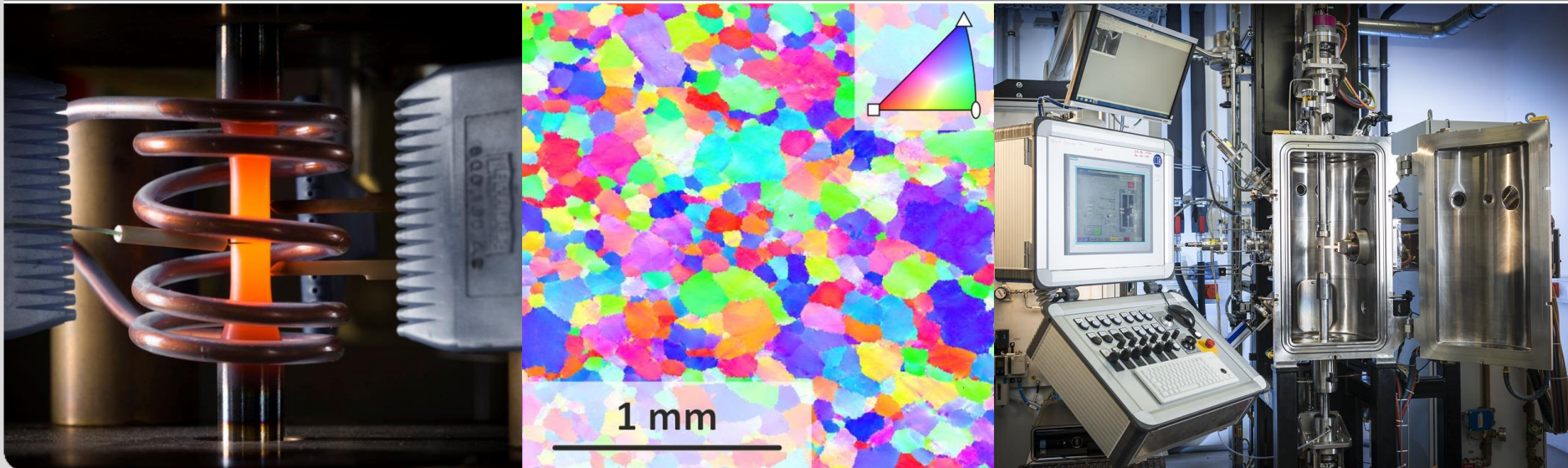


Plasticity

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 22-02-14

Institute for Applied Materials (IAM-WK)



Topics

- Historical Evolution
- Fundamental Concept
 - Slip Traces
 - (Homogenous) Shear vs. Slip
 - Types and Motion of Dislocations
 - Burgers Circuit
 - Dislocation Character
 - Volume Conservation vs. Non-Conservation
 - Slip
 - Cross-slip
 - Climb
 - Dislocation Reactions
 - Orowan Equation

Historical Evolution

- In order to provide an impression of how revolutionary the introduction of the slip and dislocation concept is (not was), some fundamental questions from the time might be recapped:
 - **How can crystalline solids deform plastic without losing their crystal structure?**
(That metallic materials are crystalline was known for a long time and proven by X-ray diffraction after 1911.)
 - **Why is the onset of plastic deformation obtained at low shear stresses?**
(That plastic deformation is mainly triggered by shear stress was already clear for a long time; note that Tresca passed away in 1885.)
 - **Why is plastic deformation instantaneous** and becomes time-dependent at high temperatures?
 - Even though defects might mediate plastic deformation, **why are the obtained strains are so high?**

Historical Evolution

- 1901-1907:
G. Weingarten, V. Volterra and many more develop the elastic theory of dislocations (though not in relation to crystal defects)
- 1926:
J. Frenkel estimates the critical shear stress for slip of a crystalline half-space against the other
- 1927:
A. E. H. Love introduces the term „dislocation“
- 1934:
E. Orowan, M. Polanyi, and Sir G. I. Taylor postulate dislocations as potential reason for low strength of metals
- 1939:
J. Burgers postulates screw dislocations
- 1950:
Ch. Frank and T. Read propose the Frank-Read mechanism
- 1956:
First direct evidence of dislocations using diffraction contrast (including the correct interpretation of what they saw) by **P. B. Hirsch, R. W. Horne, and M. J. Whelan**

Details can be found here (also highlighting the non-linearity of such historical evolution better than this slide):
J. P. Hirth: “A Brief History of Dislocation Theory”, Metallurgical Transactions A 16 (1985) 2085-2090

Historical Evolution

- Weingarten (in his important, Italian publications „Giulio“) was an Italo-German mathematician. Volterra was an Italian mathematician and mechanical physicist.
- Both were active in analysis and geometry. Various problems are related with solutions by the two scientists:
 - Volterra equations
 - Volterra rules
 - Gauß-Weingarten equations
 - Weingarten surfaces



https://de.wikipedia.org/wiki/Julius_Weingarten#/media/Datei:Julius_Weingarten.jpg
https://de.wikipedia.org/wiki/Vito_Volterra#/media/Datei:Vito_Volterra.jpg

Historical Evolution

- Orowan and Polanyi were Hungarians. Polanyi studied chemistry at TH Karlsruhe (interrupted by World War First). From 1920, he was working in Berlin and emigrated to Manchester due to pogrom against Jews after 1933. Orowan obtain a PhD in 1932 at Wien University. He left in 1933 after Hitler's rise to power (Machtergreifung) to Budapest. In 1937, he was invited by Rudolf Peierls to Birmingham and later went to Lawrence Bragg in Cambridge.
- Taylor was mainly active in hydrodynamics and many numbers and concepts in this respect are called after (this) Taylor. He was lecturer at Cambridge and research professor with the Royal Society. He was active in military research during both World Wars (e.g. Manhattan project).

https://en.wikipedia.org/wiki/G._I._Taylor#/media/File:G_I_Taylor.jpg

https://de.wikipedia.org/wiki/Michael_Polanyi#/media/Datei:Michael_Polanyi.png

https://www.tf.uni-kiel.de/matwis/amat/iss/kap_5/advanced/t5_4_1.html



Historical Evolution

- Burgers was a physicist from The Netherlands.
- He developed the concept of screw dislocations and small angle grain boundaries constructed from dislocations.

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J. M. Burgers: "Some considerations on the fields of stress connected with dislocations in a regular crystal lattice"
Proceedings of the Section of Sciences. Koninklijke Nederlandse Akademie van Wetenschappen. 42 (1939) 293-325
https://www.tf.uni-kiel.de/matwis/amat/iss/kap_5/advanced/t5_4_1.html

Historical Evolution

- Hirsch was former associate of Lawrence Bragg and lead scientist for the development of modern transmission electron microscopes.
- Hirsch's research group prepared the first images of dislocations by using diffraction contrast and delivered the first interpretation of it.
- At the time, the concept was still under debate and the experimental proof by direct imaging was an important step!



https://authors.library.caltech.edu/5456/1/hrst.mit.edu/hrs/materials/public/Whelan/Whelan_interview.htm

https://www.tf.uni-kiel.de/matwis/amat/iss/kap_5/advanced/t5_4_1.html

Historical Evolution

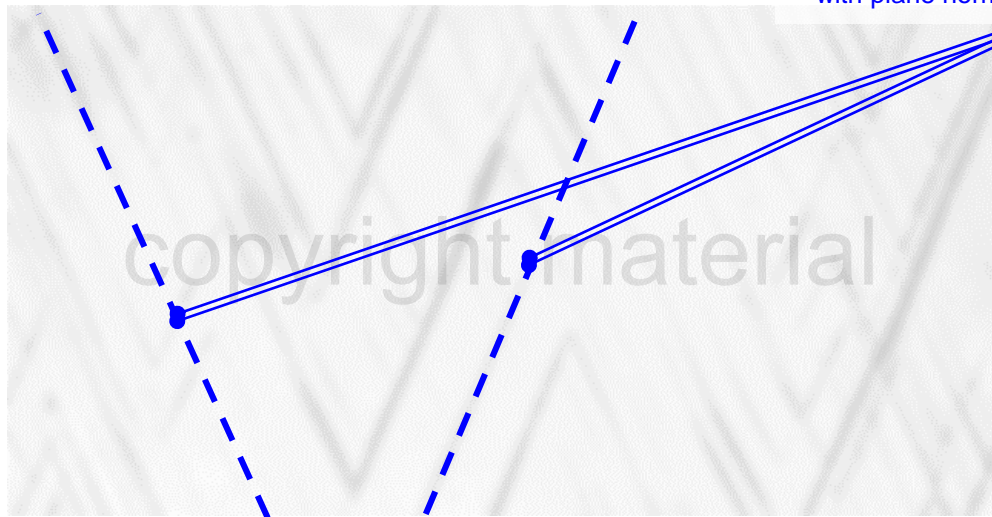
The time when dealing with dislocations was forefront solid state physics.



