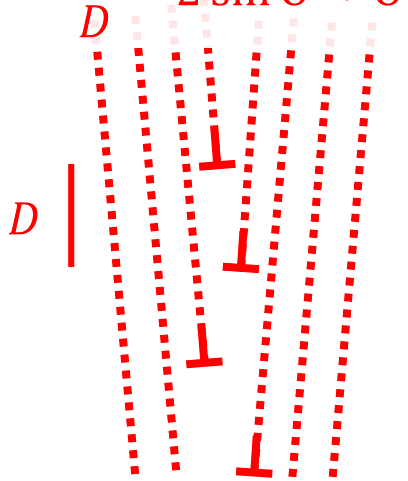


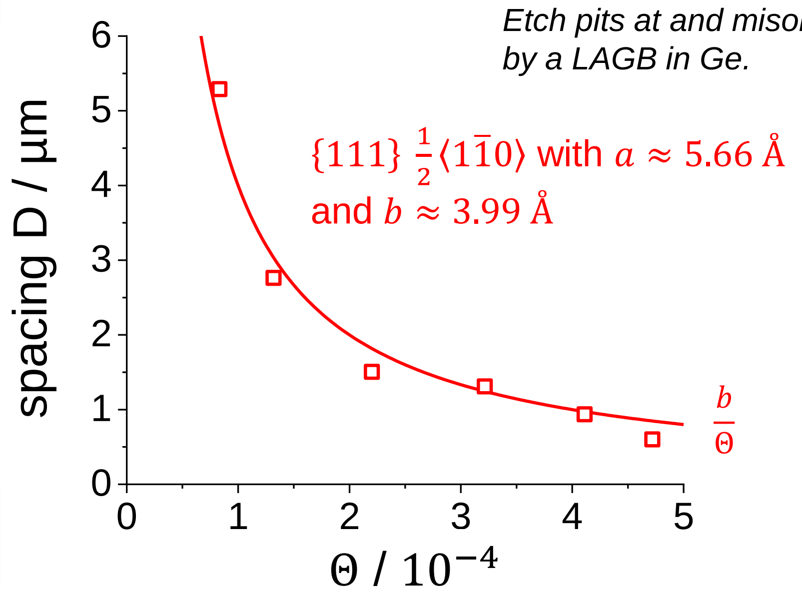
Parallel Dislocations – Low Angle Grain Boundaries

- The **stacked configuration causes an orientation change of the crystals** adjacent to the dislocations; it‘s a **low angle grain boundary** (LAGB). Since all dislocations have to be **moved cooperatively**, the **mobility of LAGB is small**.

$$\frac{b}{D} = 2\sin\Theta \approx \Theta$$



Etch pits at and misorientation by a LAGB in Ge.



adopted from: Gottstein: “Materialwissenschaft und Werkstofftechnik: Physikalische Grundlagen”, Berlin, Heidelberg: Springer Vieweg, Springer Verlag (2014)
Vogel et al., "Observation of Dislocation in Lineage Boundaries in Germanium" in Physical Review 90 (1953) 489

Parallel Dislocations – Low Angle Grain Boundaries

- The situation can also be described using Frank's formula for complex dislocation patterns containing N_i dislocations of $\boldsymbol{b}_i$:

$$\boldsymbol{d} = \sum_i N_i\, \boldsymbol{b}_i = (\boldsymbol{r} \times \boldsymbol{l})\, 2 \sin \Theta \approx (\boldsymbol{r} \times \boldsymbol{l})\, \Theta$$

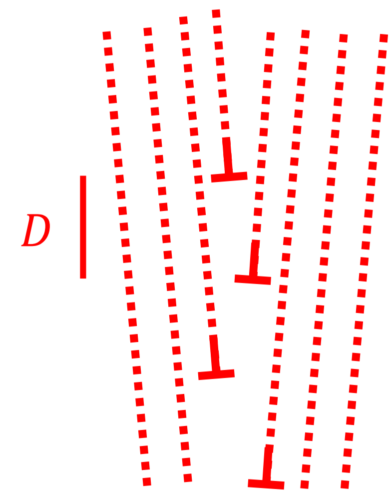
- $\boldsymbol{l}$ is the rotation axis of the boundary and $\boldsymbol{r}$ is an arbitrary vector within the boundary. N_i is given by the number of intersections of the dislocation lines with $\boldsymbol{r}$.
- The equation is restricted to flat boundaries with narrow stress field. The equation does not contain information about the distinct pattern of dislocation lines (can also be non-parallel lines).
- $\boldsymbol{n}$ is the normal vector of the boundary and, hence, $\boldsymbol{n} \parallel \boldsymbol{l}$ are a twist boundaries and $\boldsymbol{n} \perp \boldsymbol{l}$ are a tilt boundaries.

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

Parallel Dislocations – Low Angle Grain Boundaries

- A single set of dislocations: $\boldsymbol{d} = N\,\boldsymbol{b} \approx (\boldsymbol{r} \times \boldsymbol{l})\,\Theta$

- $\boldsymbol{b} \perp \boldsymbol{n}$ since $\boldsymbol{r}$ lies arbitrary within the boundary.
- Since $(\boldsymbol{r} \times \boldsymbol{l}) = \boldsymbol{0}$ when $\boldsymbol{r} \,||\, \boldsymbol{l}$, the dislocation lines must be parallel to $\boldsymbol{l}$ (no intersections of the dislocations and $\boldsymbol{r}$).
- The boundary must be a tilt boundary with only edge dislocations as seen on two slides before: $N\,\boldsymbol{b} \approx \big((\boldsymbol{l} \times \boldsymbol{n}) \times \boldsymbol{l}\big)\, r\,\Theta = \boldsymbol{n}\, r\,\Theta$, when $r = |\boldsymbol{r}|$, finally $D = \frac{r}{N} = \frac{b}{\Theta}$.



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

Parallel Dislocations – Low Angle Grain Boundaries

- Two sets of dislocations: $\boldsymbol{d} = N_1\, \boldsymbol{b}_1 + N_2\, \boldsymbol{b}_2 \approx (\boldsymbol{r} \times \boldsymbol{l})\, \Theta$

$$(N_1\, \boldsymbol{b}_1 + N_2\, \boldsymbol{b}_2) \cdot\ (\boldsymbol{b}_1 \times \boldsymbol{b}_2) \approx \Theta\, (\boldsymbol{r} \times \boldsymbol{l}) \cdot (\boldsymbol{b}_1 \times \boldsymbol{b}_2)$$

expand the equation by $\cdot\, (\boldsymbol{b}_1 \times \boldsymbol{b}_2)$

$$0 = (\boldsymbol{r} \times \boldsymbol{l})\ \cdot\ (\boldsymbol{b}_1 \times \boldsymbol{b}_2)$$

$$\boldsymbol{r} \cdot \big(\boldsymbol{l} \times (\boldsymbol{b}_1 \times \boldsymbol{b}_2)\big) = 0$$

- This is satisfied whenever $\boldsymbol{r}\ ||\ \big(\boldsymbol{l} \times (\boldsymbol{b}_1 \times \boldsymbol{b}_2)\big)$.

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

Parallel Dislocations – Low Angle Grain Boundaries

- Case (1): tilt boundary formed from two sets of edge dislocations

- $\boldsymbol{l}$ and $\boldsymbol{b}_1 \times \boldsymbol{b}_2$ lie within the boundary plane

Asymmetric tilt boundary in a cubic crystal by two sets of dislocations.

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

Parallel Dislocations – Low Angle Grain Boundaries

- Case (2): $\boldsymbol{l}$ is parallel to $\boldsymbol{b}_1 \times \boldsymbol{b}_2$

- For the case that $\boldsymbol{l} \,||\, \boldsymbol{n}$, a pure twist boundary is formed.
- For additionally $\boldsymbol{b}_1 \perp \boldsymbol{b}_2$, the boundary is formed only from screw dislocations:

Atom positions resulting from rigid rotation through angle Θ; open circles represent atoms just above the boundary and solid circles those just below.

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

Parallel Dislocations – Low Angle Grain Boundaries

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Accommodation of the mismatch (in the boundary!) by two sets of parallel screw dislocations labeled S-S.

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

Parallel Dislocations – Low Angle Grain Boundaries

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Gottstein: "Materialwissenschaft und Werkstofftechnik: Physikalische Grundlagen", Berlin, Heidelberg: Springer Vieweg, Springer Verlag (2014)

Parallel Dislocations – Low Angle Grain Boundaries

- Case (2): $\boldsymbol{l}$ is parallel to $\boldsymbol{b}_1 \times \boldsymbol{b}_2$

Take-home messages:

- In contrast to edge dislocations, **there are at least two sets of screw dislocations needed** in order **to built up a symmetric (twist) boundary**.
- Dislocations or dislocation components (especially screws or screw components) **might not contribute to the orientation change but do contribute to the energy** of the pattern!

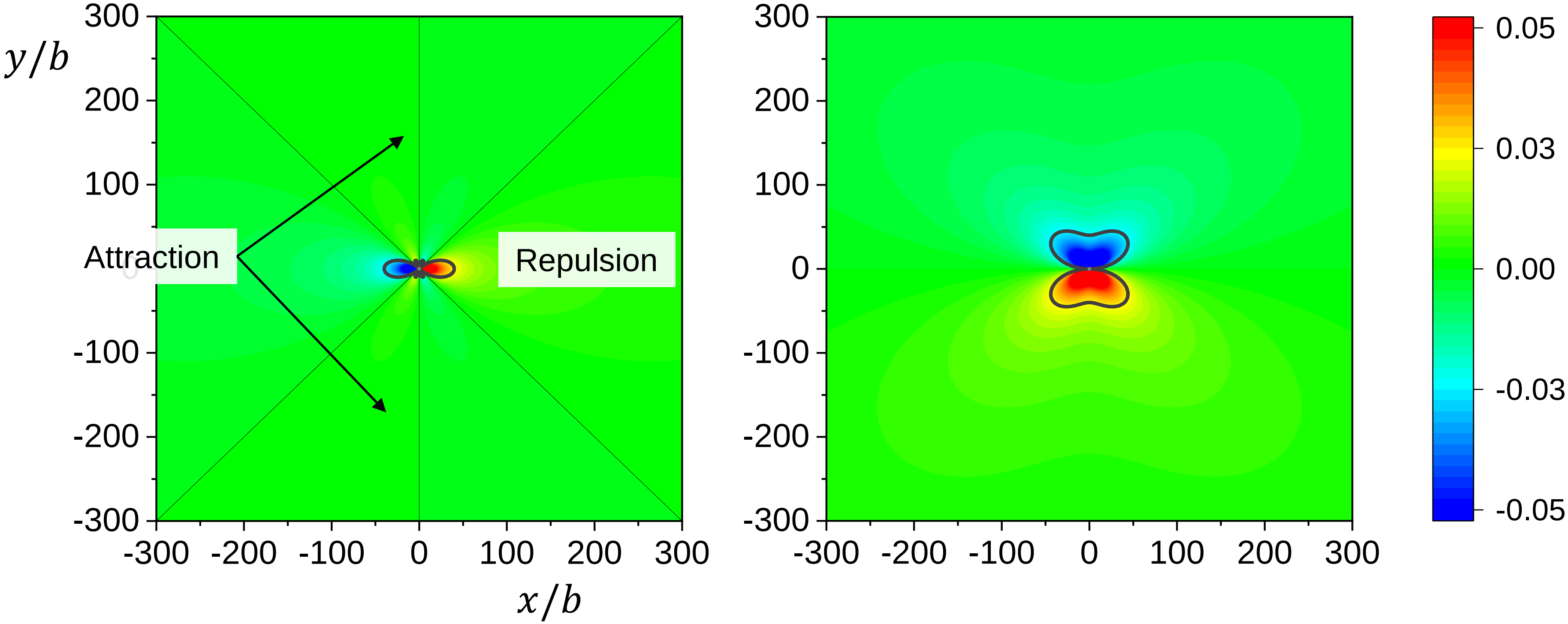
Accommodation of the mismatch (in the boundary!) by two sets of parallel screw dislocations labeled S-S.

Gottstein: "Materialwissenschaft und Werkstofftechnik: Physikalische Grundlagen", Berlin, Heidelberg: Springer Vieweg, Springer Verlag (2014)

Parallel Dislocations – Low Angle Grain Boundaries

glide interaction | *climb interaction*

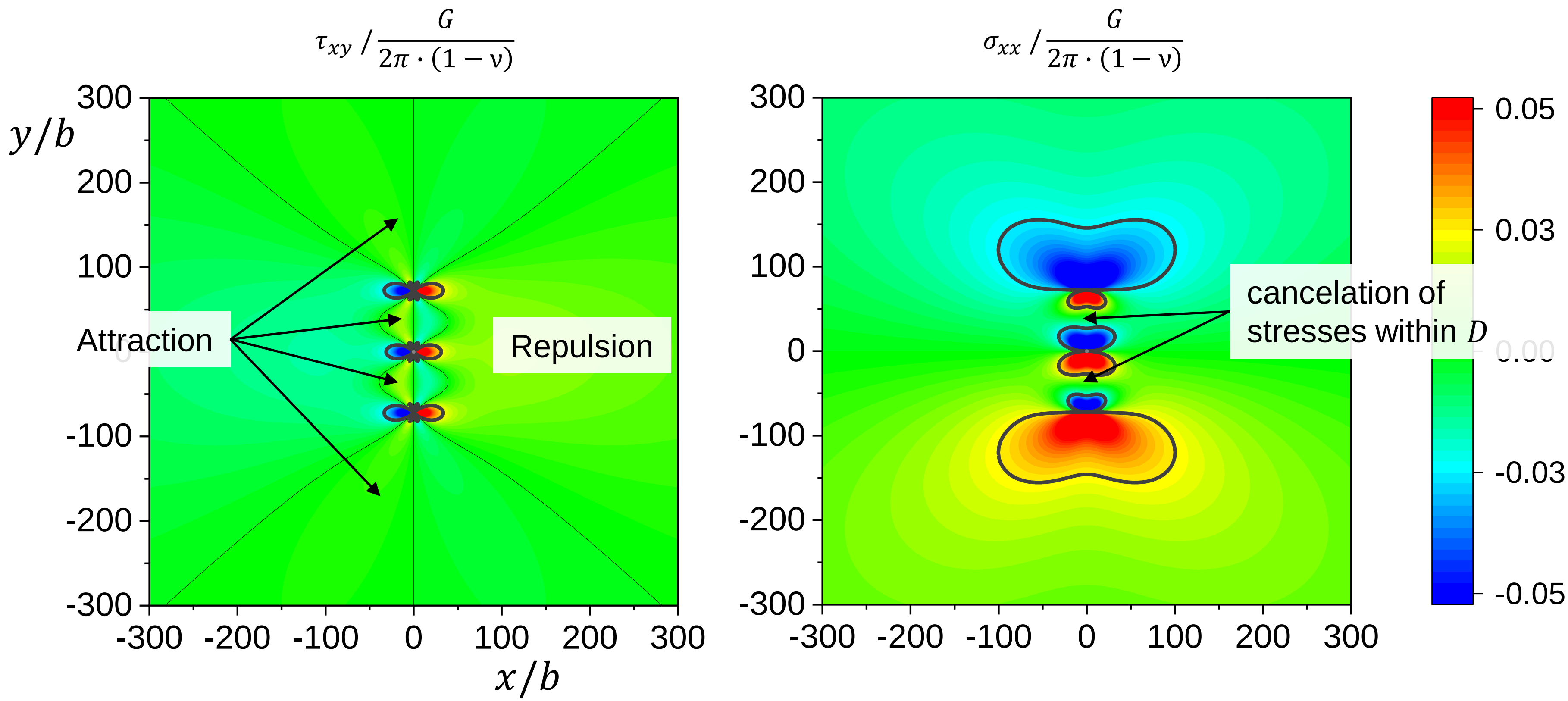
$\tau_{xy} / \frac{G}{2\pi \cdot (1-\nu)}$ | $\sigma_{xx} / \frac{G}{2\pi \cdot (1-\nu)}$



Remember: $\frac{\boldsymbol{F}}{L} = \begin{pmatrix} \pm\, b\, \tau_{xy} \\ \mp\, b\, \sigma_{xx} \\ 0 \end{pmatrix}$

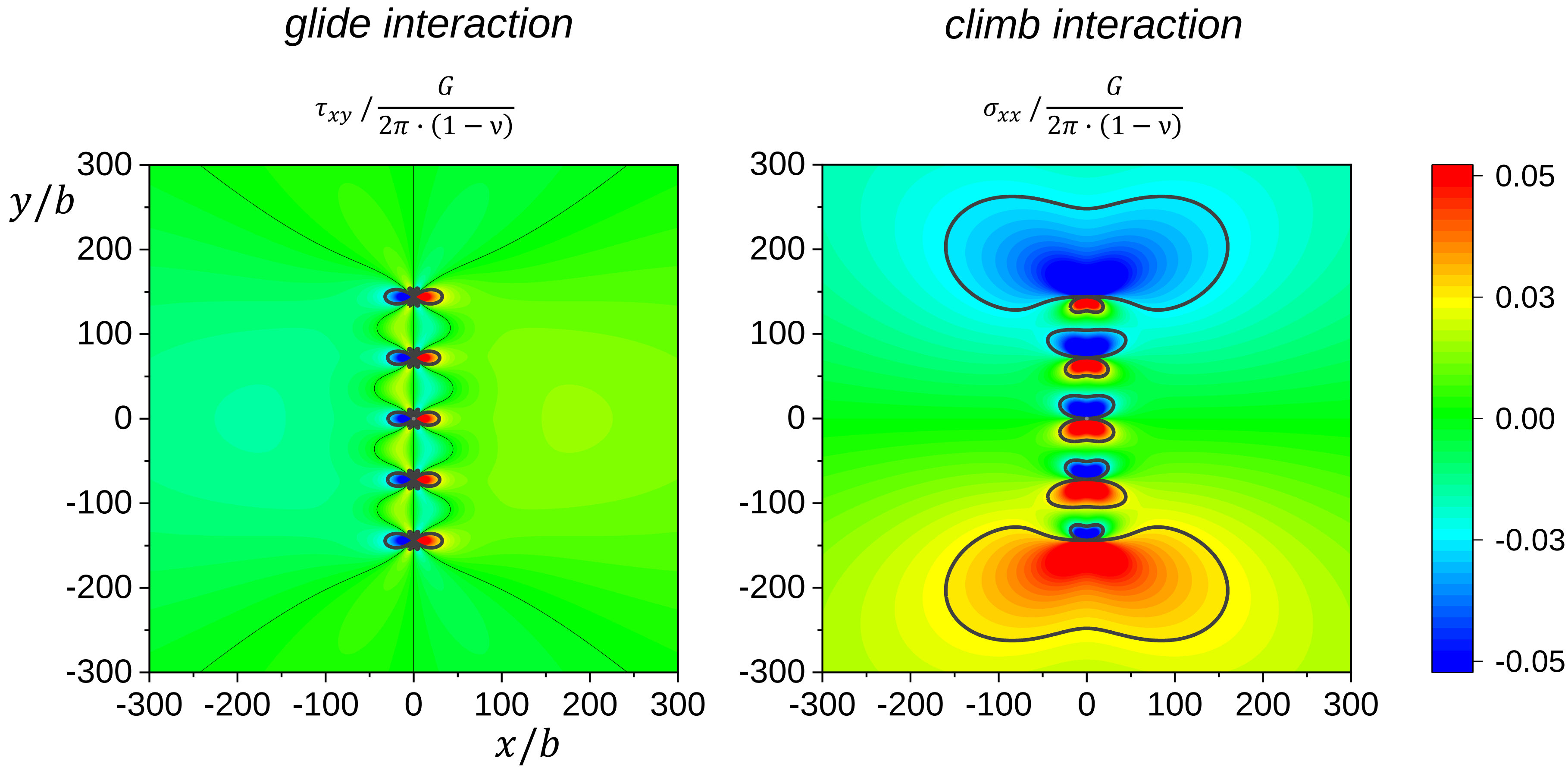
Parallel Dislocations – Low Angle Grain Boundaries