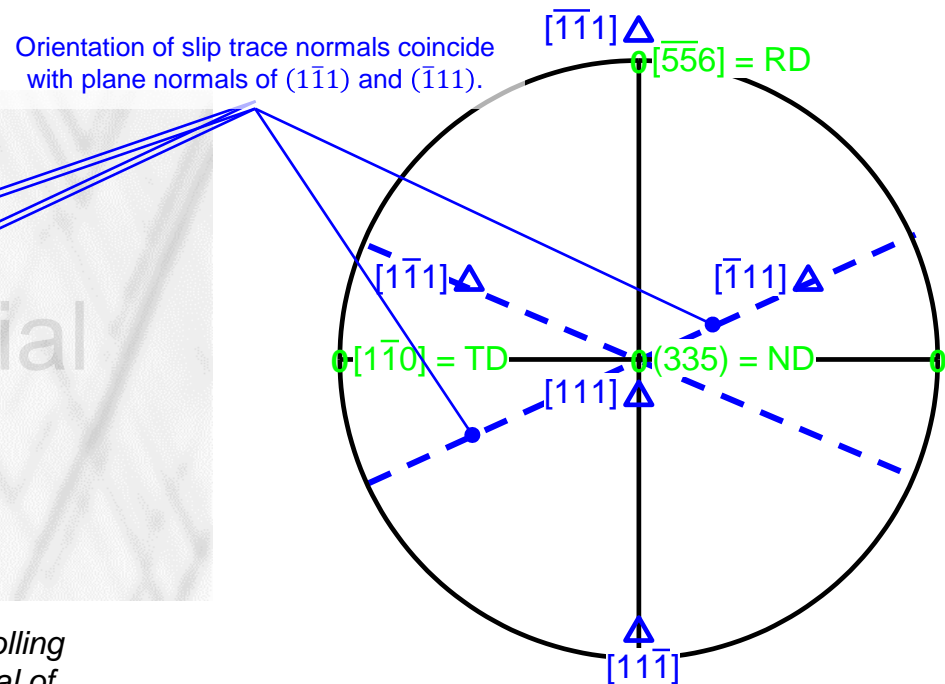
G. Coopmans - <http://www.hilliontchernobyl.com/solvay1951.htm>
https://en.wikipedia.org/wiki/Egon_Orowan#/media/File:Solvay_conference_1951_g.jpg

Slip Traces

- It was recognized very early that polished, metallic single crystals (e.g. Czochralski (1916/1918) or Bridgman method (1925)) or polycrystals exhibit distinct straight microscopic features on deformed surfaces, called **slip traces**.



Slip traces on the surface of (view onto the rolling plane) of a slightly deformed Cu single crystal of $\{335\}\langle\bar{5}\bar{5}6\rangle$ orientation.



G. Y. Chin, W. F. Hosford, D. R. Mendorf: "Accommodation of constraint deformation in fcc metals by slip and twinning", Proceedings of the Royal Society A 309 (1969) 433-456

Slip Traces

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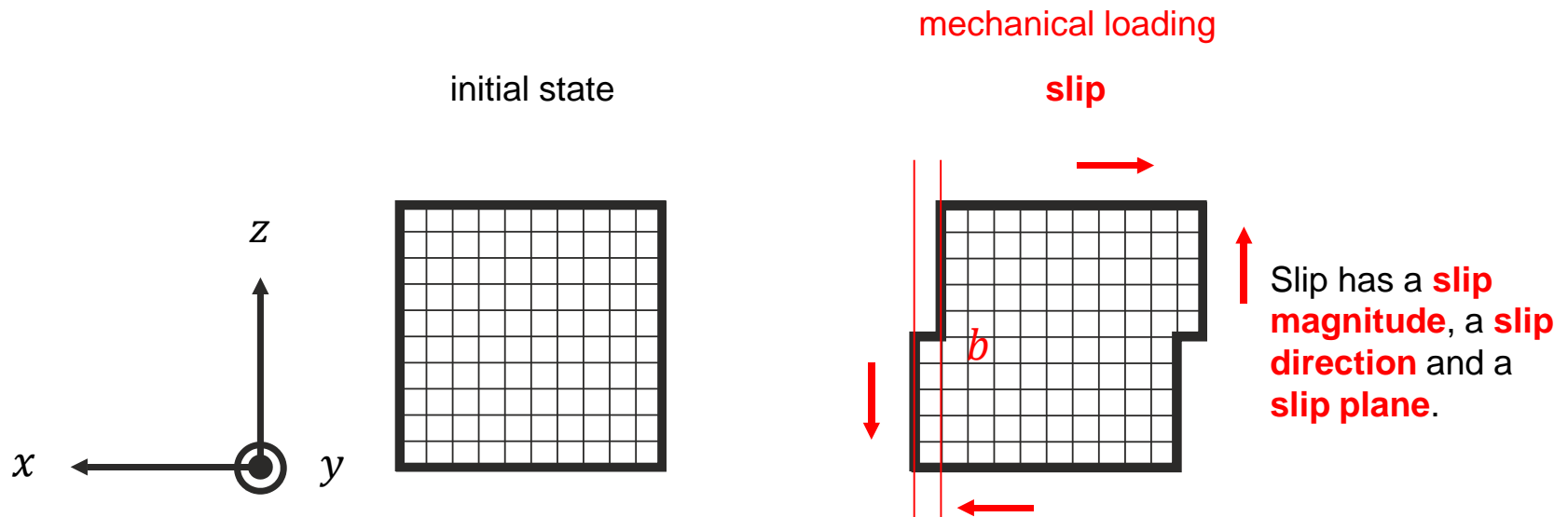


Maximum shear strain from locally resolved strain measurements on polished and speckle-marked surfaces of 304L after uniaxial plastic deformation: 1.6 % (left) and 6 % (right) in total strain.

F. D. Gioacchino & J. Q. da Fonseca: "An experimental study of the polycrystalline plasticity of austenitic stainless steel", International Journal of Plasticity 74 (2015) 92-109