glide interaction *climb interaction*



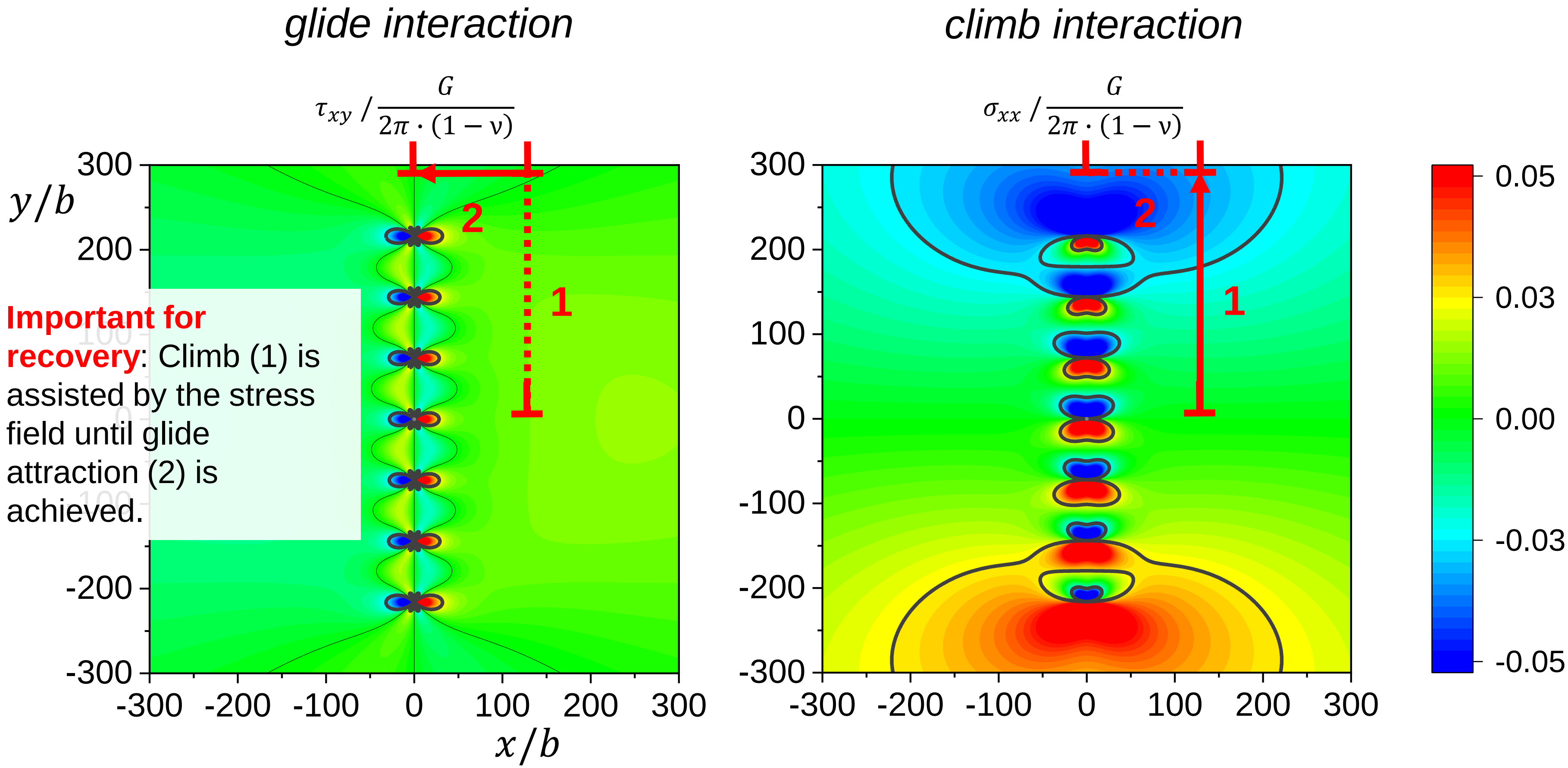
Three, stacked edge dislocations with $D = 72b$ ($\Theta \approx 0.8°$).

Parallel Dislocations – Low Angle Grain Boundaries



Five, stacked edge dislocations with $D = 72b$ ($\Theta \approx 0.8°$).

Parallel Dislocations – Low Angle Grain Boundaries



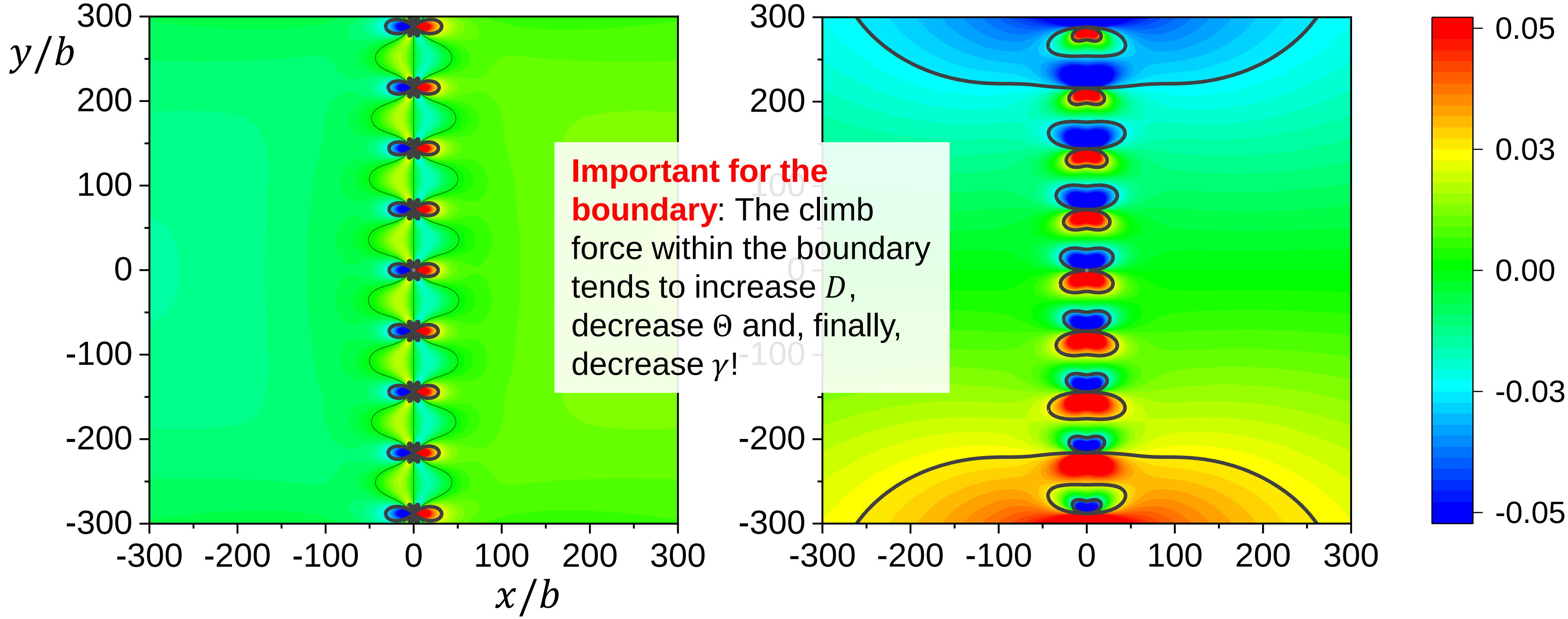
Important for recovery: Climb (1) is assisted by the stress field until glide attraction (2) is achieved.

Seven, stacked edge dislocations with $D = 72b$ ($\Theta \approx 0.8°$).

Parallel Dislocations – Low Angle Grain Boundaries

glide interaction | *climb interaction*

$\tau_{xy} \,/\, \frac{G}{2\pi \cdot (1-\nu)}$ | $\sigma_{xx} \,/\, \frac{G}{2\pi \cdot (1-\nu)}$



Important for the boundary: The climb force within the boundary tends to increase D, decrease Θ and, finally, decrease γ!

Nine, stacked edge dislocations with $D = 72b$ ($\Theta \approx 0.8°$).

Parallel Dislocations – Low Angle Grain Boundaries

- Read-Shockley's formula describes the specific grain boundary of an asymmetric tilt boundary as a function of the misorientation by the summation of the elastic energy of the dislocations in the boundary:

$$\gamma = \frac{G\, b}{4\pi\,(1-\nu)} (\cos\phi + \sin\phi)\, \Theta\, (A(\phi) - \ln\Theta)$$

- This is approximately:

$$\gamma \approx \frac{\alpha\, G\, b}{4\pi\,(1-\nu)}\, \Theta\, (1 - \ln\Theta)$$

Asymmetric tilt boundary in a cubic crystal by two sets of dislocations.

D. Hull, D. J. Bacon: "Introduction to Dislocations", Amsterdam, etc.: Elsevier (2011)
W. T. Read & W. Shockley: "Dislocation model of crystal grain boundaries", Physical Review 78 (1950) 275-289

Shockley, Bardeen, and the Bell labs …

- Shockley made major contributions to solid state physics of semiconductors and crystal defects. In 1956, he was awarded Nobel prize for the development of the transistor together with Bardeen and Brattain. The entire research group of Shockley at Bell labs revolutionized the world by their work on the fundamentals and applications of semiconductors. Late in his life, he was involve in publications on race, intelligence and eugenics.
- Apart from the Nobel prize for the transistor, Bardeen was awarded with a second Nobel prize (there are only three other persons with more than one Nobel prize: M. Skłodowska Curie; L. Pauling, F. Sanger) for the development of the development of the BCS (Bardeen-Cooper-Shrieffer) theory of super conductors. The Bardeen-Herring climb source (later in Ch. 4) traces back to his work.

https://de.wikipedia.org/wiki/Datei:William_Shockley,_Stanford_University.jpg
https://en.wikipedia.org/wiki/John_Bardeen#/media/File:Bardeen.jpg

Parallel Dislocations – Low Angle Grain Boundaries

- Rough estimates for Cu:

$G \approx 50\ \mathrm{GPa},\ b \approx 2.5\ \text{Å}$:

$$\frac{G\, b}{4\pi\,(1-\nu)} \approx 1420\ \mathrm{mJ/m^2}$$

At $\Theta \approx 10° = 0.174$:

$$\frac{G\, b}{4\pi\,(1-\nu)}\,\Theta(1-\ln\Theta) \approx 680\ \mathrm{mJ/m^2}$$

D. Hull, D. J. Bacon: “Introduction to Dislocations”, Amsterdam, etc.: Elsevier (2011)
W. T. Read & W. Shockley: “Dislocation model of crystal grain boundaries”, Physical Review 78 (1950) 275-289

Parallel Dislocations – Low Angle Grain Boundaries

- Rough estimates for Al:

$G \approx 25\ \text{GPa},\ b \approx 2.9\ \text{Å}$:

$$\frac{G\ b}{4\pi\ (1-\nu)} \approx 825\ \text{mJ/m}^2$$

at $\Theta \approx 10° = 0.174$:

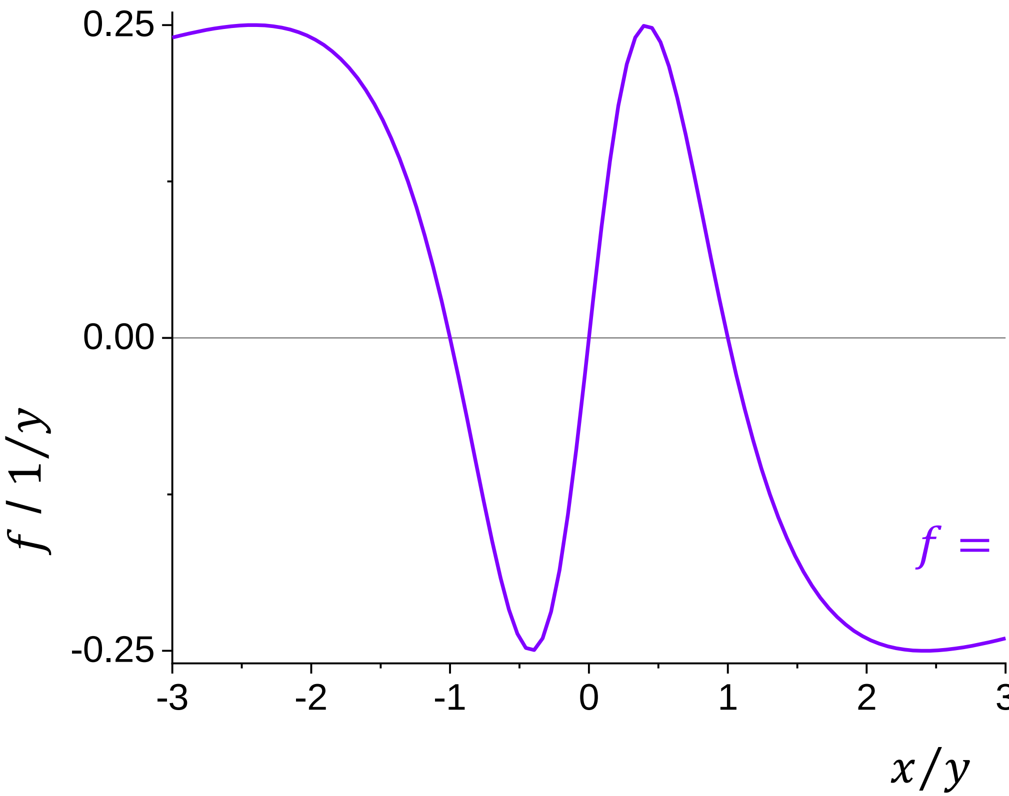
$$\frac{G\ b}{4\pi\ (1-\nu)}\ \Theta\ (1 - \ln\Theta) \approx 394\ \text{mJ/m}^2$$

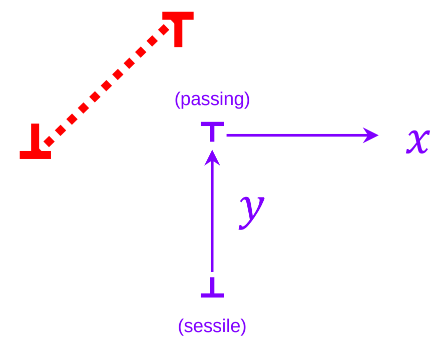
Gottstein: “Materialwissenschaft und Werkstofftechnik: Physikalische Grundlagen”, Berlin, Heidelberg: Springer Vieweg, Springer Verlag (2014)

Parallel Dislocations – Dipoles

- **Dipoles are antiparallel edge dislocations metastable arranged at an angle of 45°.**

Lateral dependence of the interaction force between a passing and a sessile dislocation. Note that the force is normalized by the reciprocal distance of the dislocations.



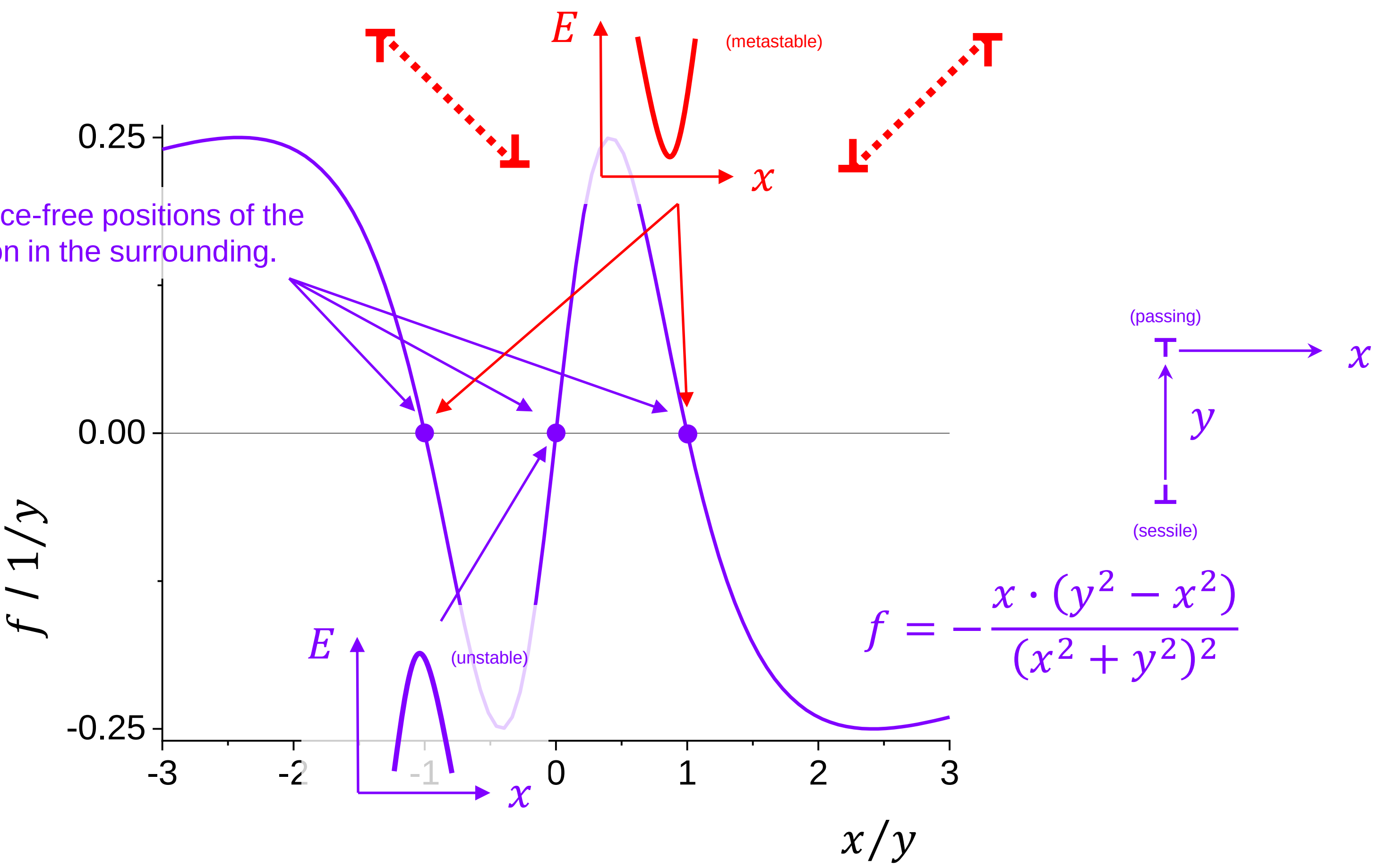


$$f = -\frac{x \cdot (y^2 - x^2)}{(x^2 + y^2)^2}$$

Parallel Dislocations – Dipoles

- **Dipoles are antiparallel edge dislocations metastable arranged at an angle of 45°.**

Lateral dependence of the interaction force between a passing and a sessile dislocation. Note that the force is normalized by the reciprocal distance of the dislocations.



Further Notes

- The important configurations described before are metastable. The zero transition of force is not sufficient to characterize the metastable configuration. It must be associated with a minimum of energy. In case of a maximum, the configuration is unstable!
- For an advanced discussion, also image forces on dislocations would have to be considered. In the vicinity of surfaces or discontinuities, the dislocation experiences a force by the surface. The math leads to terms equivalent to an attraction by a mirrored dislocation outside the body (similar to problems in electrical engineering).
- For the lecture, there is only little advance by considering this. Anyhow, in TEM experiments you have to consider that surfaces might attract dislocations as a practical relevance of this.