Slip Traces

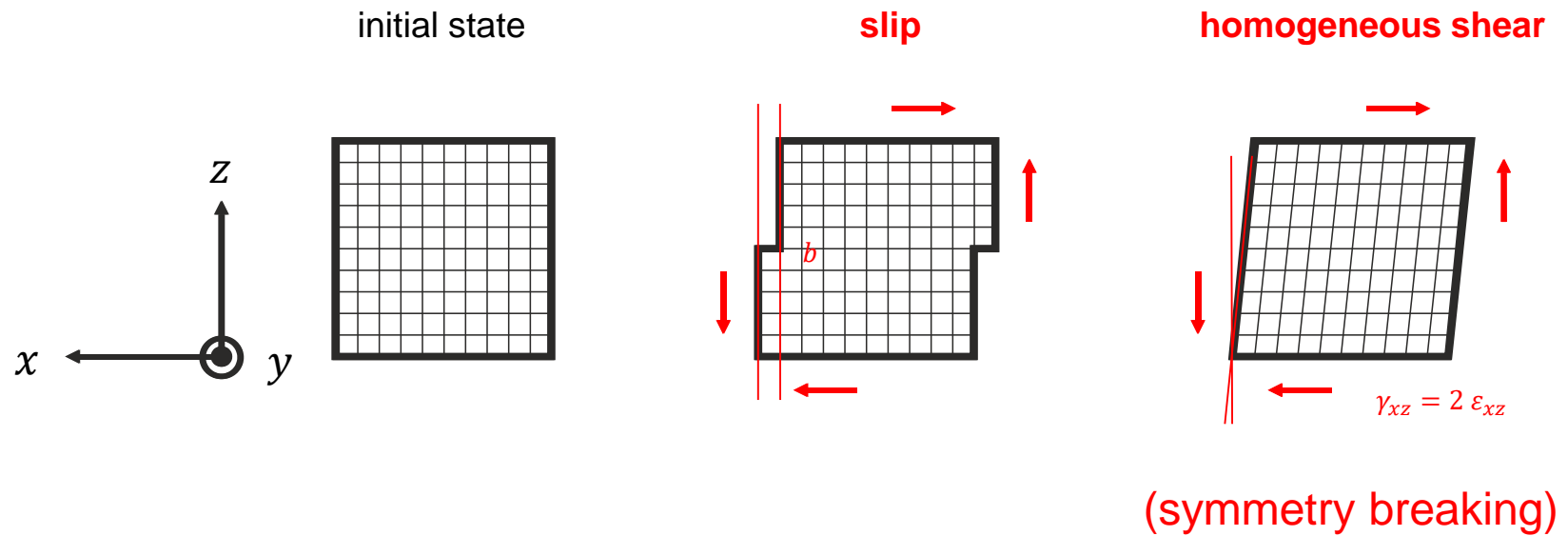
- Slip traces were identified being associated with **small steps on the surface** of the materials as a result of an **elementary slip process**.
- The fundamental process is **shear controlled**.
- It is important to note that the **crystal structure remains unaffected!** This would not be the case if homogeneous shear occurs.



Note that shear stresses request four force arrows for force *and* torque balance! Two arrows only lead to rigid body rotation without deformation.

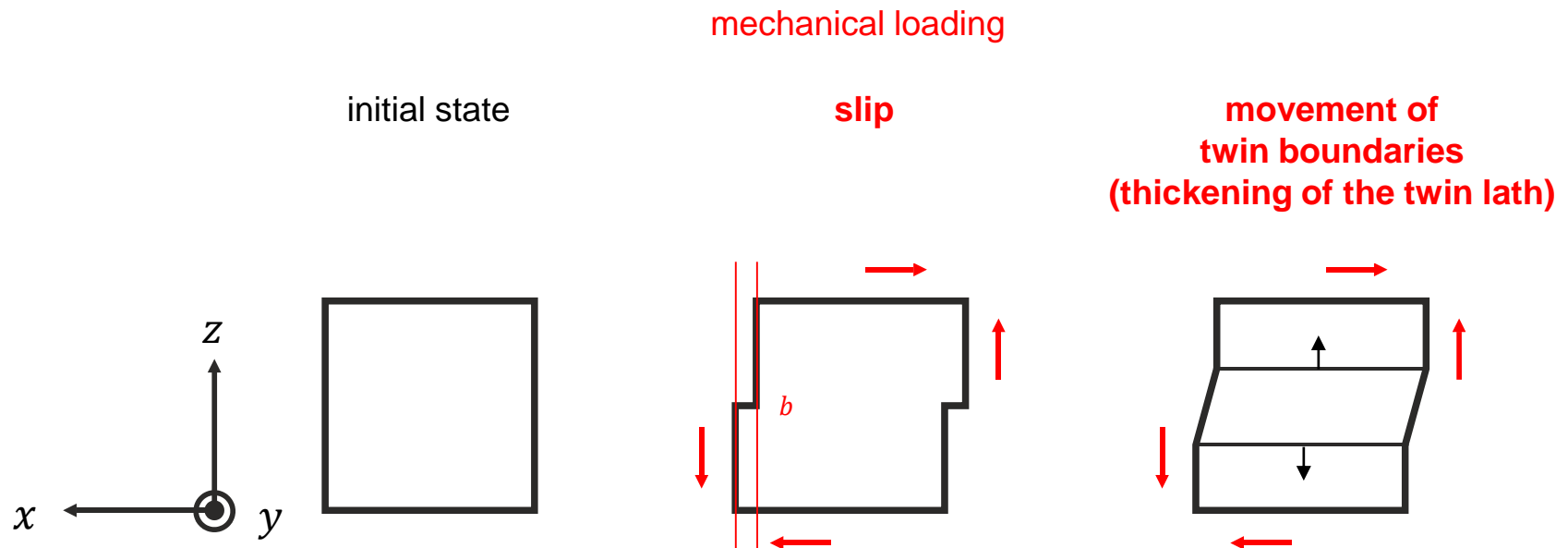
Slip Traces

- For comparison:



Slip Traces, Shear Bands, Twin Bands, etc.

- Apart from dislocation motion on distinct crystallographic planes (slip), localized deformation can also lead to line-like features on deformed surfaces:



Slip Traces, Shear Bands, Twin Bands, etc.

- Thickening of thin twin laths results in similar surface patterns as for dislocation slip. They cannot be easily resolved as being twin laths by means of light optical microscopy. (Note that the twinning plane is also a major slip plane in some cases.)
- Hence, both phenomena were frequently false interpreted. The line-like features terminate at grain boundaries in both cases.
- See for example Blewitt's first report on the appearance of deformation twinning in Cu single crystals at 4.2 K in 1957: only after verification of the twin orientation by X-ray diffraction, the scientific community was fine with the observation of deformation twinning in fcc metals; Cottrell and Bilby excluded deformation twinning in fcc metals by geometrical reasons in advance to Blewitt's experiments.



T. H. Blewitt, R. R. Coltman, J. K. Redman: "Low-Temperature Deformation of Copper Single Crystals",
Journal of Applied Physics 28 (1957) 651-660

Slip Traces, Shear Bands, Twin Bands, etc.

- Under certain conditions (for example rolling of some metals and alloys), pronounced localization of plastic deformation occurs. These features can also alter surface topography and appear line-like but are shear bands.



Shear band formation by localization of plastic deformation during crystal plasticity simulation of sheets consisting of Cu single crystals $\{112\}\{11\bar{1}\}$ and Nb single crystals $\{111\}\{11\bar{2}\}$ subsequent to thickness reduction of 50 %.

N. Jia, D. Raabe, X. Zhao: "Crystal plasticity modeling of size effects in rolled multilayered Cu-Nb composites", Acta Materialia 111 (2016) 116-128

Slip Traces, Shear Bands, Twin Bands, etc.

- Shear bands do usually not terminate at grain boundaries. Under certain conditions, shear bands can propagate during plastic deformation (for example Lüders bands).