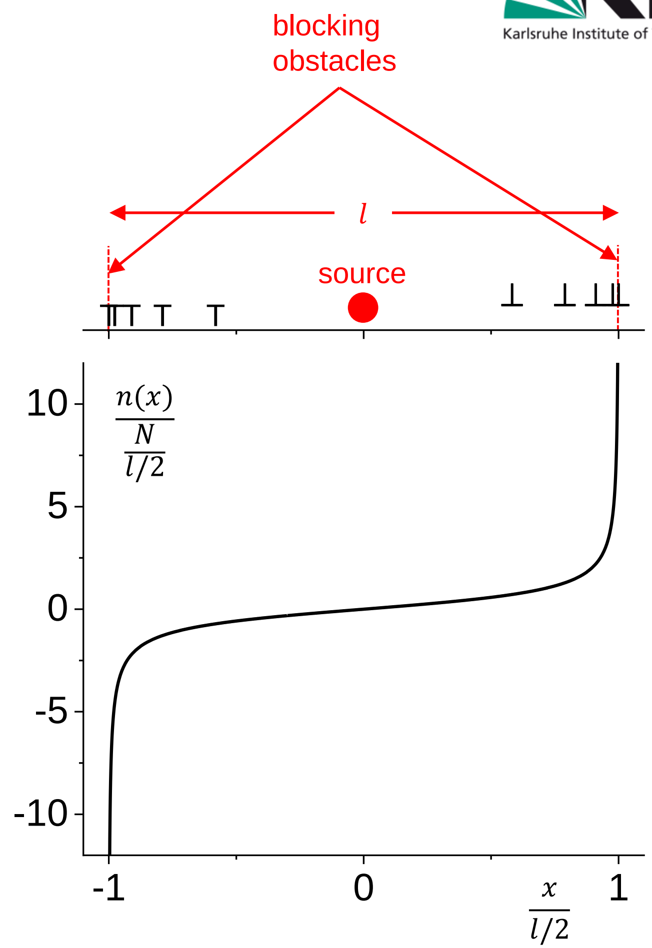
Parallel Dislocations – Pile-Ups

- When dislocations emitted from a glide source meet a barrier, **the dislocations cannot combine due to same sign**. Instead they form a (double) pile up.
- The (lateral) distribution of (edge) dislocations follows under the applied stress τ due to their interaction:

$$n(x) = \frac{(1-\nu)}{G\,b}\,\tau\,\frac{x}{\sqrt{\left(\frac{l}{2}\right)^2 - x^2}}$$

- The total number of dislocations (of equal sign) in the pile up at τ is:

$$N = \int_0^{\frac{l}{2}} n(x)\,dx = \frac{(1-\nu)\,l}{G\,b}\,\tau$$



Pile up from a glide source and the corresponding distribution of dislocations in the pile up as a function of the applied stress.

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

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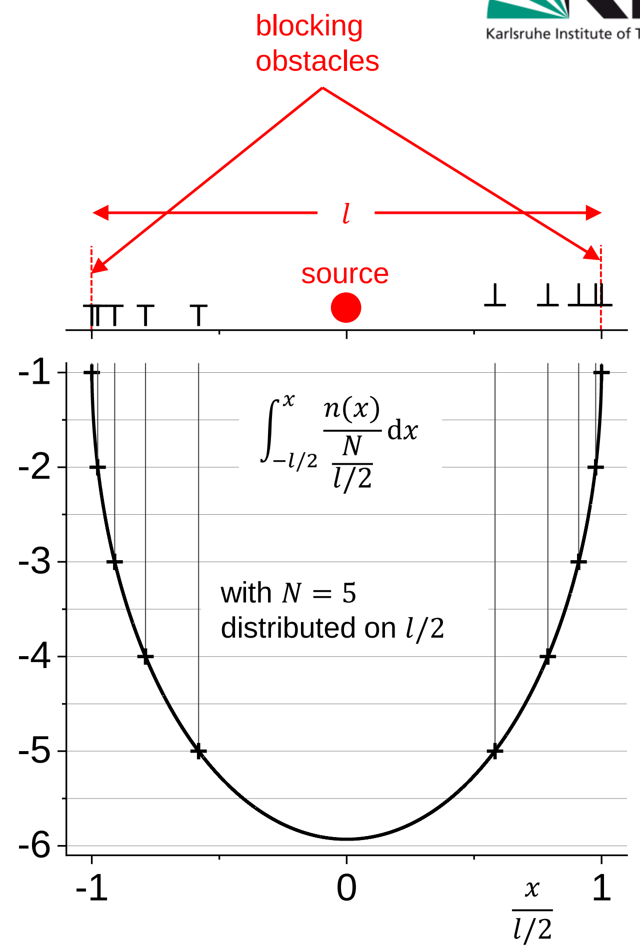

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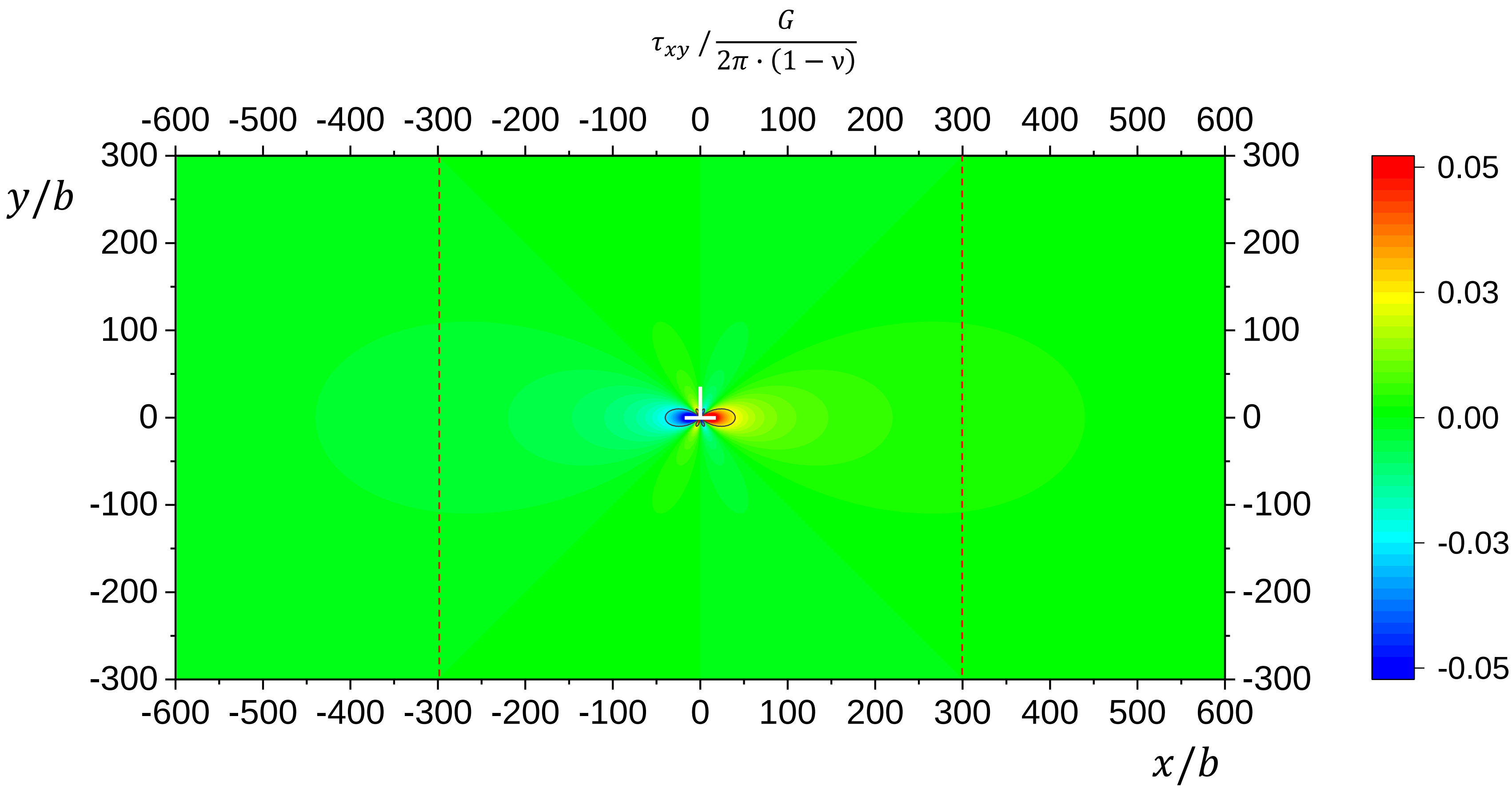
Gottstein: “Materialwissenschaft und Werkstofftechnik: Physikalische Grundlagen”, Berlin, Heidelberg: Springer Vieweg, Springer Verlag (2014)

Parallel Dislocations – Pile Ups

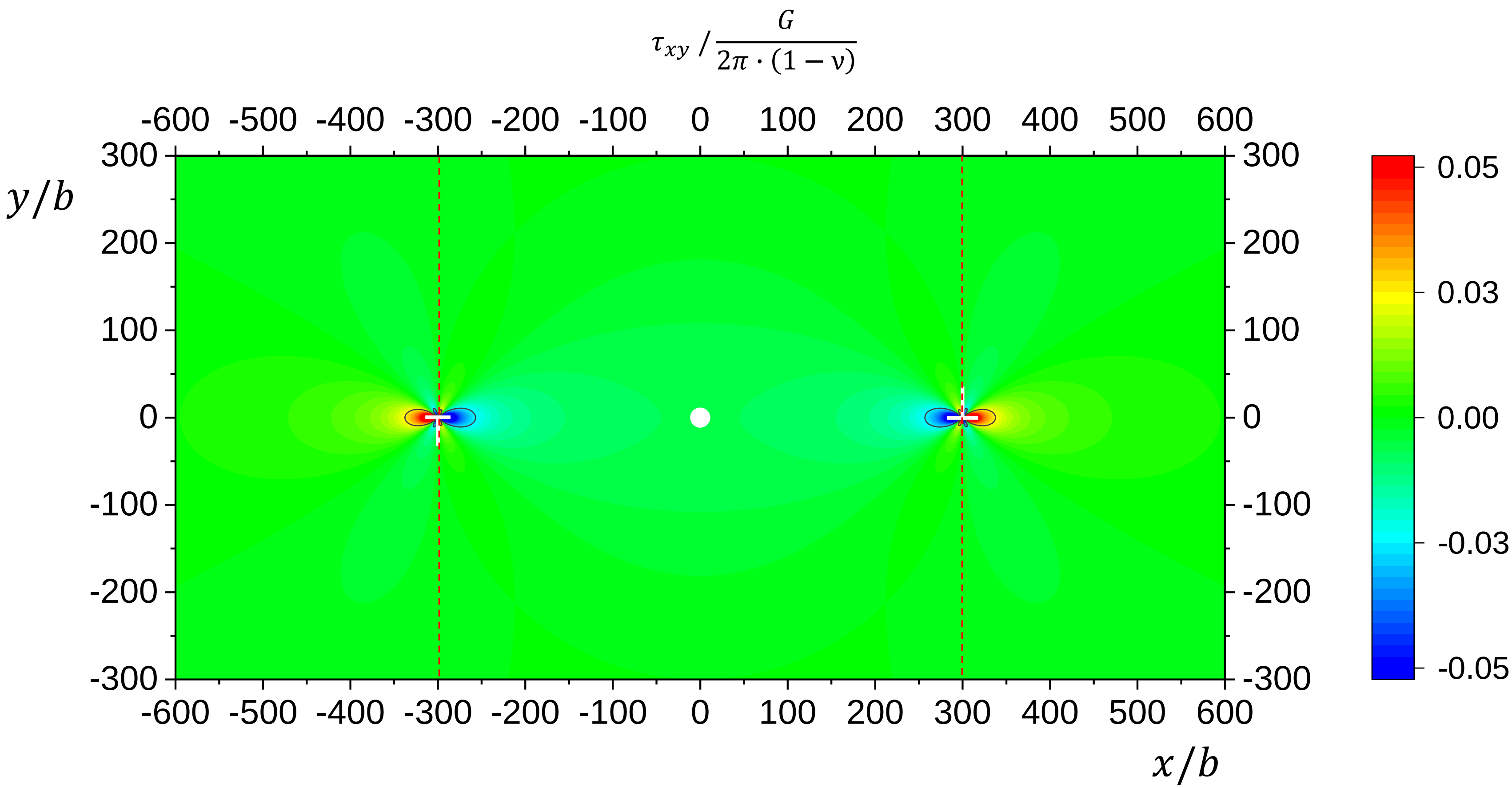
glide interaction



Single edge dislocation.

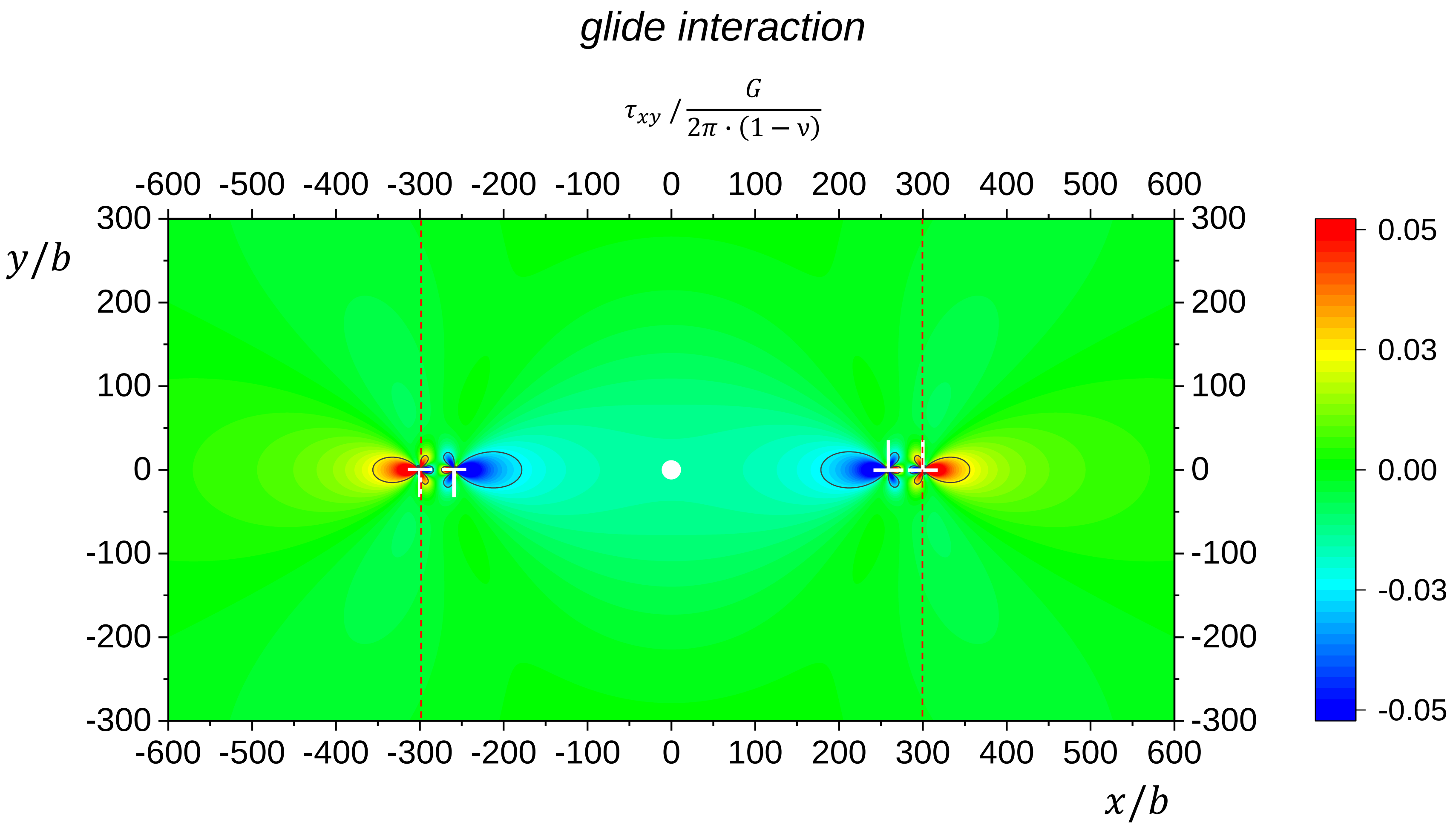
Parallel Dislocations – Pile Ups

glide interaction



One dislocation in a double pile up: $N = 1,\ l = 600b,\ \tau = \frac{1}{600}\frac{Gb}{1-\nu}$.

Parallel Dislocations – Pile Ups

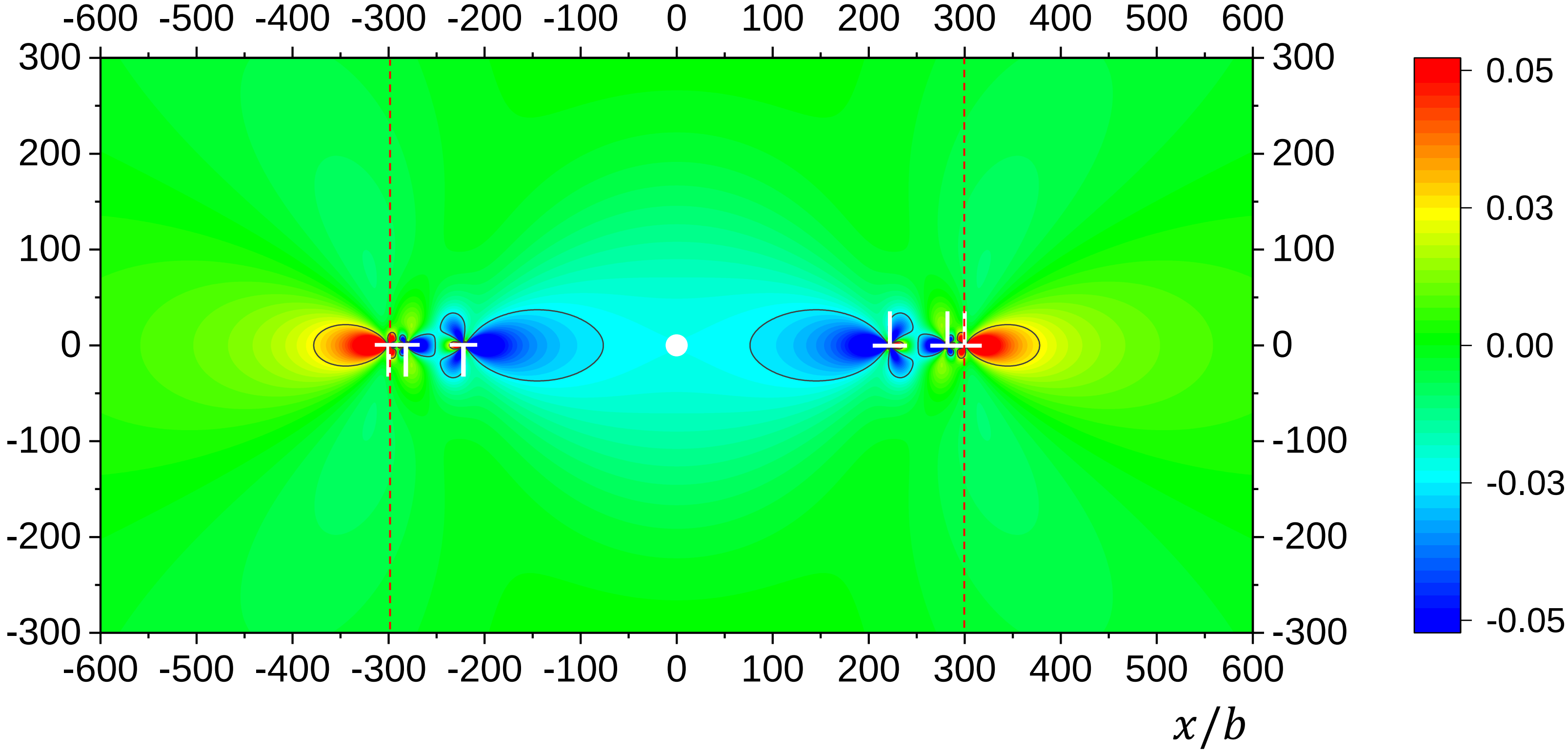


Two dislocations in a double pile up: $N = 2,\ l = 600b,\ \tau = \frac{1}{300}\frac{Gb}{1-\nu}$.