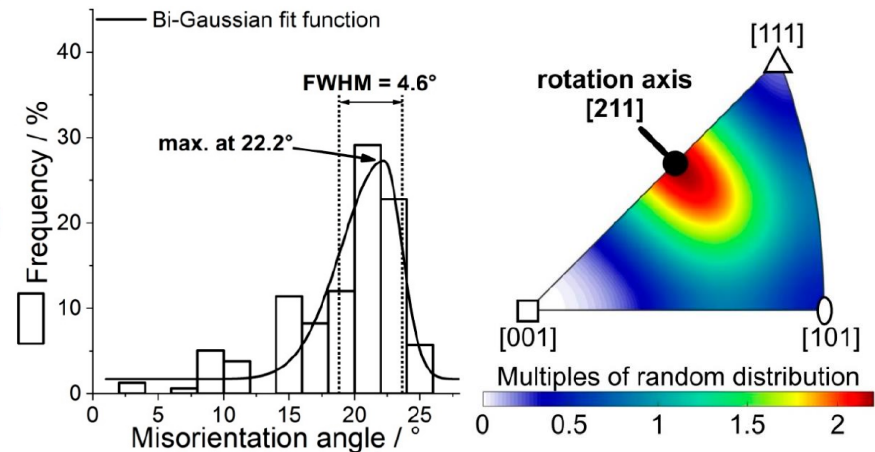
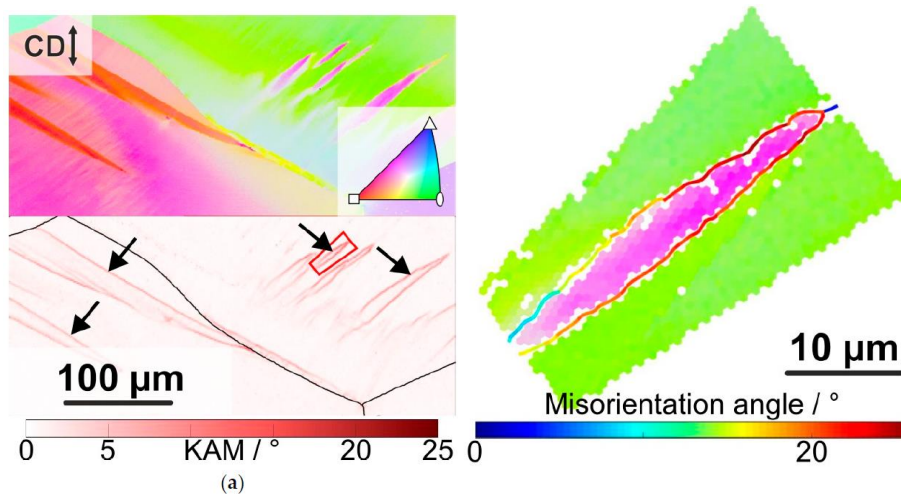


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Slip Traces, Shear Bands, Twin Bands, etc.

- Kink bands are formed in some metals and alloys (A2 for example) due to intense localization of slip to a single slip system:



Kink bands forming in A2 HfNbTaTiZr single-phase high entropy alloy subsequent to compression testing (compression direction CD) at room temperature to 9.8 % total plastic strain. The misorientation distribution and inverse pole figure highlights the correlation to the active slip systems in A2 metals and alloys, e.g. $\{112\}\{11\bar{1}\}$.

H. Chen et al.: "Influence of Temperature and Plastic Strain on Deformation Mechanisms and Kink Band Formation in Homogenized HfNbTaTiZr", Crystals 11 (2021) 81

Slip Traces, Shear Bands, Twin Bands, etc.

- **Shear bands, twin bands, kink bands can be etched/contrasted after polishing** due to increased local defect density (twin boundaries, dislocation density, etc.).
- **Slip traces are gone after polishing** (apart from some locally stuck dislocations segments which might get etched).

Slip Traces

- Hence, **plastic deformation is obviously localized to distinct crystallographic planes** and has a certain (small) magnitude.
- The necessary, **critical shear stress to activate slip** (= movement of one half crystal against the other) **is very high**:

$$\tau_c \approx \frac{G}{2\pi}$$

- This is far beyond the critical stresses to activate plastic deformation in most common metals and alloys (average magnitudes will be point of discussion later in the lecture).
- Thus, there is a need for a defect to mediate the localization and the lower barrier for activation.

Note that J. Frenkel studied different cases (of elastic properties/interatomic potentials) and the one noted above is the most simple. It corresponds to the common text book version.

In both, English and German literature, the term „theoretical strength“ is frequently used. The term is misleading and leads to false interpretation of the result. The process does not determine an upper bound for (macroscopic) strength. The spontaneous nucleation of dislocations is possible even in the case of otherwise perfect crystals preventing to reach the above mentioned stress limit.

J. Frenkel: “Zur Theorie der Elastizitätsgrenze und der Festigkeit kristallinischer Körper“, Zeitschrift für Physik 37 (1926) 572-609

Dislocations as Carriers of Plast. Deformation

- Even before the officially accepted parallel proposal of dislocations by Polanyi, Orowan and Taylor, there were few reports on it before (as often seen for major developments):

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M. Polanyi in Zeitschrift für Physik 89 (1934) 660-664
E. Orowan in Zeitschrift für Physik 89 (1934) 634-659
G. I. Taylor in Proceedings of the Royal Society of London 145 (1934) 1-18

Polanyi comments on the work of Taylor but also work of Prandtl und Dehlinger before 1933/34.

Dislocations as Carriers of Plast. Deformation

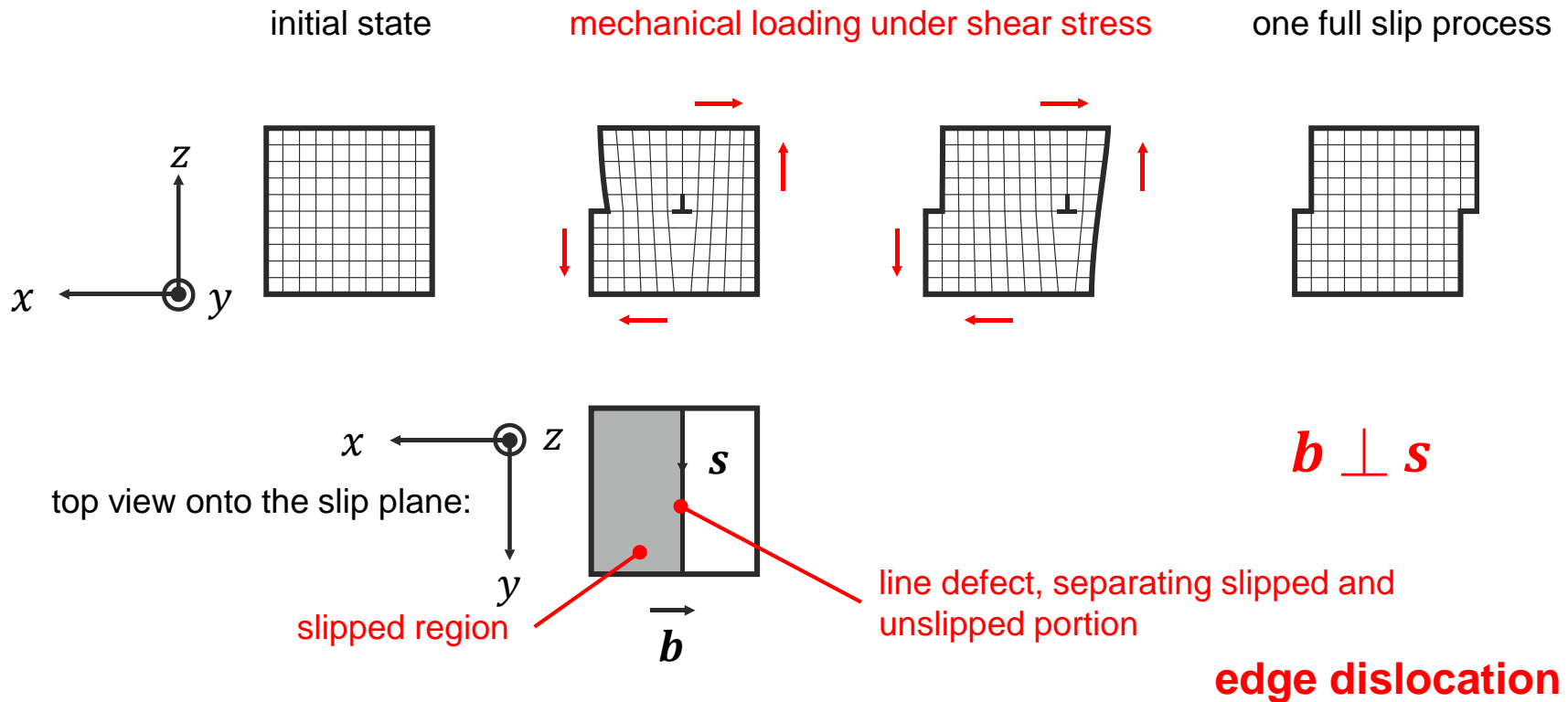
- Even before the officially accepted parallel proposal of dislocations by Polanyi, Orowan and Taylor, there were few reports on it before (as often seen for major developments):