Parallel Dislocations – Pile Ups

glide interaction

$$\tau_{xy} \,/\, \frac{G}{2\pi \cdot (1-\nu)}$$

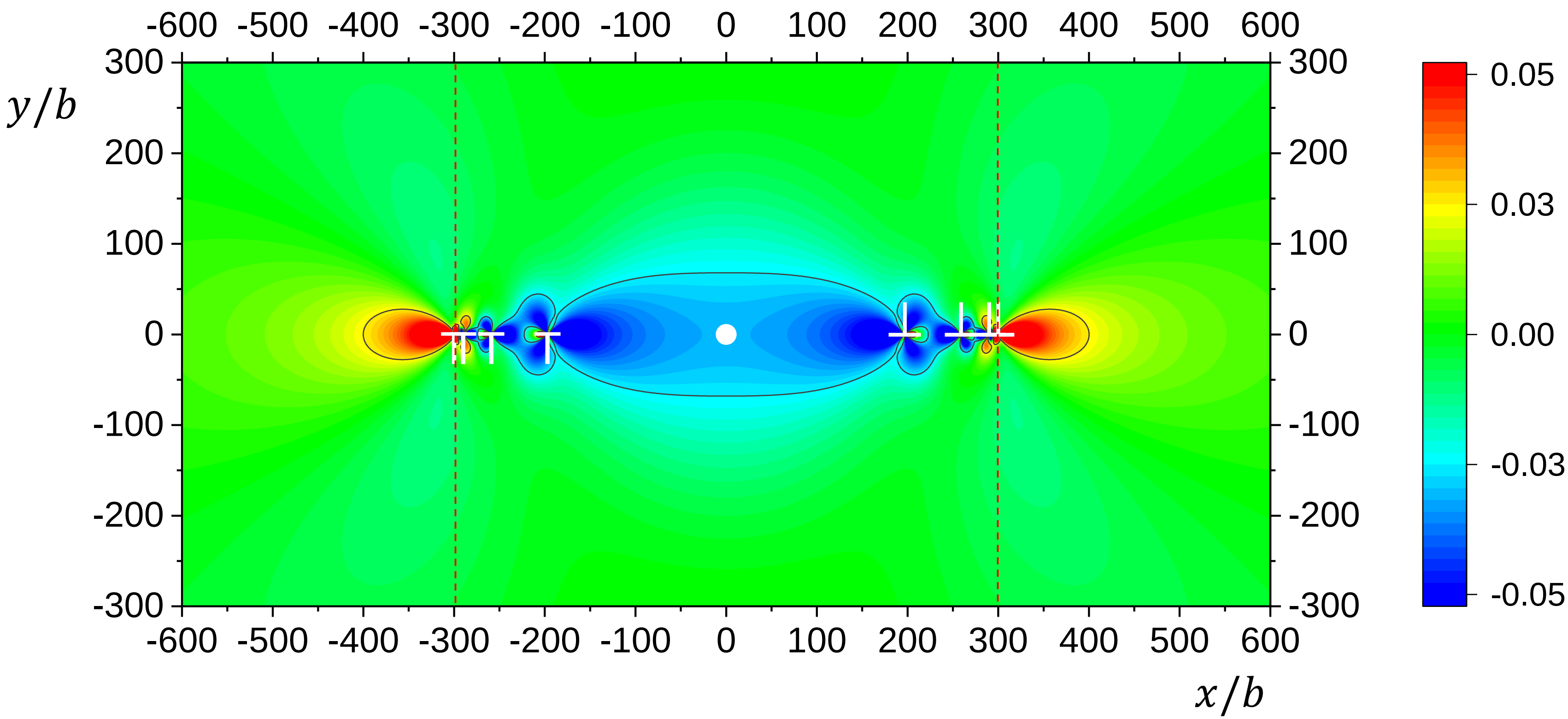


Three dislocations in a double pile up: $N = 3,\ l = 600b,\ \tau = \frac{1}{200}\frac{Gb}{1-\nu}$.

Parallel Dislocations – Pile Ups

glide interaction

$$\tau_{xy} \Big/ \frac{G}{2\pi \cdot (1-\nu)}$$

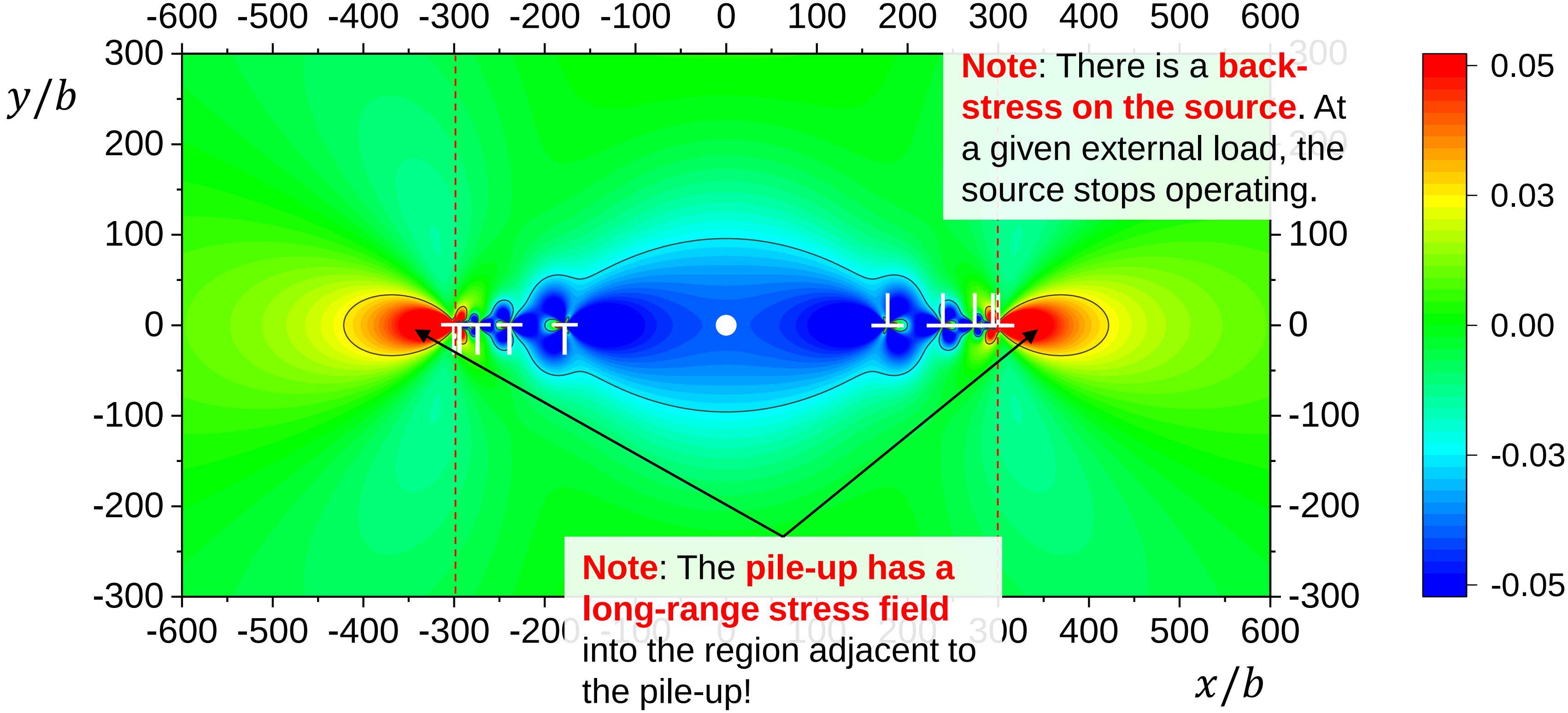


Four dislocations in a double pile up: $N = 4,\ l = 600b,\ \tau = \frac{1}{150}\frac{Gb}{1-\nu}$.

Parallel Dislocations – Pile Ups

glide interaction

$\tau_{xy} / \frac{G}{2\pi \cdot (1-\nu)}$



Note: There is a **back-stress on the source**. At a given external load, the source stops operating.

Note: The **pile-up has a long-range stress field** into the region adjacent to the pile-up!

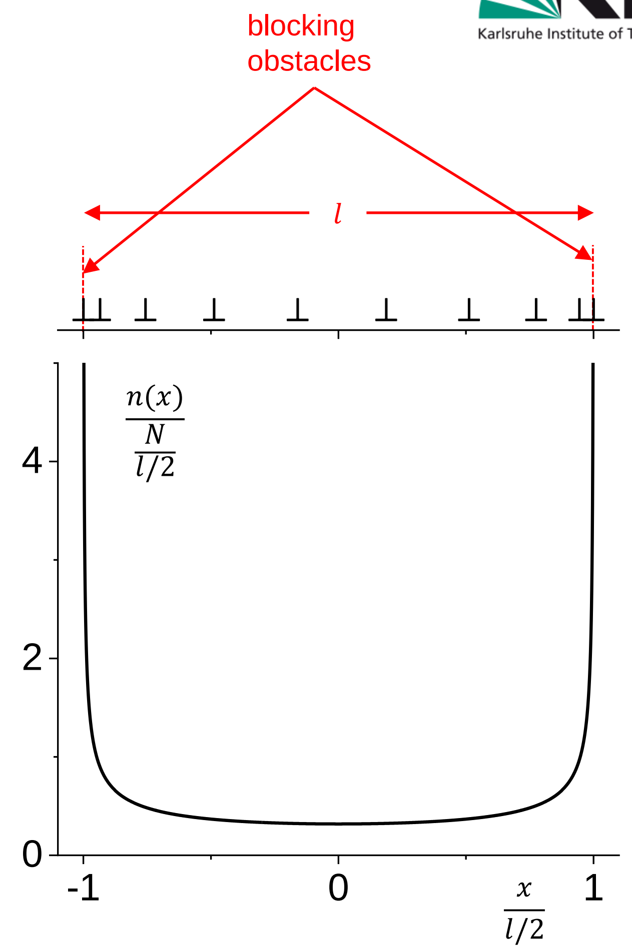
Five dislocations in a double pile up: $N = 5,\ l = 600b,\ \tau = \frac{1}{200}\frac{Gb}{1-\nu}$.

Parallel Dislocations – Pile Ups

- The (single) pile-up exists without stress by the repulsion of the dislocations with a lateral distribution of:

$$n(x) = \frac{2N}{\pi\, l \sqrt{\left(\frac{l}{2}\right)^2 - x^2}}$$

- The single pile-up acts as a single super dislocation with $b_S = N\, b$.



Pile-up from a glide source and the according distribution of dislocations in the pile-up as a function of the applied stress.

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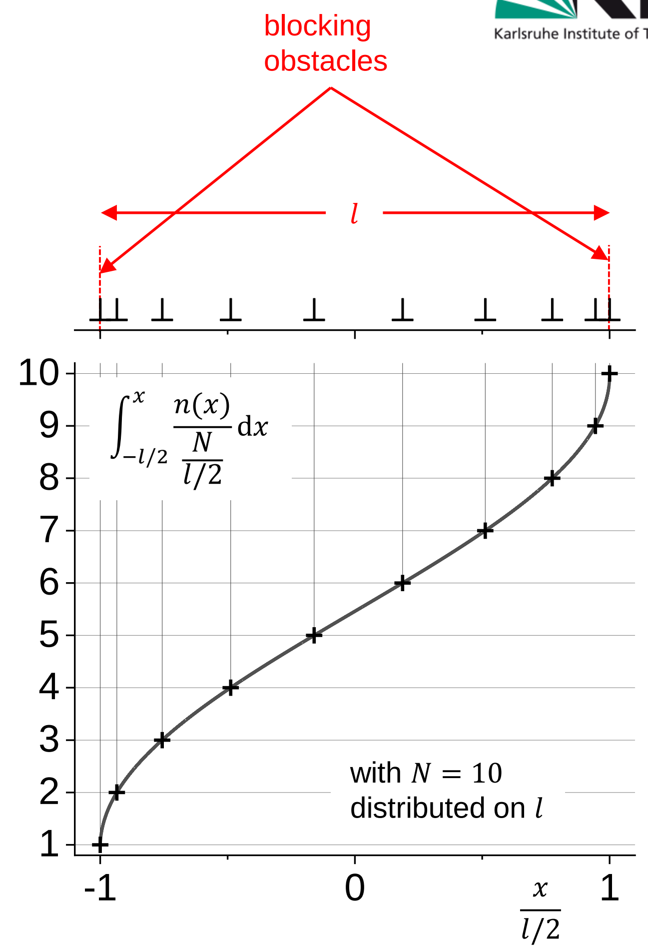

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Parallel Dislocations – Pile Ups

glide interaction

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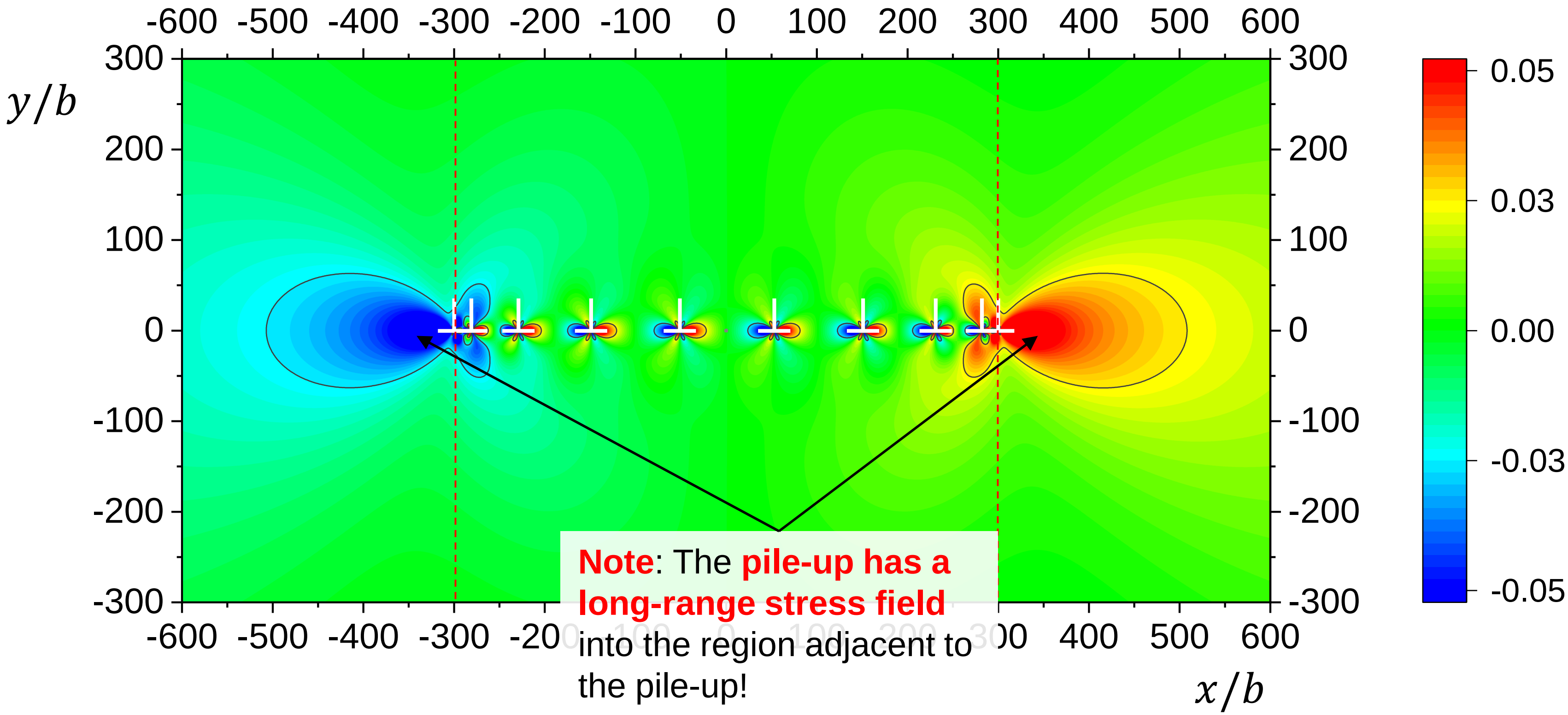


Note: The **pile-up has a long-range stress field** into the region adjacent to the pile-up!

Ten dislocations in a double pile up: $N = 10,\ l = 600b,\ \tau = 0.$

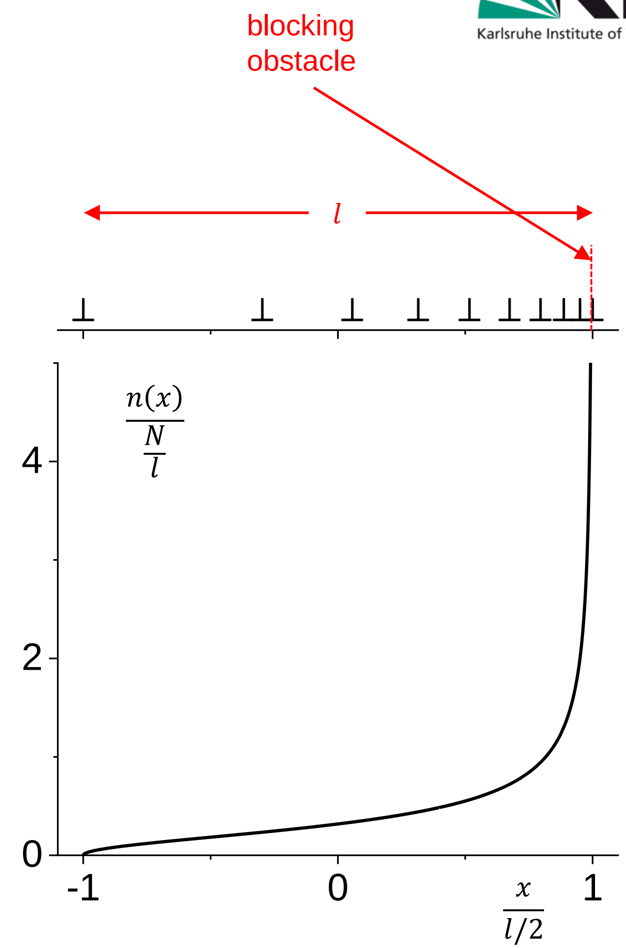
Parallel Dislocations – Pile Ups

- Under applied stress, the (single) pile-up changes and exhibits following asymmetric lateral distribution then:

$$n(x) = \frac{2(1-\nu)}{G\ b}\ \tau \sqrt{\frac{\frac{l}{2}+x}{\frac{l}{2}-x}}$$

- Note that the dislocations will in this case distribute over the length l for a given number of dislocations N and an applied stress τ:

$$l = \frac{G\ N\ b}{\pi\ (1-\nu)\ \tau}$$



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Parallel Dislocations – Pile Ups

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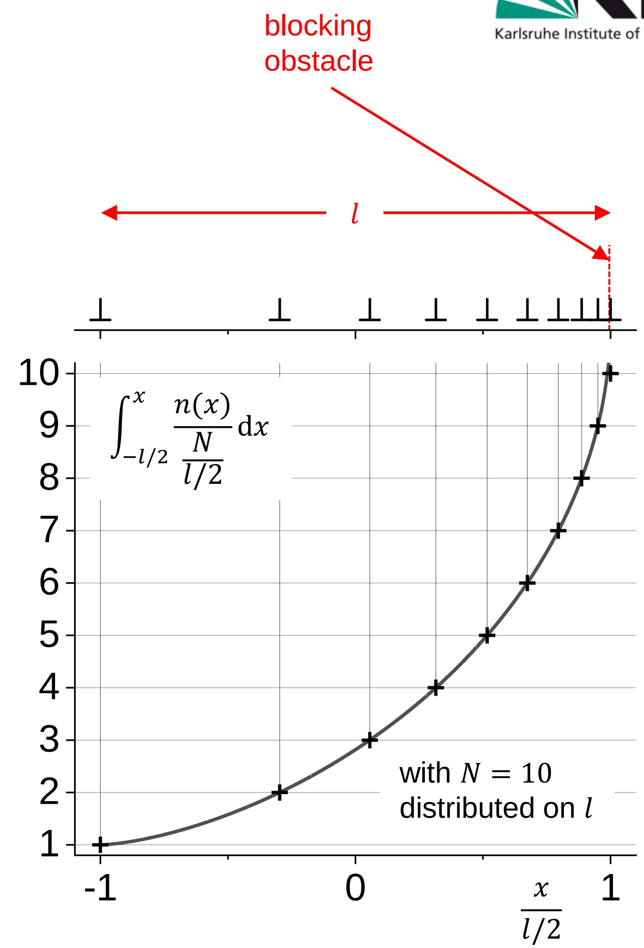

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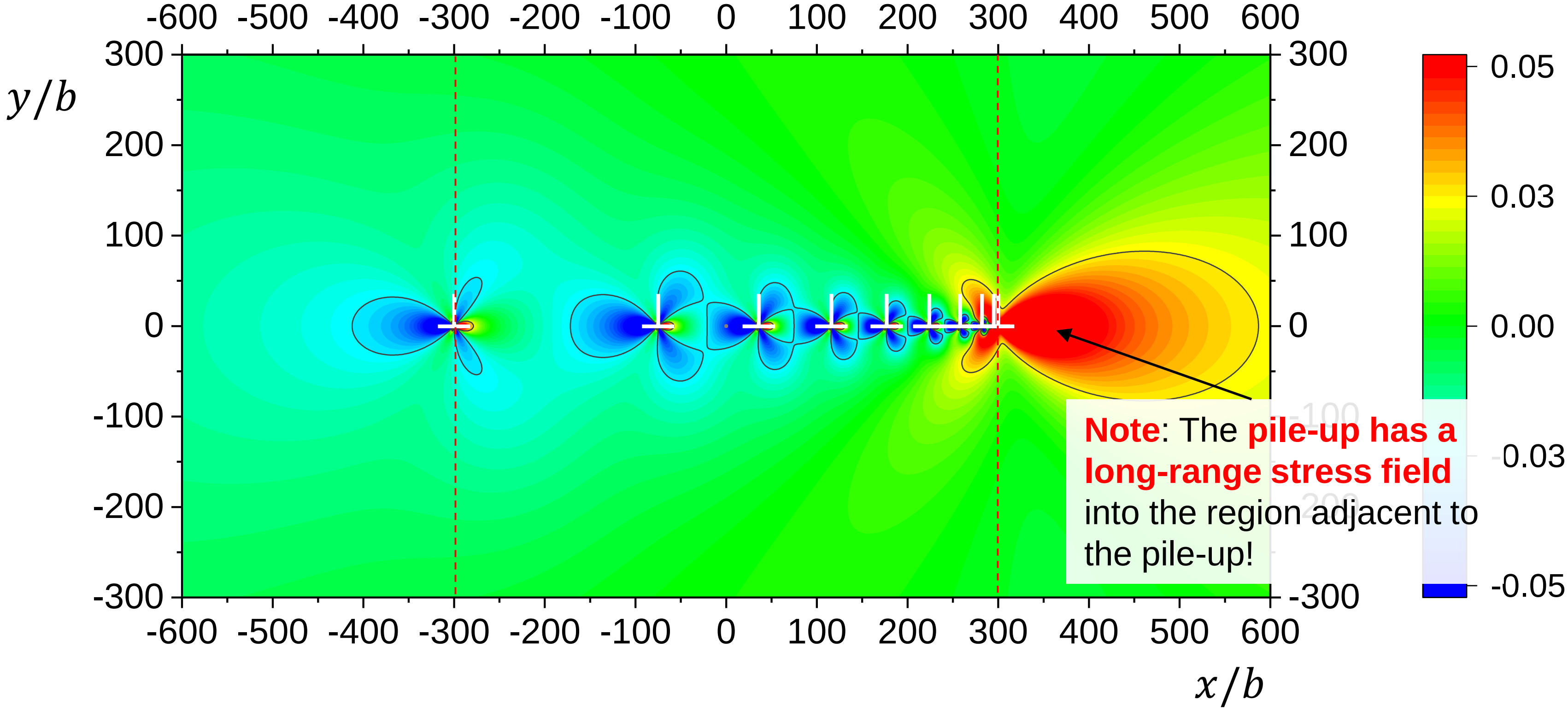


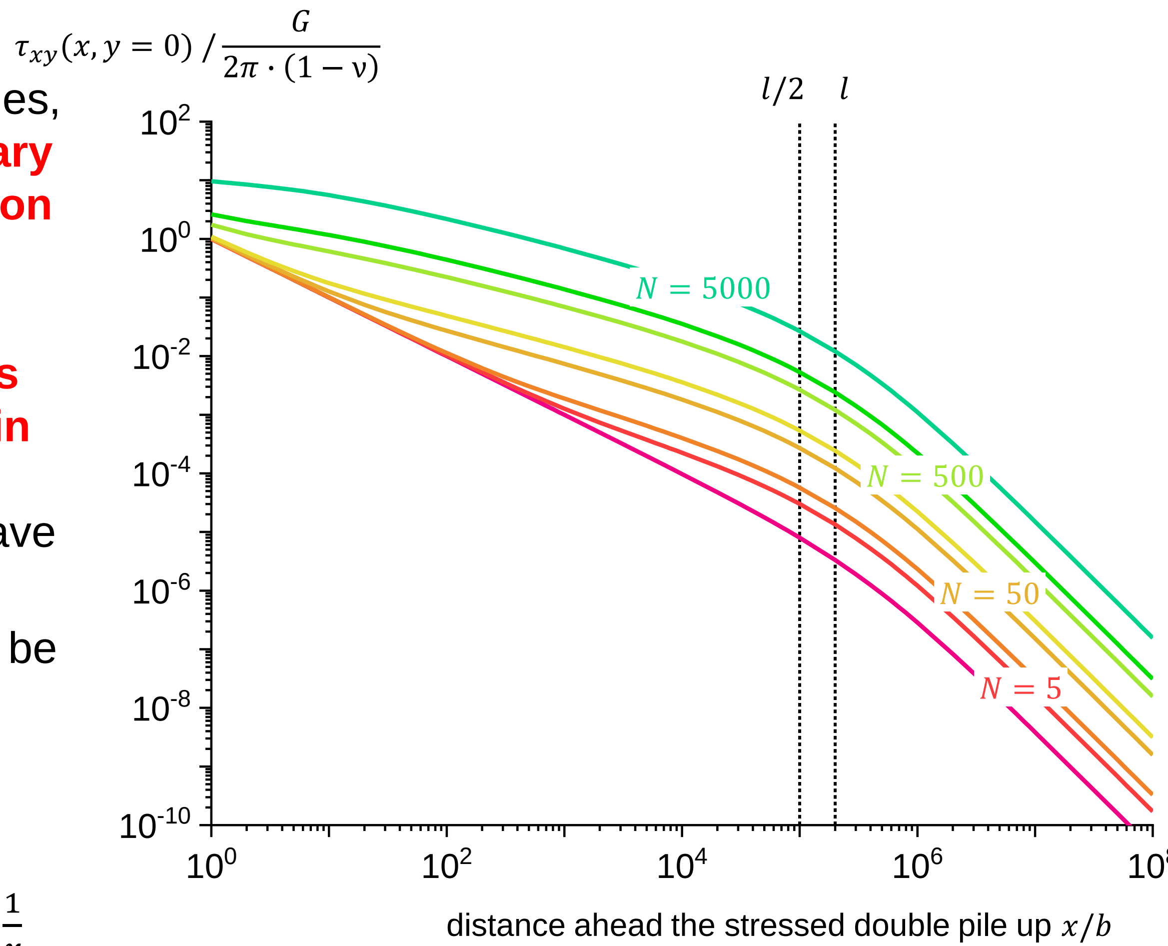
Ten dislocations in a double pile up: $N = 10,\ l = 600b,\ \tau = \frac{1}{188}\frac{Gb}{1-\nu}$.

Grain Boundary Strengthening

- The interpretation of **grain boundary strengthening with the empirical Hall-Petch relationship** $\sigma_\mathrm{y} = \sigma_0 + \frac{k}{\sqrt{D}}$ (see fundamental lectures) **can be based on** the **stress fields ahead pile ups**.
- In all instances, a **grain with operating sources** are considered that produce pile ups at its grain boundary. The length of the pile up corresponds to roughly the grain size D in case of a double pile up or half of the grain size $D/2$ in case of a stressed single pile up.
- In some cases, **neighboring grains might be unfavorable for slip** due to their orientation.
- **Macroscopic yield** (as it is necessary for σ_y) is only observed, **when all grains exhibit slip** activity. Hence, the **stress fields of pile ups** need to **operate dislocation sources** (Ch. 4f) **in the neighboring grains**.

Grain Boundary Strengthening

- As seen on the previous slides, **a pile up at a grain boundary leads to a stress distribution in the neighboring grain**.
- It can be obtained by the **superposition of the stress fields by the dislocations in the pile up** (in principle all stress components would have to be considered).
- **Three distinct regions** can be obtained:
  - a stress concentration immediate in/at the grain boundary τ_{GB}
  - a near-field $\tau_{\mathrm{NF}} \propto \frac{1}{\sqrt{x}}$ or $\propto \frac{1}{x}$
  - a far-field $\tau_{\mathrm{FF}} \propto \frac{1}{x^2}$



Examples for the stress distributions ahead double pile ups for $l/2 = 200000b$ and several N dislocations. Note that other components of the stress fields might also be considered and the angular distribution omitted here. x starts at the grain boundary.

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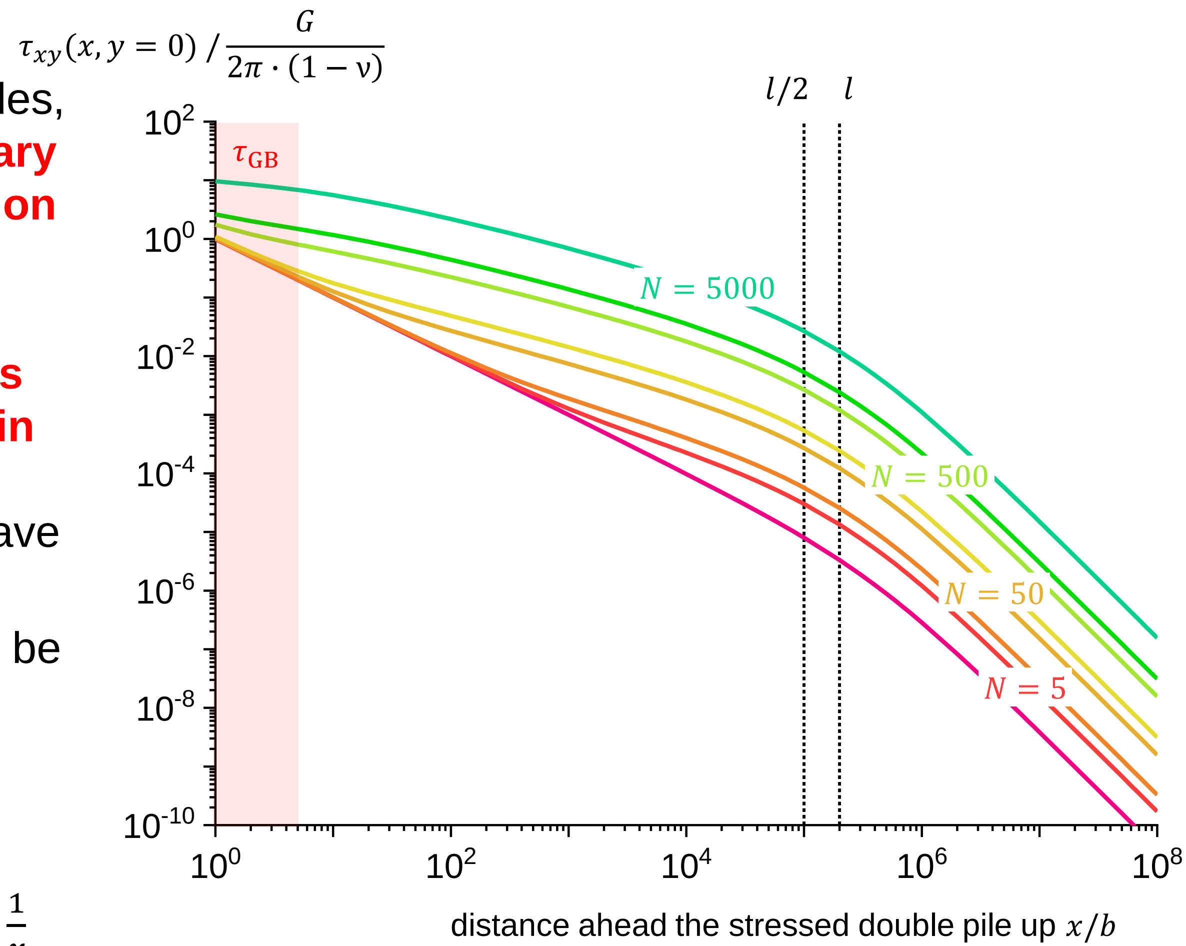

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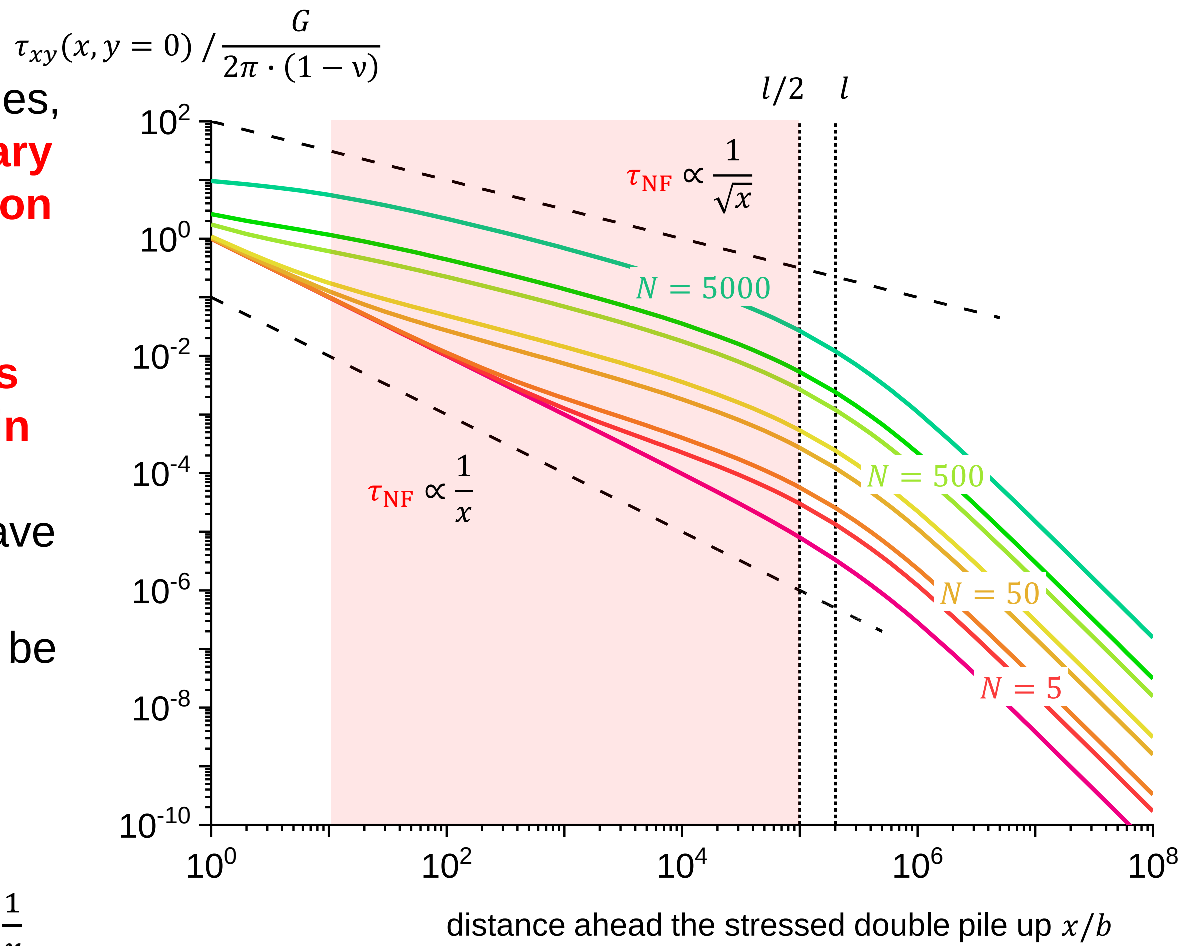