J. M. Burgers: "Some considerations on the fields of stress connected with dislocations in a regular crystal lattice", Proceedings of the Section of Sciences. Koninklijke Nederlandse Akademie van Wetenschappen 42 (1939) 293-325

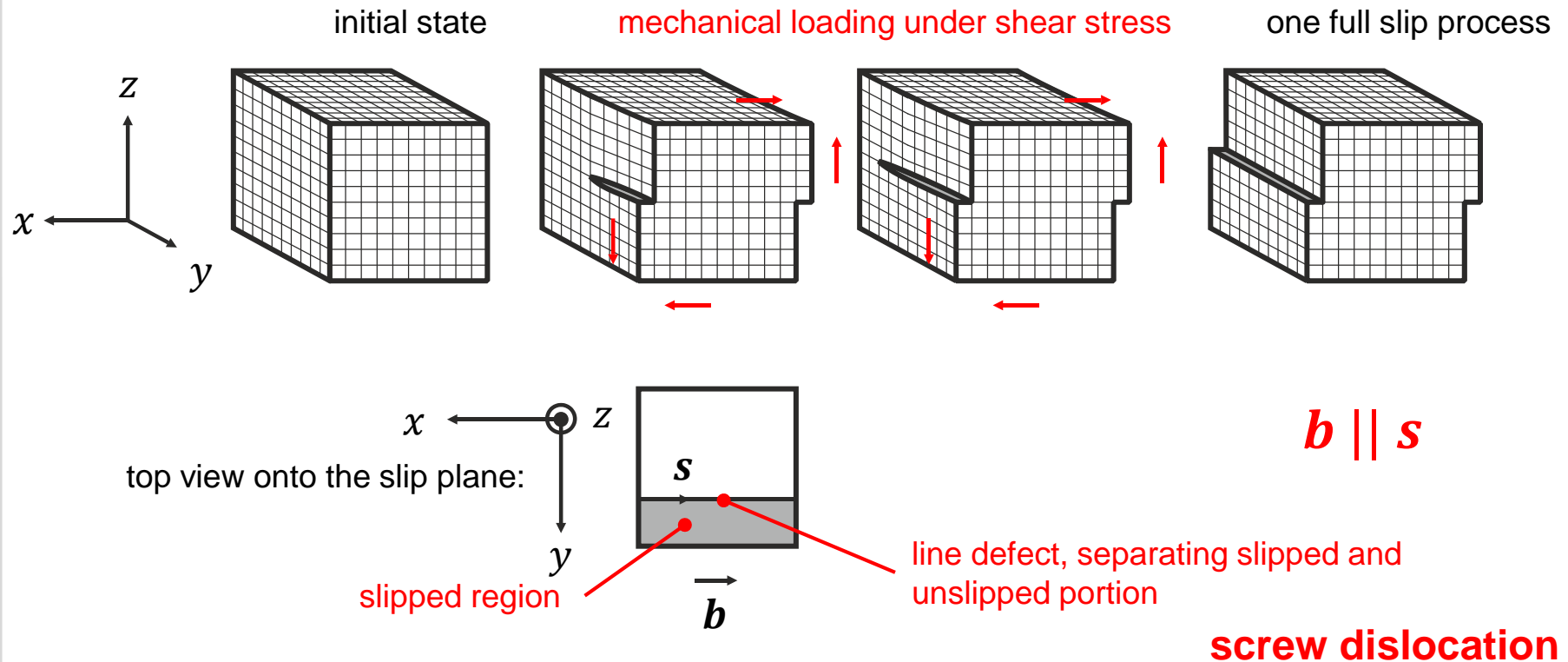
Concept: Types and Motion

- By the movement of the dislocation, the **slip process** of one half crystal against the other **becomes easier** since **only atomic bindings along the dislocation line have to be cut and reassembled** (instead of all in the entire slip plane).



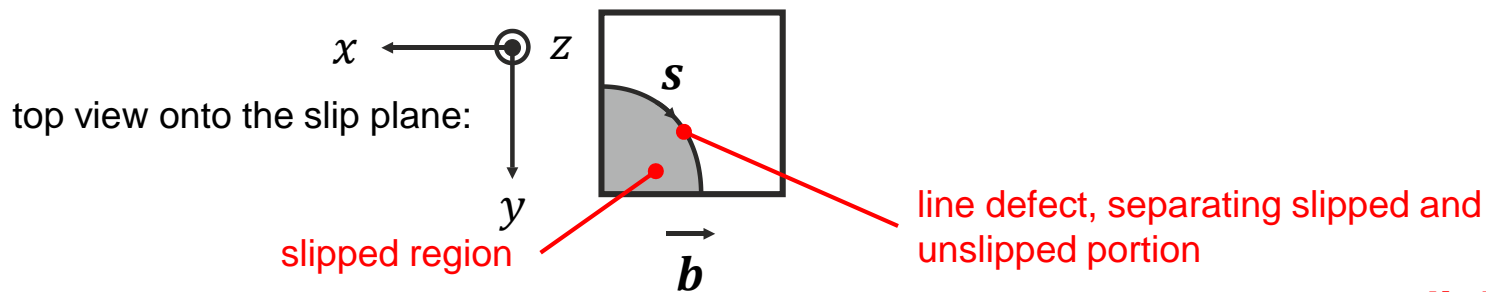
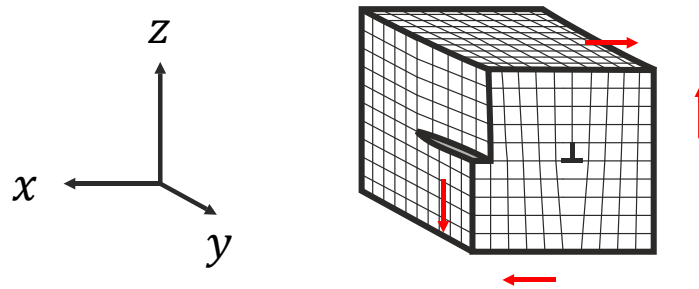
Concept: Types and Motion

- Same happens for the **screw dislocation** but with a **movement of the defect perpendicular to the situation before**:



Concept: Types and Motion

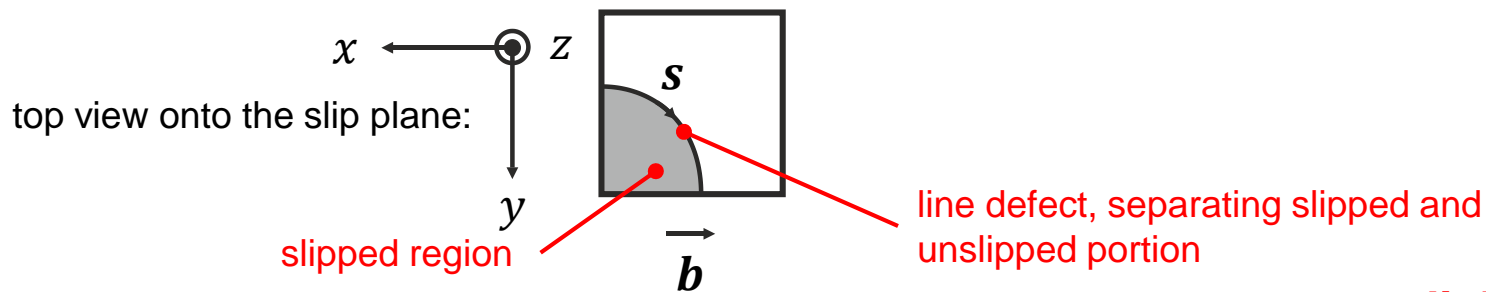
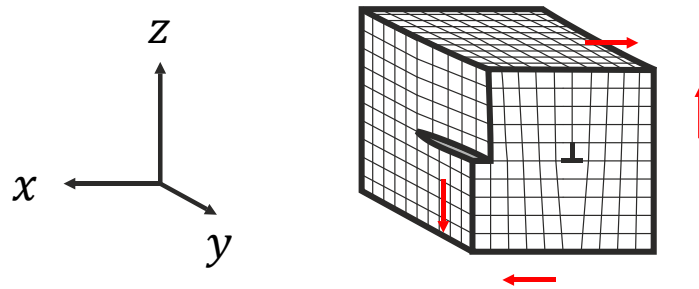
- Also in the case of the **mixed dislocation**, the same macroscopic deformation is realized. This is obvious, since **plane, direction and magnitude of the macroscopic deformation is determined by the slip operation**, not by the line defect mediating the process! **Therefore, the Burgers vector cannot change along the dislocation line.**