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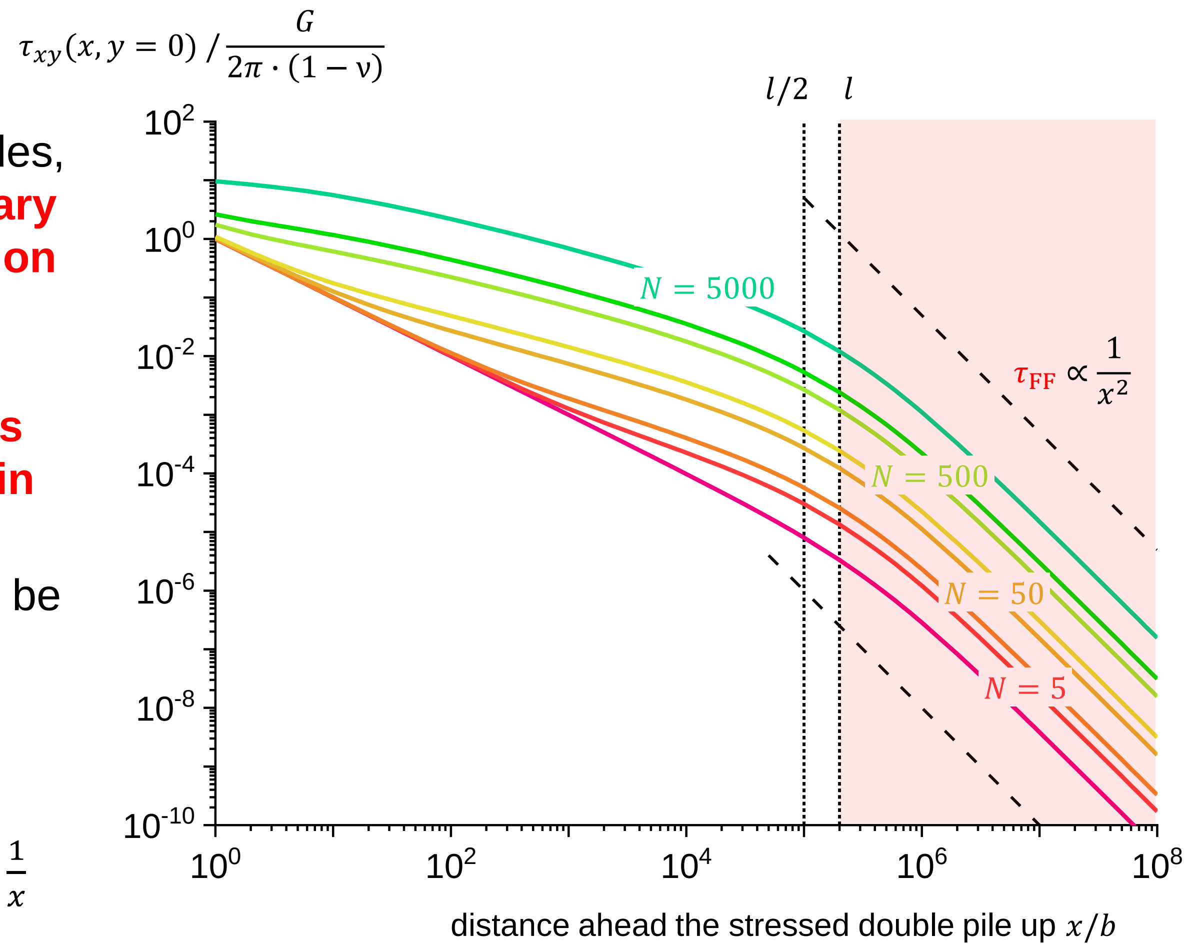

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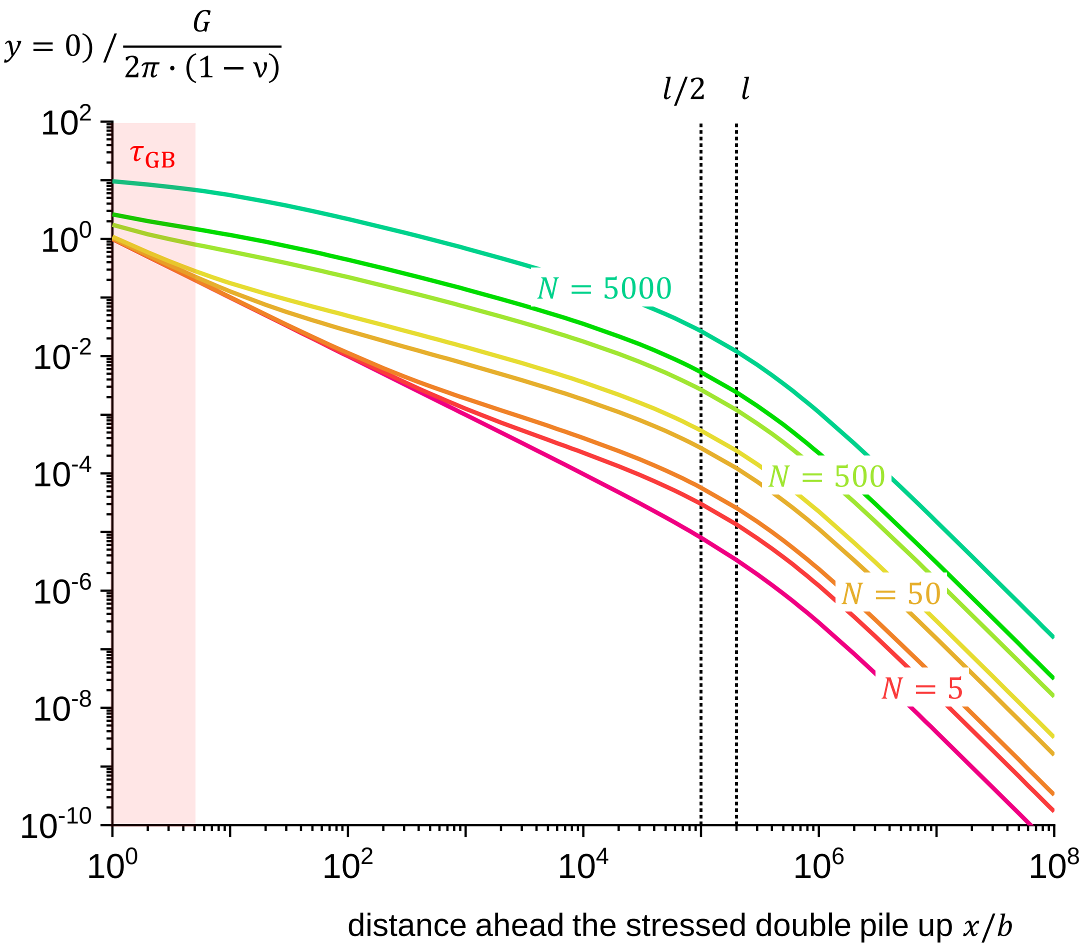
Grain Boundary Strengthening – grain boundary source

- The τ_{GB} might reach a critical stress τ_{GBS} to **activate a grain boundary dislocation source** (Ch. 4f).
- τ_{GBS} can be considered high in comparison to stresses to operate other types of dislocation sources. As a very rough estimate $\tau_{\mathrm{GBS}} \approx \frac{G}{2\pi}$ might be assumed.



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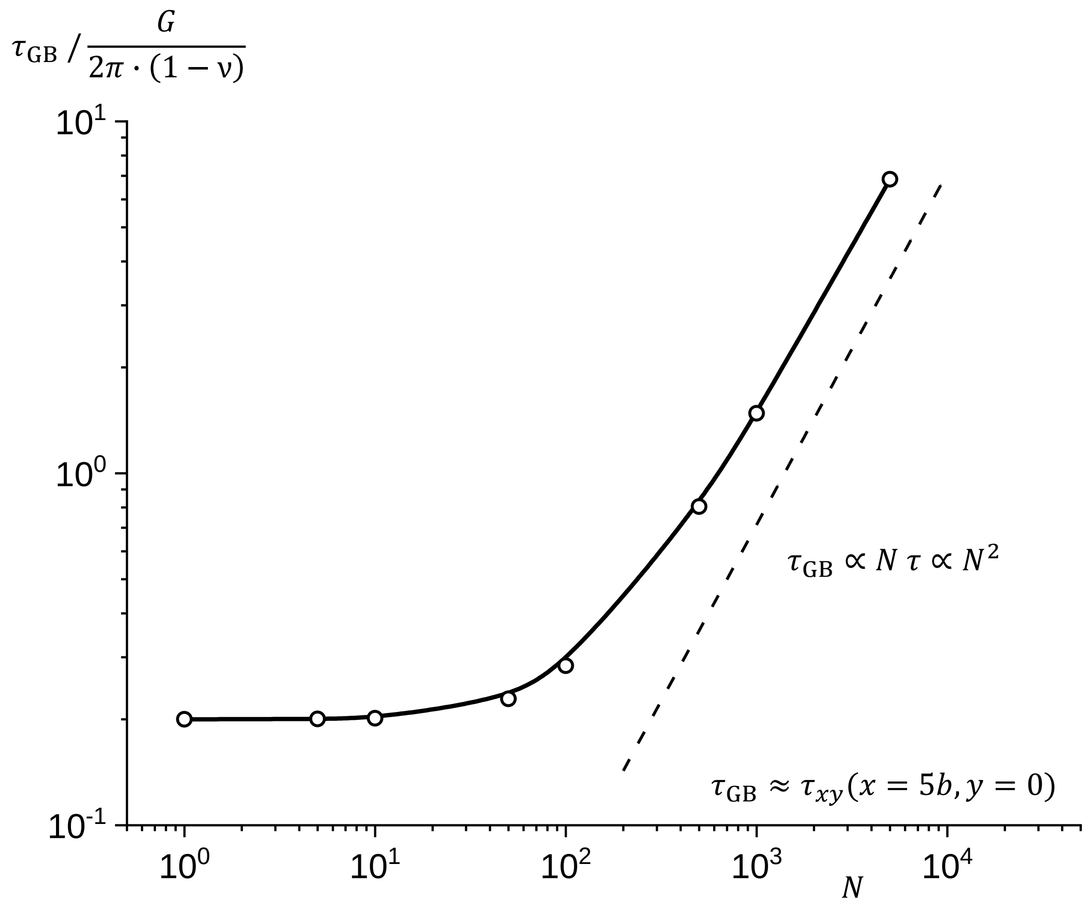


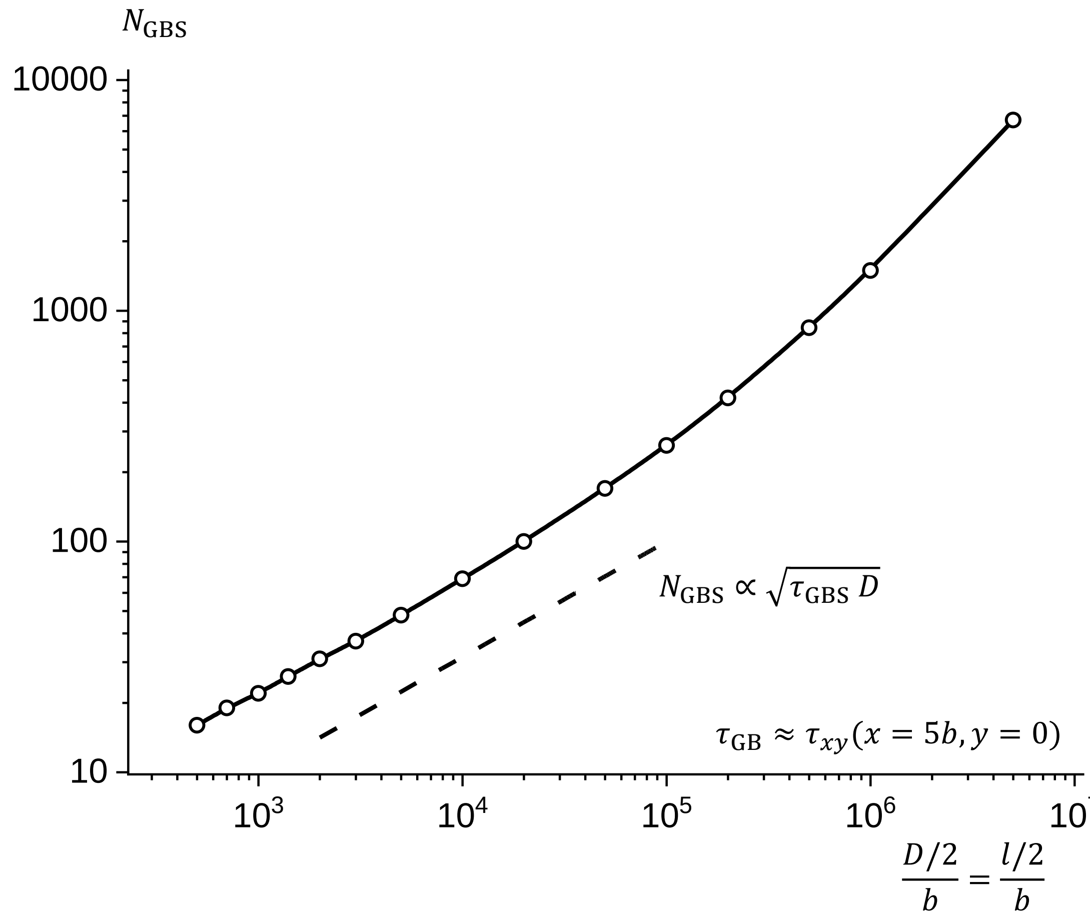
Stress in the grain boundary τ_{GB} ahead a pile up of $D/2 = l/2 = 200000b$ as function number of dislocations in the pile up N.

Grain Boundary Strengthening – grain boundary source

- The number of dislocations in the pile up N_{GBS} to obtain $\tau_{\mathrm{GB}}|_{N=N_{\mathrm{GBS}}} = \tau_{\mathrm{GBS}}$ depends on the length of the pile up l and, thus, grain size D.
- The applied stress τ_{y} to obtain this N_{GBS} dislocations in the pile up is (see previous slides on the pile ups):

$$\tau_{\mathrm{y}} = \frac{N_{\mathrm{GBS}}\, b}{l} \frac{G}{(1-\nu)}$$

- Note that the applied critical stress τ_{y} is orders of magnitude lower than τ_{GB}.

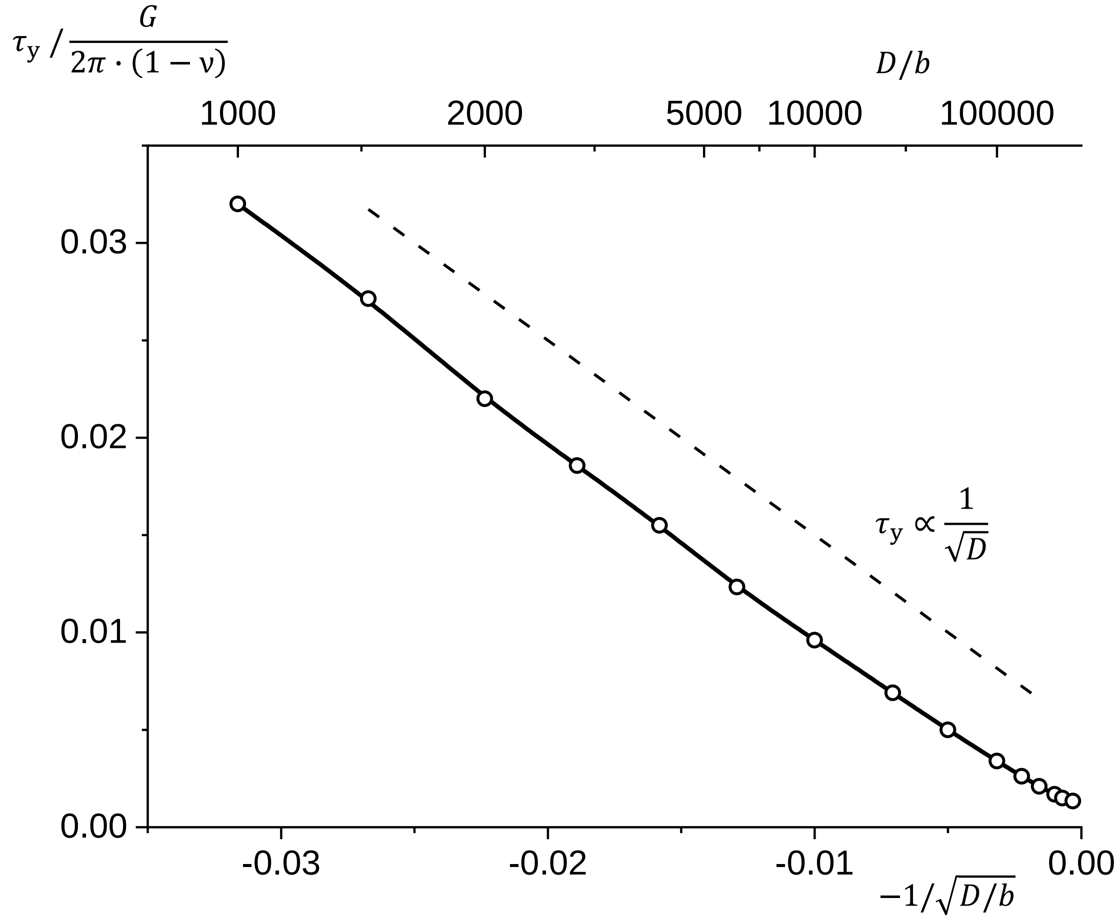


Number of dislocations in the pile up N_{GBS} necessary to operate a grain boundary dislocation source with $\tau_{\mathrm{GB}} = \tau_{\mathrm{GBS}} \approx \frac{G}{2\pi}$.

Grain Boundary Strengthening – grain boundary source

- Indeed, the applied stress τ_y to obtain N_{GBS} dislocations and, thus, to initiate yielding in the pile up follows $1/\sqrt{D}$:

$$\tau_y \propto \frac{1}{\sqrt{D}}$$



Necessary applied stress τ_y to operate the grain boundary source. Yielding occurs.

Grain Boundary Strengthening – grain boundary source

- The rough estimate using:

$$\tau_{\mathrm{GB}} \approx N\,\tau = \frac{(1-\nu)\,D}{G\,b}\tau^2$$

- with

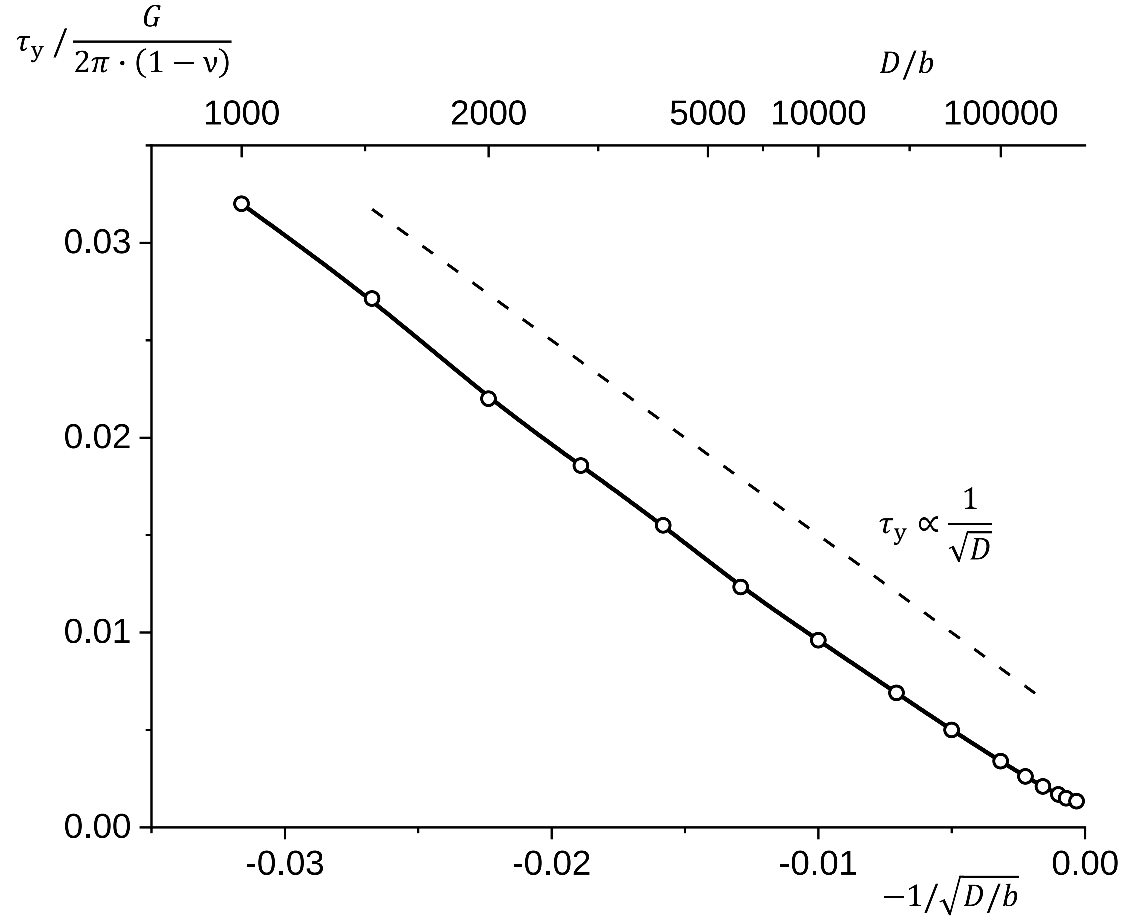
$$\tau_{\mathrm{GB}}\Big|_{\tau=\tau_{\mathrm{y}}} = \tau_{\mathrm{GBS}}$$

- yields

$$\tau_{\mathrm{y}} = \sqrt{\frac{\tau_{\mathrm{GBS}}\,G\,b}{(1-\nu)}\frac{1}{\sqrt{D}}}$$

- Assuming $\tau_{\mathrm{GBS}} \approx \frac{G}{2\pi}$:

$$\tau_{\mathrm{y}} \approx \sqrt{\frac{G^2\,b}{2\pi(1-\nu)}\frac{1}{\sqrt{D}}}$$



Necessary applied stress τ_{y} to operate the grain boundary source. Yielding occurs.

Grain Boundary Strengthening – grain boundary source

Karlsruhe Institute of Technology

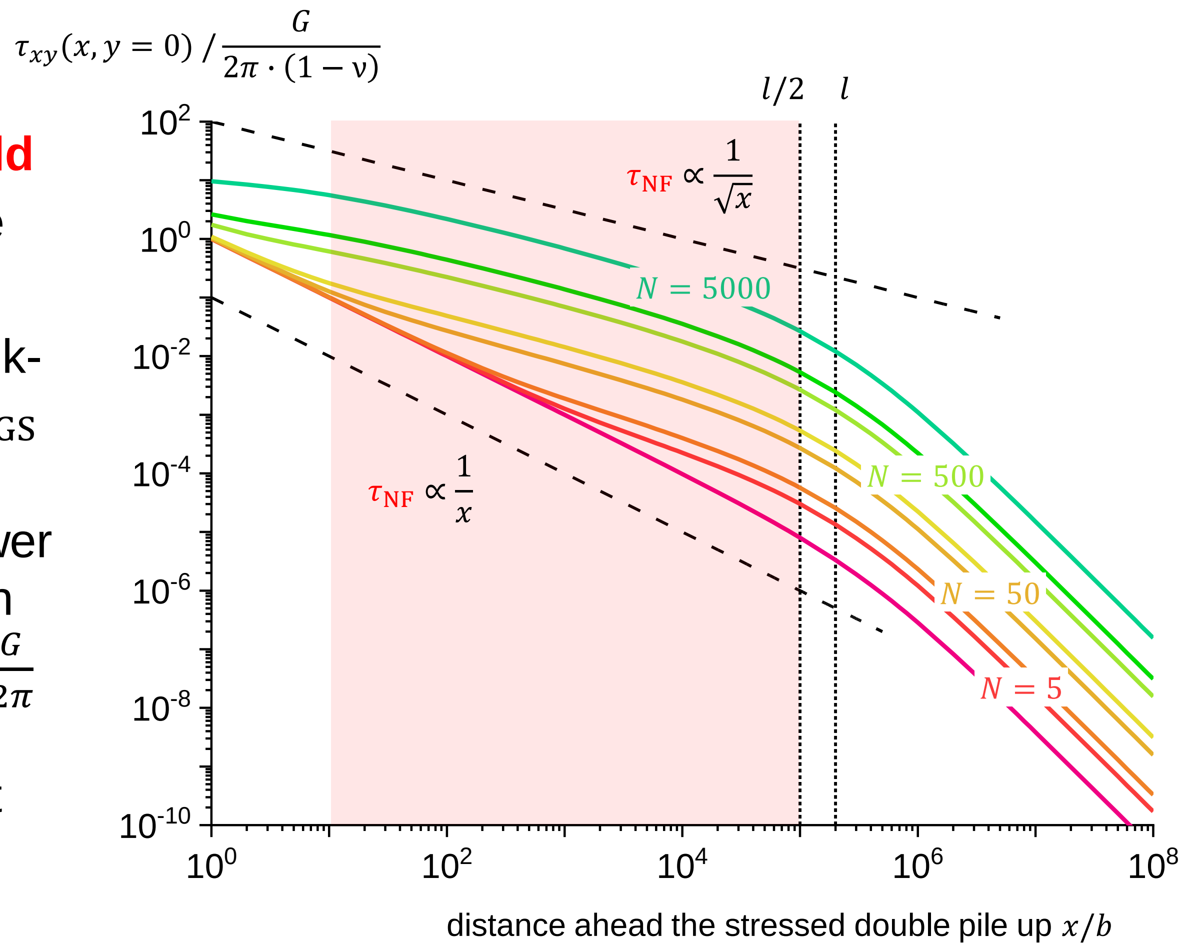
- For example, data for Cu with $G \approx 50\ \mathrm{GPa}$, $b \approx 2.5\ \mathrm{Å}$, $\nu \approx 0.3$ yields:
$$\tau_\mathrm{y} \approx \frac{0.38\ \mathrm{MPa}\sqrt{\mathrm{m}}}{\sqrt{D}}$$
- Transfer to macroscopic yield strength in tensile tests (normal stresses) can be obtained by multiplication with the Taylor factor M_T ($M_\mathrm{T} = 3.06$ for A1 and A2 assuming simple slip systems, Ch. 6a):
$$\sigma_\mathrm{y} = M_\mathrm{T}\,\tau_\mathrm{y} = \frac{1.15\ \mathrm{MPa}\sqrt{\mathrm{m}}}{\sqrt{D}}$$
- Apart from all roughness of this estimate, the order of magnitude is almost met.

metal	σ_0 / MPa	k / MPa$\sqrt{\mathrm{m}}$	k / $G\sqrt{b}$
A1 (fcc, Cu prototype)			
Ni	80	0.23	0.2
Cu	**40**	**0.11**	**0.1**
Ag	60	0.1	0.2
Au	150	0.08	0.2
Al	10	0.09	0.2
A2 (bcc, W prototype)			
V	150	0.38	0.5
Nb	120	0.34	0.5
Ta	80	0.76	0.7
Cr	320	0.8	0.4
Mo	270	0.63	0.3
W	800	1	0.4
Fe	130	0.31	0.2

Z. C. Cordero, B. E. Knight and C. A. Schuh: "Six decades of the Hall–Petch effect – a survey of grain-size strengthening studies on pure metals", International Materials Reviews 61 (2016) 495-51

Grain Boundary Strengthening – glide source

- Alternatively, the **near field stress $\tau_{\mathrm{NF}} \propto \frac{1}{\sqrt{x}}$** of the pile up might **activate a glide source** (for example Frank-Read Source, Ch. 4f) at τ_{GS} in the adjacent grain.
- τ_{GS} can be considered lower than τ_{GBS}. As a very rough estimate $\tau_{\mathrm{GS}} \approx 2Gb\sqrt{\rho} \ll \frac{G}{2\pi}$ might be assumed (with ρ being the density of forest dislocations, no plastic deformation has taken place).



Examples for the stress distributions ahead double pile ups for $l/2 = 200000b$ and several N dislocations. Note that other components of the stress fields might also be considered and the angular distribution omitted here. x starts at the grain boundary.

Grain Boundary Strengthening – glide source

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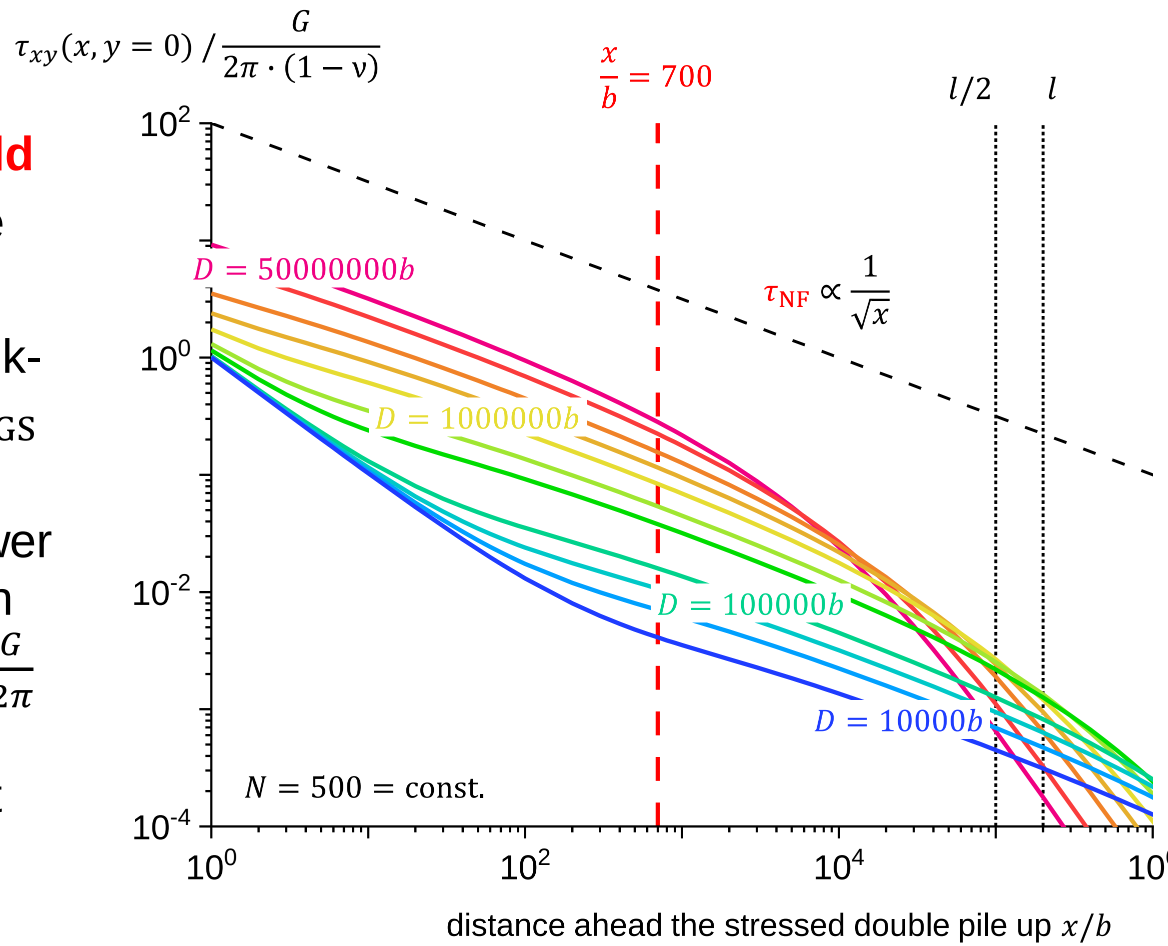


Examples for the stress distributions ahead double pile ups for several grain sizes $D = l$ at $N = 500$ dislocations. x starts at the grain boundary.

Grain Boundary Strengthening – glide source

- For a constant distance ahead the pile up, the near field stress can be approximated by $\left(N = \frac{(1-\nu)\, l}{G\, b}\, \tau\right.$ from the previous slides):

$$\tau_{\mathrm{NF}} \propto \sqrt{D}\, \tau \propto \frac{N}{\sqrt{D}}$$

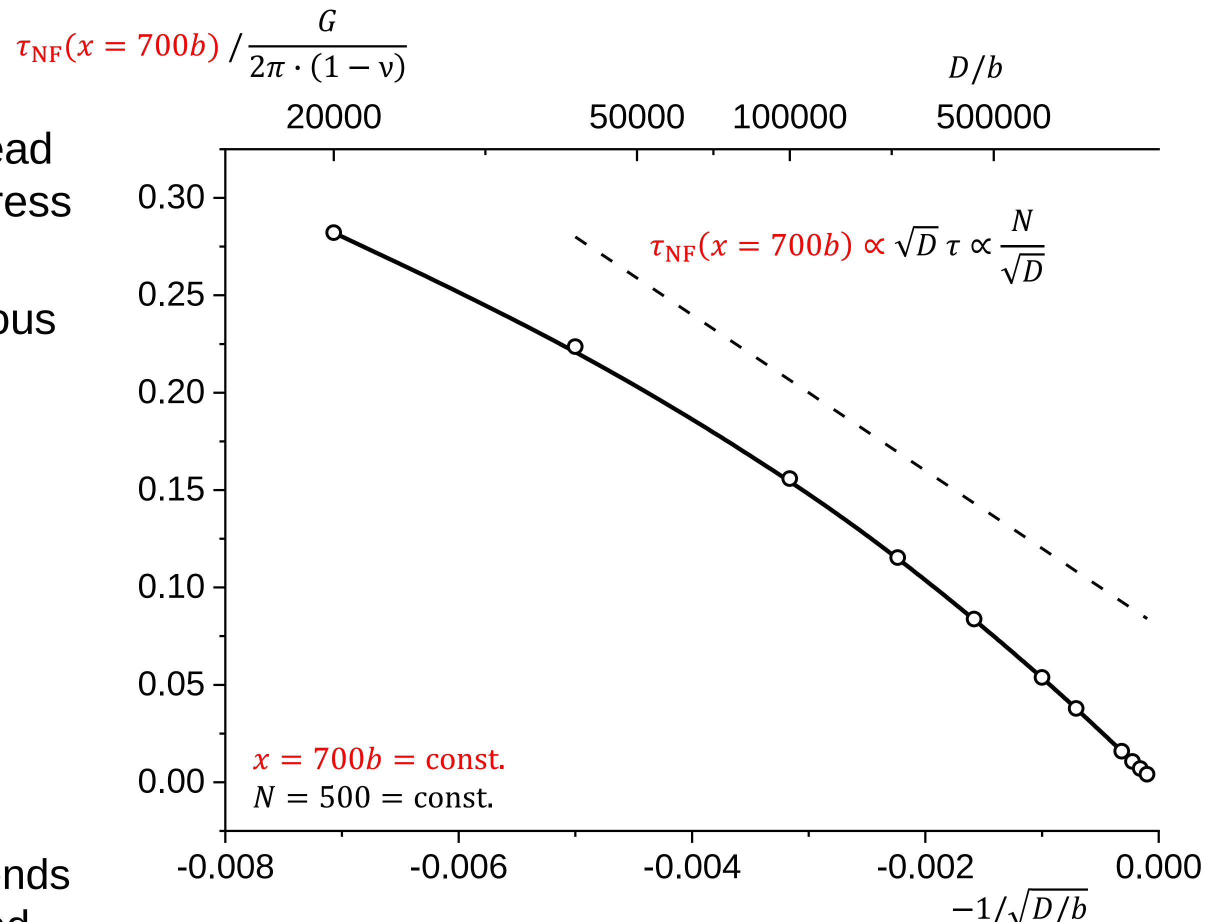
- For the onset of yielding by

$$\tau_{\mathrm{NF}}\Big|_{\tau=\tau_{\mathrm{y}}} = \tau_{\mathrm{GS}}$$

- one obtains:

$$\tau_{\mathrm{y}} \propto \frac{1}{\sqrt{D}}$$

- Note that the result still depends on the chosen distance ahead the pile by $\tau_{\mathrm{y}} \propto \sqrt{x}$.



Necessary applied stress τ_{y} to operate the grain boundary source. Yielding occurs.

Intersection Reactions of Dislocations

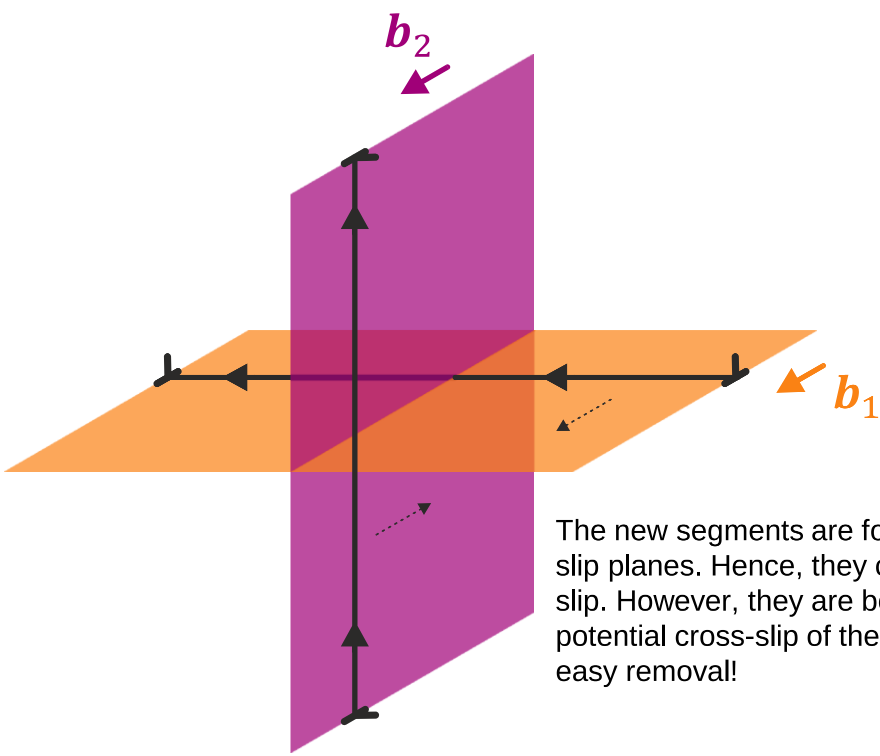
- Even in well-recovered crystals, dislocations exists (as we have seen in Ch. 4c). Hence, any moving dislocation has to intersect with these non-parallel "**forest dislocations**".
- The reaction products follow the rule: **the displacement field of one dislocation acts on the dislocation line of the other intersected dislocation**.
- Important configurations with $\boldsymbol{s}_1 \perp \boldsymbol{s}_2$ are:
  - Two edge dislocations with $\boldsymbol{b}_1 \parallel \boldsymbol{b}_2$
  - Two edge dislocation with $\boldsymbol{b}_1 \perp \boldsymbol{b}_2$
  - Edge and screw dislocation with $\boldsymbol{b}_1 \perp \boldsymbol{b}_2$
  - Two screw dislocations with $\boldsymbol{b}_1 \perp \boldsymbol{b}_2$

Intersection Reactions of Dislocations

- If the Burgers vector of the intersecting dislocation is parallel to dislocation line of the intersected dislocation, there is no interaction product: a line cannot be distorted along the line!
- If the Burgers vector of the intersecting dislocation is inclined with respect to the dislocation line of the intersected dislocation, the reaction product is of the length and the direction of the Burgers vector of the cutting dislocation. Since the Burgers vector is unique to the dislocation, the new dislocation segment has the same Burgers vector as the intersected dislocation.
- There are two possibilities of interaction products:
  - **Kinks**: dislocation segments **in the slip plane** of the intersected dislocation. Kinks are glissile and can easily be removed.
  - **Jogs**: dislocation segments **not lying in the slip plane** of the intersected dislocation. Cross-slip or climb are needed to (re)move the jog.