screw dislocation

Concept: Types and Motion

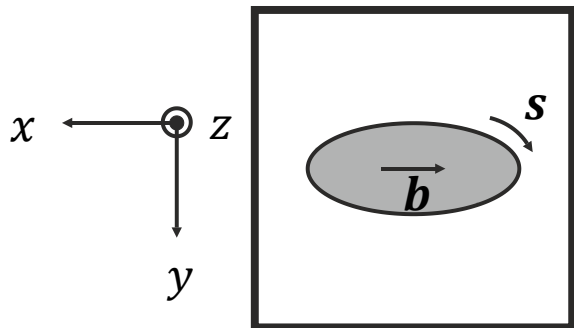
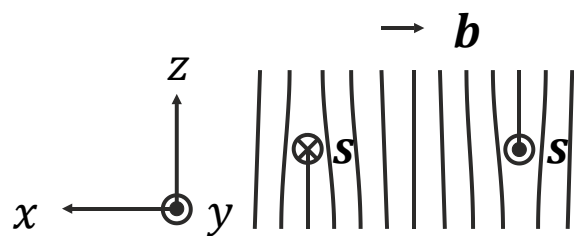
- The **definition of the dislocation line** is simple: **the dislocation separates the slipped from the unslipped portion of the crystal**. Since there is **no continuous transition from the slipped to the unslipped region, dislocations can only terminate at discontinuities of the crystal**, like surfaces, boundaries, etc. **They do not end within the crystal!**



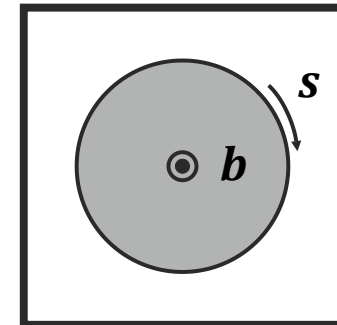
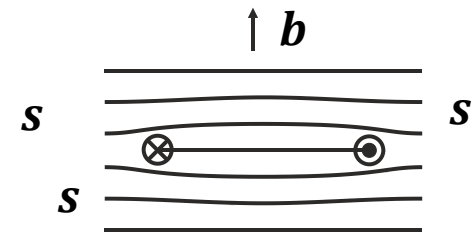
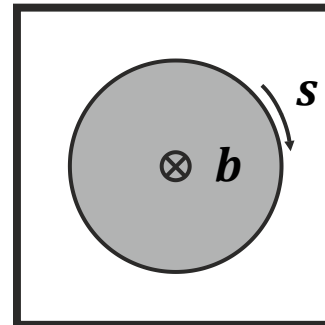
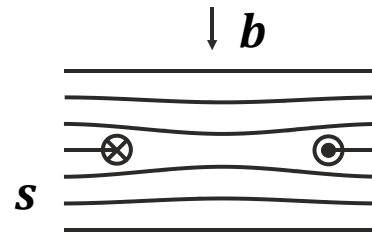
screw dislocation

Concept: Types and Motion

- A special line **configuration without ends** in real space is the **loop**. Obviously, dislocation loops are possible. Since the Burgers vector must be the same for the entire loop, there are only two possibilities: **mixed and edge loops**. There are no screw loops possible.



mixed loop (glissile loop)

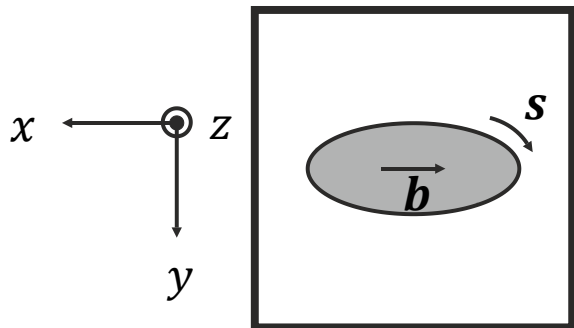
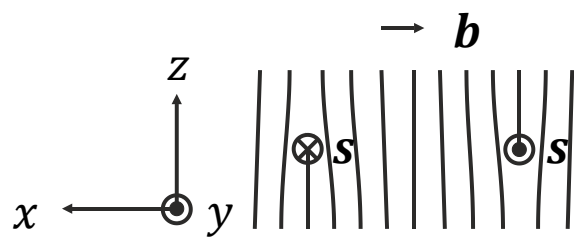


edge loop (prismatic loop)

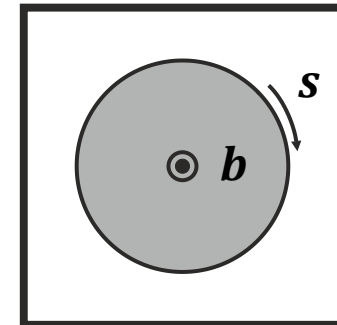
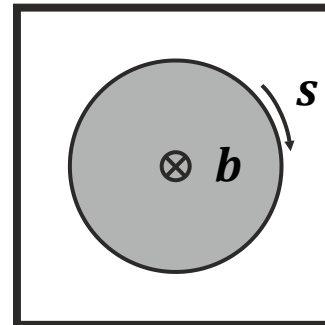
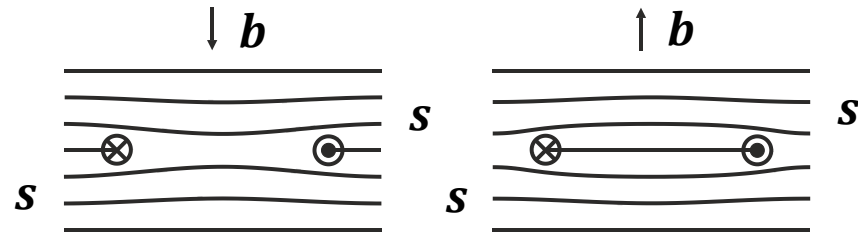
The term prismatic loop results from the shape of the slip planes which form a cylinder (complex prism) in 3D.

Concept: Types and Motion

- Mixed loops result for example from **glide sources** (Frank-Read) or when **Orowan mechanism** at precipitates is active. Prismatic loops are formed by **agglomeration of interstitials** (“positive”, “extrinsic”, right image) or **vacancies** (“negative”, “intrinsic”, left image). They can also form from **climb sources** (Bardeen-Herring).



mixed loop (glissile loop)