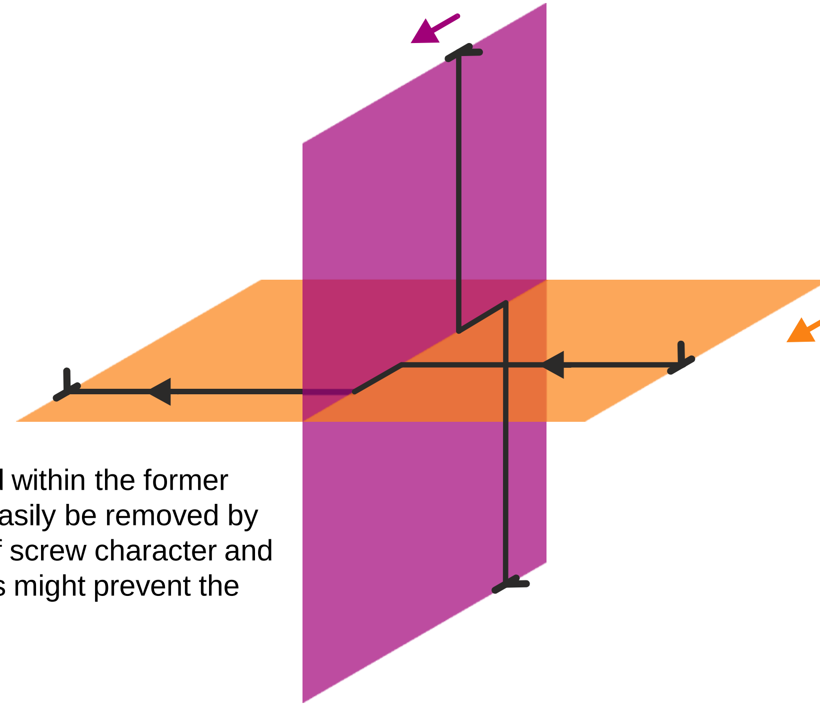
Intersection Reactions of Dislocations

- $\boldsymbol{s}_1 \perp \boldsymbol{s}_2$ and $\boldsymbol{b}_1 \parallel \boldsymbol{b}_2$ with edge dislocations:



The new segments are formed within the former slip planes. Hence, they can easily be removed by slip. However, they are both of screw character and potential cross-slip of the kinks might prevent the easy removal!

before cutting



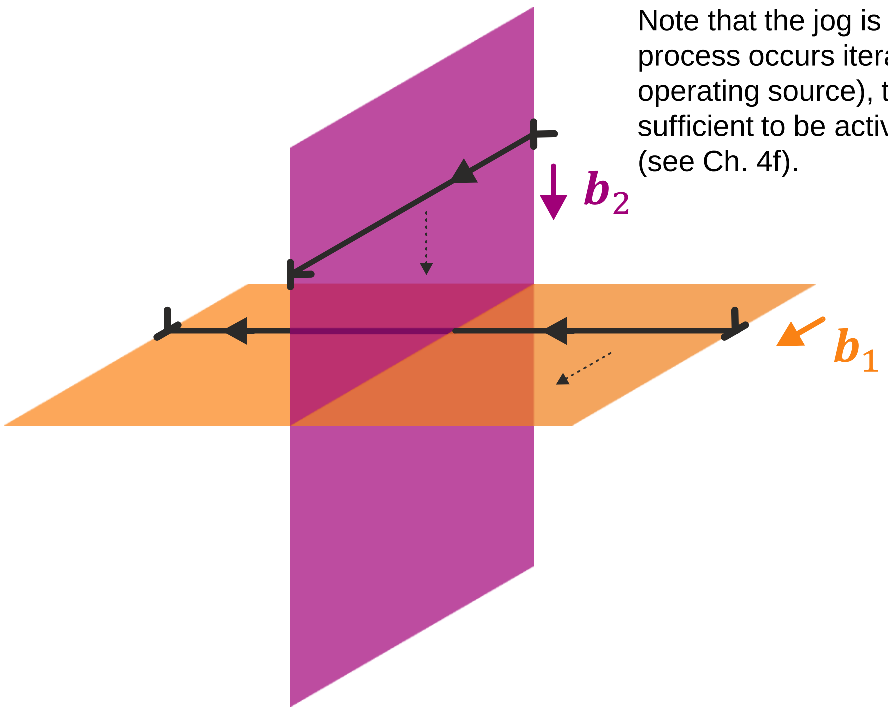
after cutting

Intersection Reactions of Dislocations

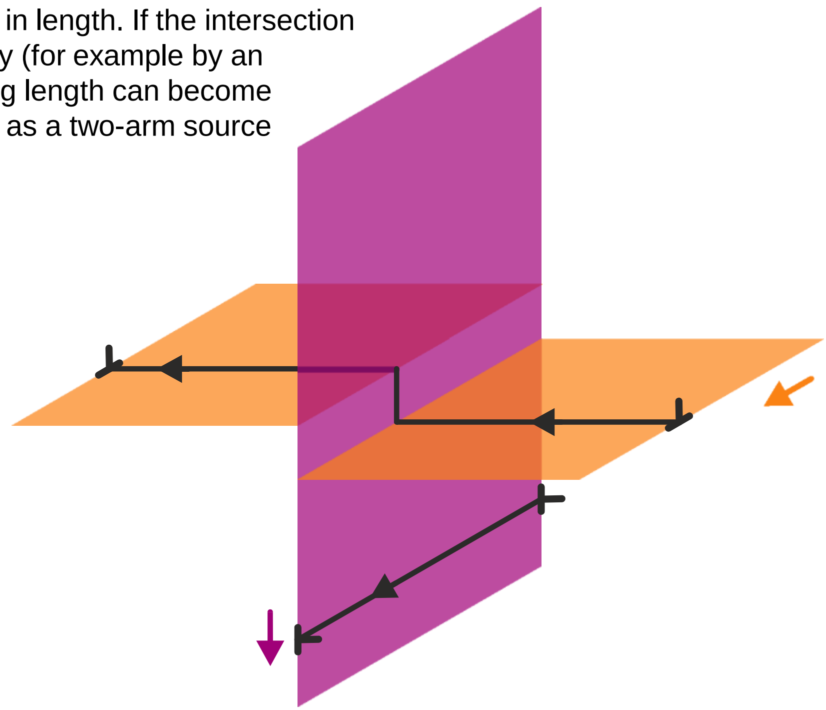
- $\boldsymbol{s}_1 \perp \boldsymbol{s}_2$ and $\boldsymbol{b}_1 \perp \boldsymbol{b}_2$ with edge dislocations:

There is only one new segment itself not being within the former slip plane. The jog (edge character) needs climb to be (re)moved.

Note that the jog is of b_2 in length. If the intersection process occurs iteratively (for example by an operating source), the jog length can become sufficient to be activated as a two-arm source (see Ch. 4f).



before cutting



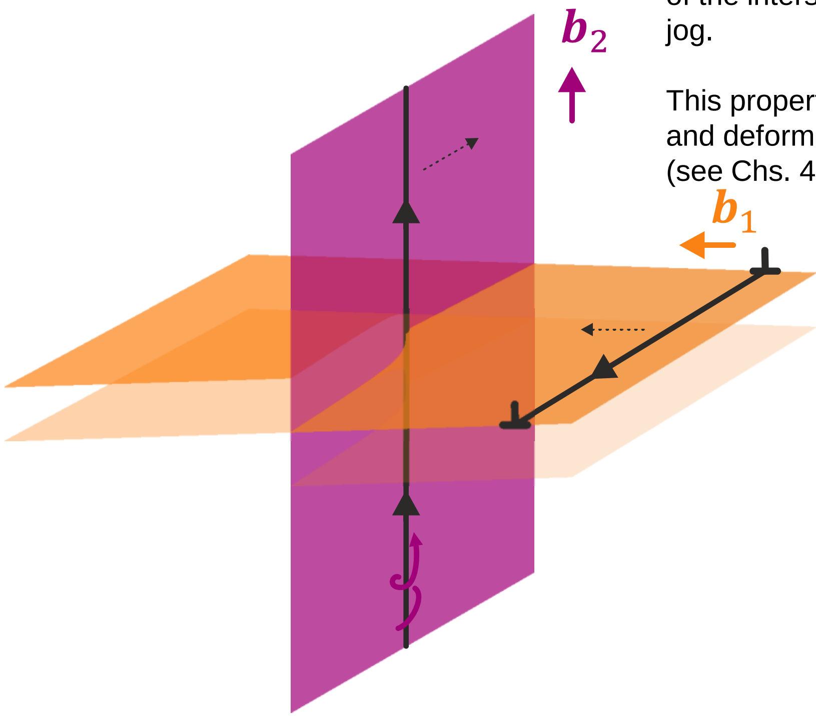
after cutting

Intersection Reactions of Dislocations

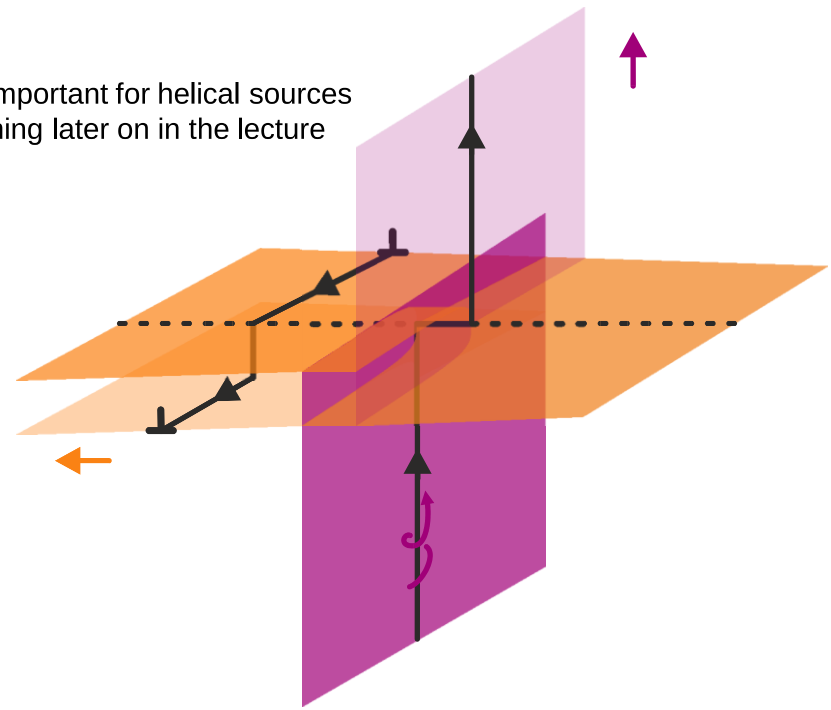
- Perpendicular edge and screw dislocations:

The screw dislocation induces a screw-like deformation of the slip plane of the edge dislocation. This leads to a change of the slip plane of the intersecting dislocation and the formation of a jog.

This property will be important for helical sources and deformation twinning later on in the lecture (see Chs. 4f and 7a).



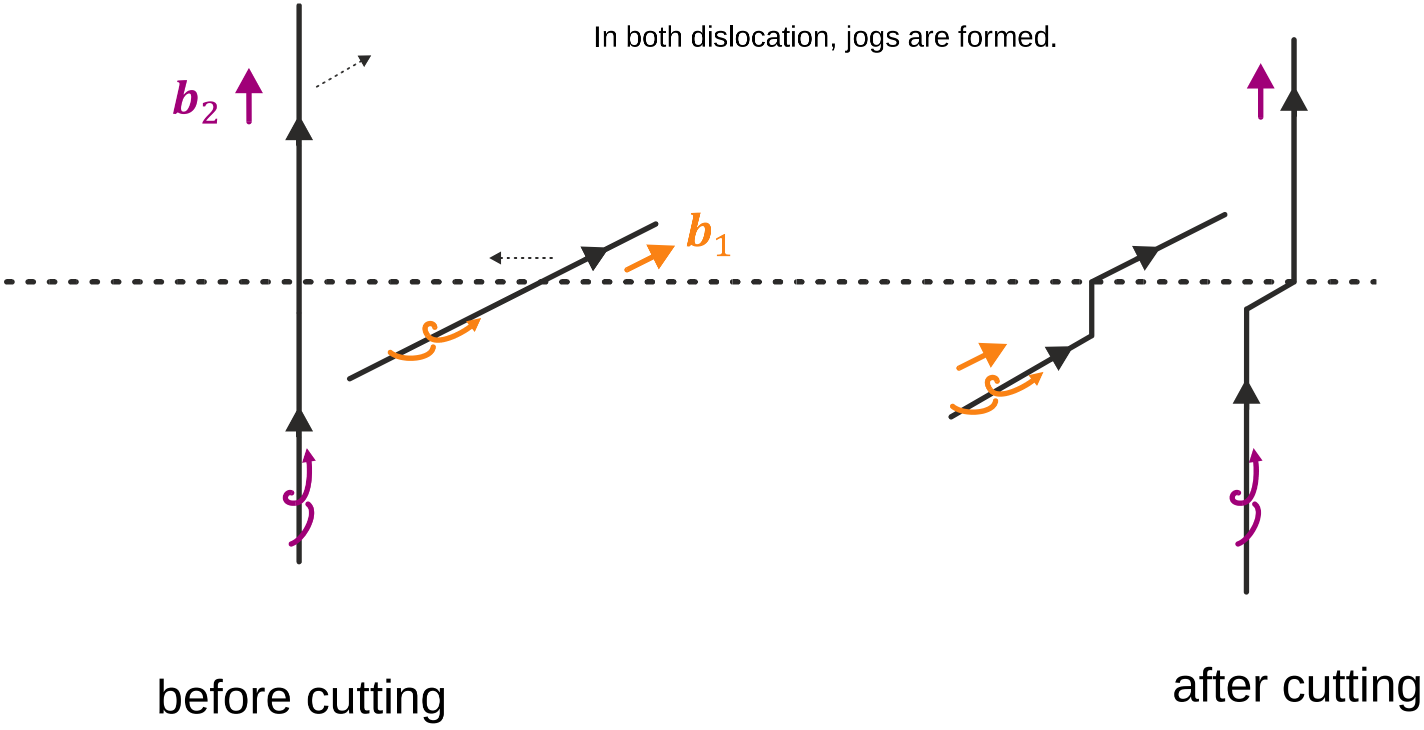
before cutting



after cutting

Intersection Reactions of Dislocations

- $\boldsymbol{s}_1 \perp \boldsymbol{s}_2$ and $\boldsymbol{b}_1 \perp \boldsymbol{b}_2$ with screw dislocations:



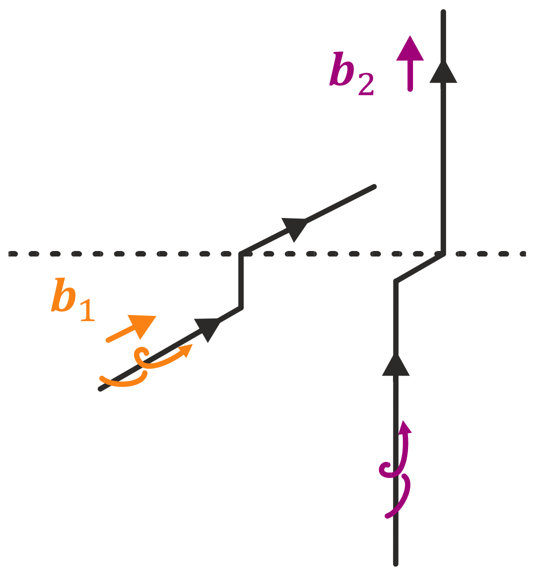
Dislocation Strengthening

- During the intersection process, new dislocation segments might be formed. These segments of b in length are associated with a line energy $\frac{W}{L} \propto G\, b^2$ and, therefore, the total energy is increased by $W \propto G\, b^3$.
- This excess energy is provided by the external load: $W = F \cdot b \propto \tau\, b\, L_f \cdot b$; L_f is the free path of the glissile dislocations.
- The intersection process is another contribution to dislocation strengthening:

$$\tau \propto \frac{G\, b}{L_f} \approx G\, b\, \sqrt{\rho}$$

Vacancy Generation by Jogged Screws

- Note that the further movement of the jogged screw dislocation with $\boldsymbol{b}_1$ requires climb of the edge jog portion.
- Hence, the moving jog leaves a trail of vacancies behind.
- At sufficiently low temperatures, the otherwise mobile screw dislocations become markedly slowed down. This might be one important contribution to serrated plastic deformation at cryogenic temperatures (< 35 K, see Ch. 5).



after cutting

Vacancy Generation by Jogged Screws

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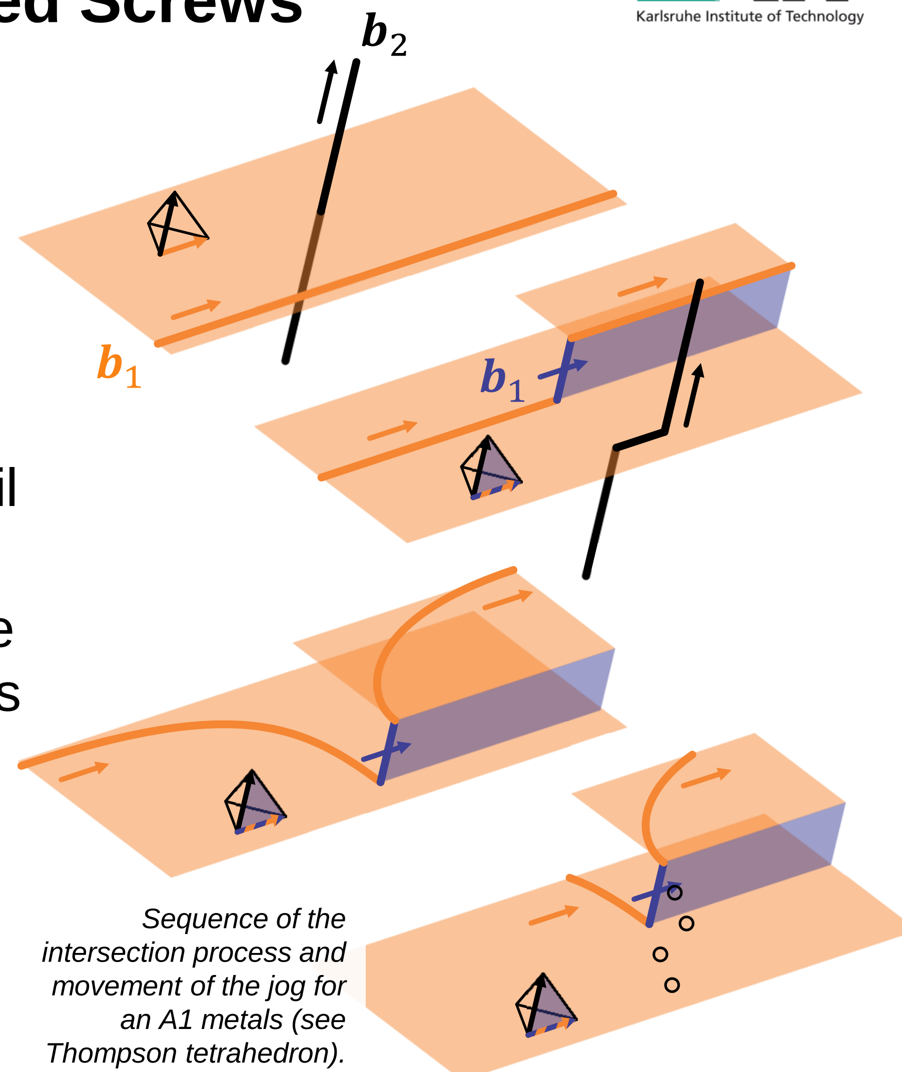

Sequence of the intersection process and movement of the jog for an A1 metals (see Thompson tetrahedron).

A. S. Tirunilai: “Dislocation-based serrated plastic flow of high entropy alloys at cryogenic temperatures”, Acta Materialia 200 (2020) 980-991

Summary

- The **interaction of dislocations** provides two important contributions to **dislocation strengthening**: passing by and cutting. The **stress ahead of pile-ups** contributes to **grain boundary strengthening**.
- Parallel dislocations can form **metastable configurations** that play a significant **role in dislocation patterning** during plastic deformation.