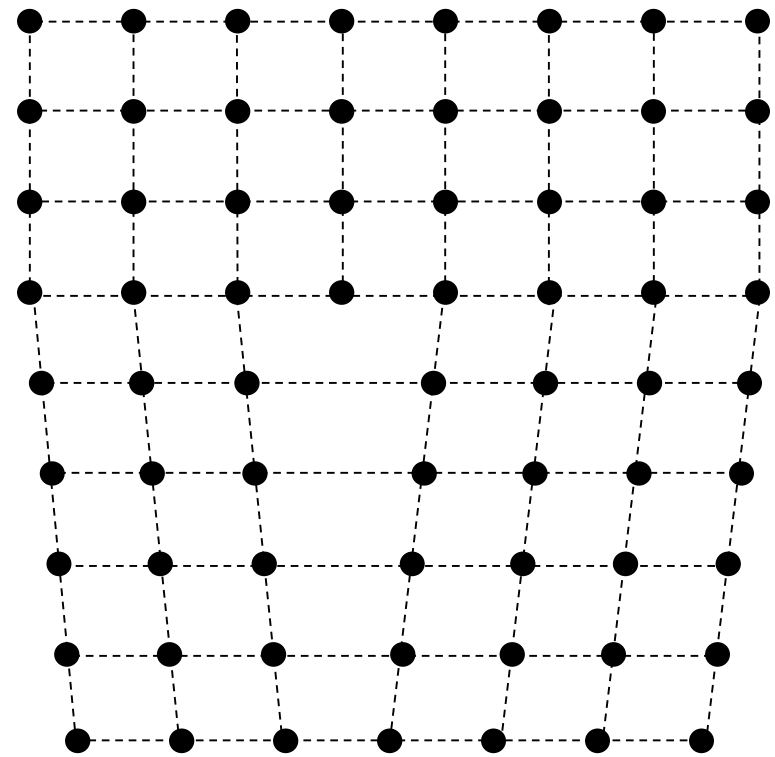
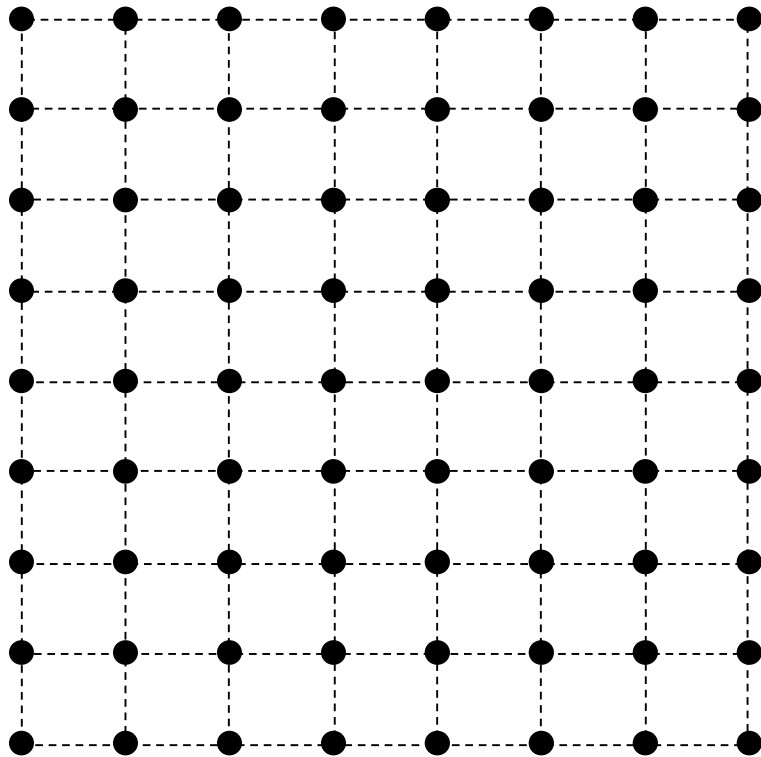


edge loop (prismatic loop)

Burgers Circuit

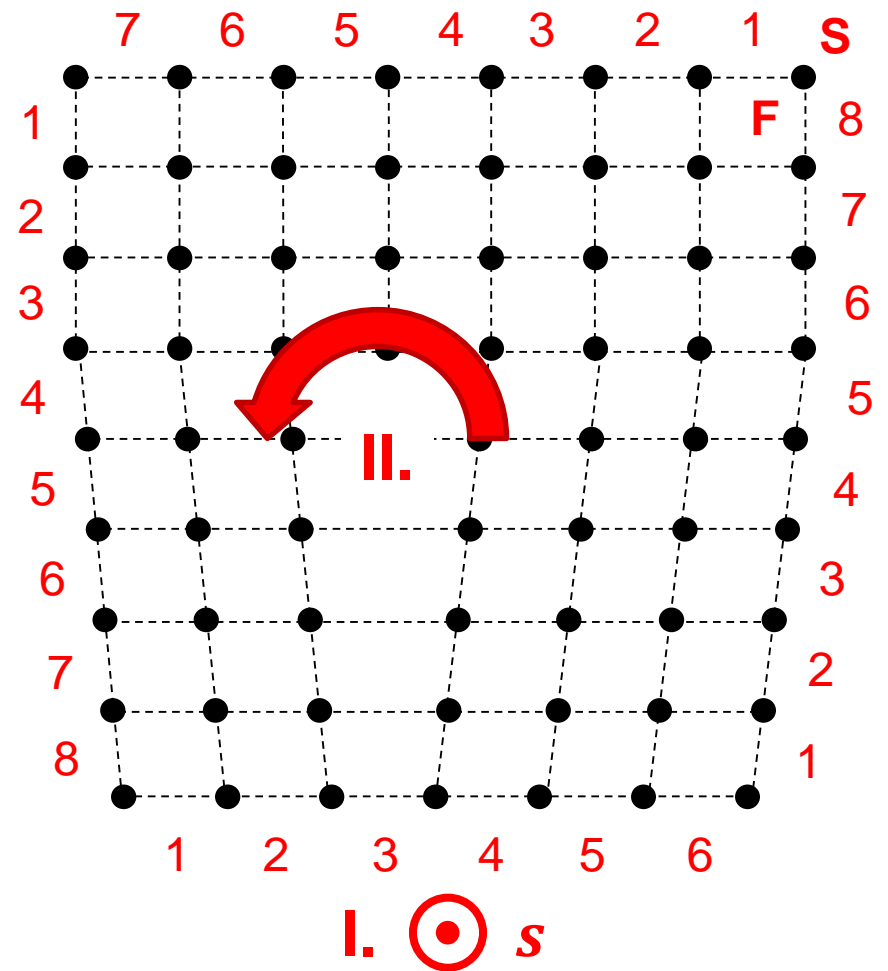
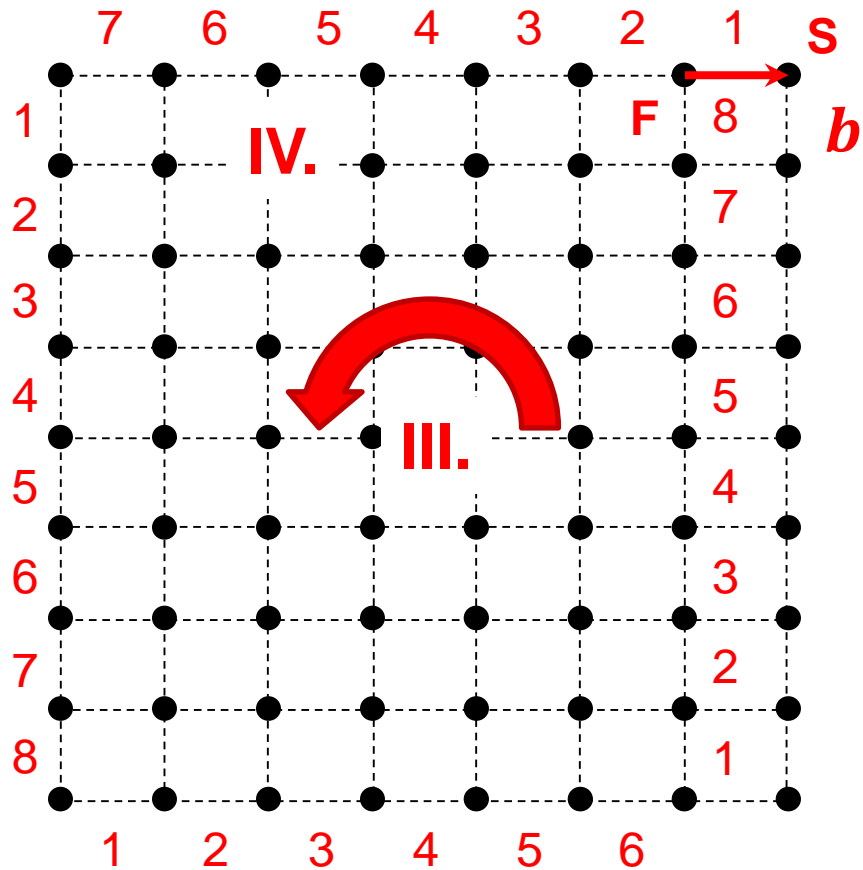
- The **Burgers circuit** is frequent source of mistakes in interpretation due to its **arbitrariness without proper definition**. There are many ways to perform the circuit(s) depending on what is set in the beginning:
 - **What is the direction of the circuit?** (right-handed RH, left-handed LH)
 - **Is the circuit closed from finish-to-start (FS) or from start-to-finish (SF)?**
 - **Is the circuit closed in the distorted (slipped) crystal** (“local Burgers vector” $\mathbf{b} = \oint_C \frac{\partial \mathbf{u}}{\partial l} dl$) **or in the perfect crystal** (“Burgers vector”)?
- All equations used in the lecture are made for Burgers vectors determined in the perfect crystal with RH/FS.
- Note that the length of the local Burgers vector depends on the choice of the circuit. Therefore, it is usually not recommended for Cauchy-type mechanics.

Burgers Circuit



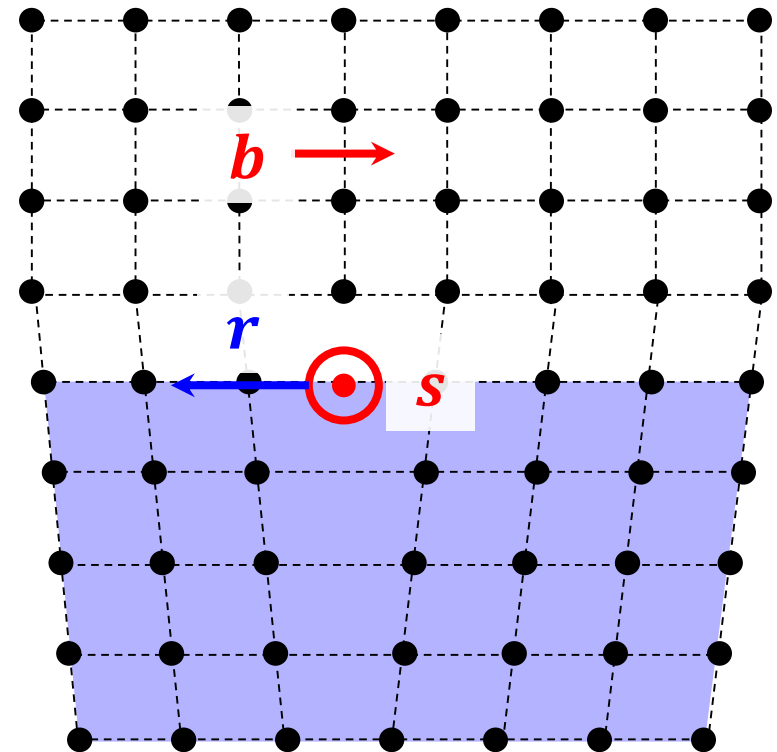
Close it in the perfect crystal with RH/FS!

Burgers Circuit



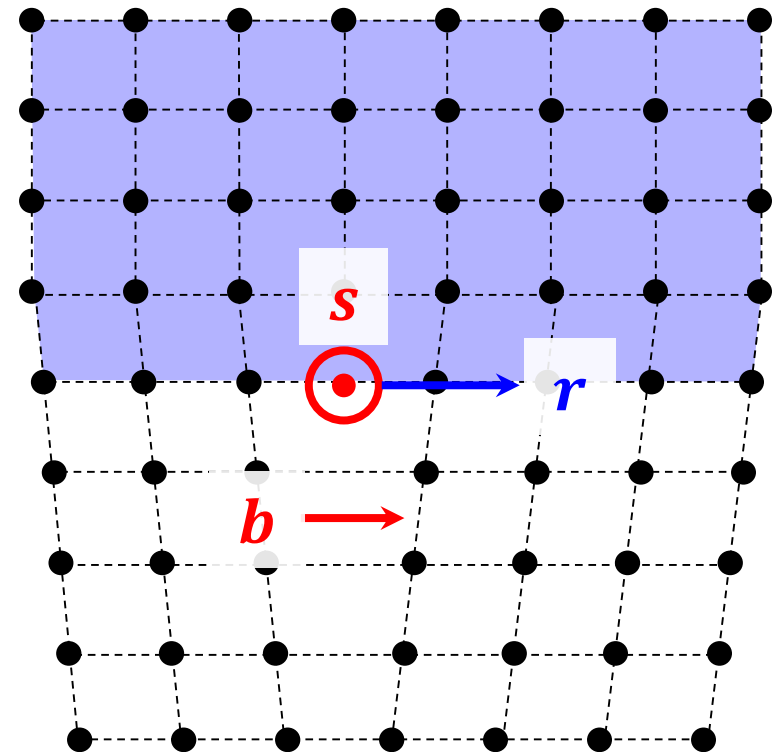
Burgers Circuit

- The **cross product** of dislocation **line vector s** and **direction of motion of the line r** denotes the **half crystal that is shifted** along the **Burgers vector b** .

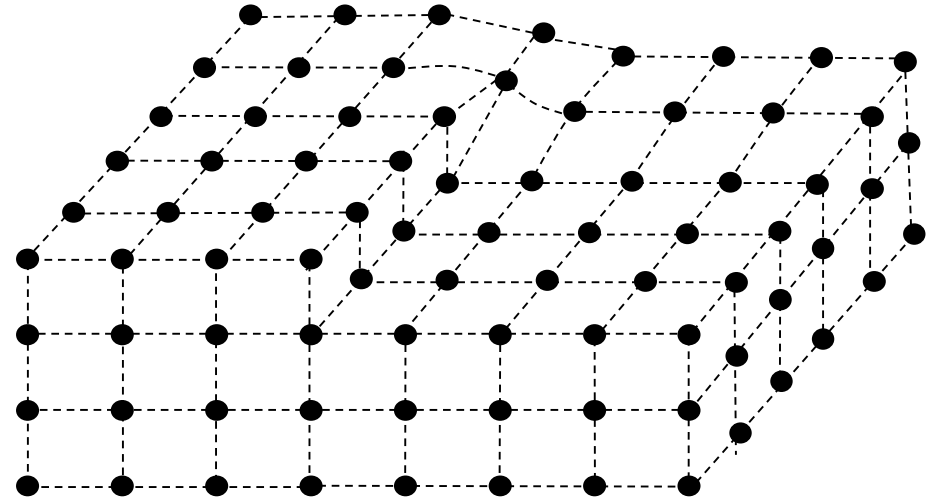
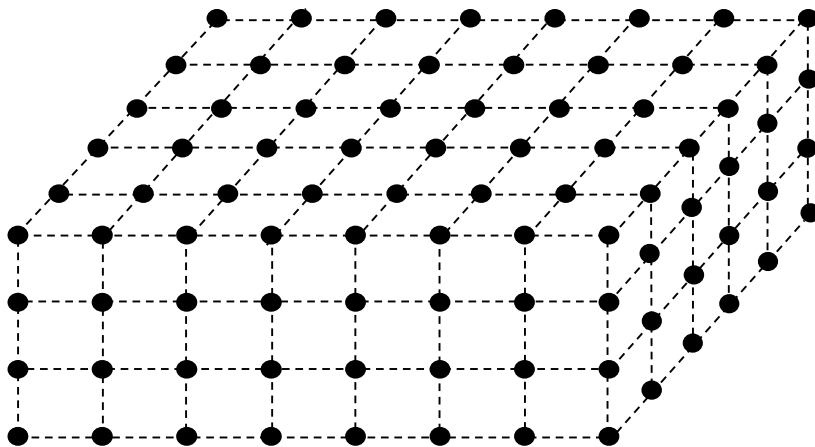


Burgers Circuit

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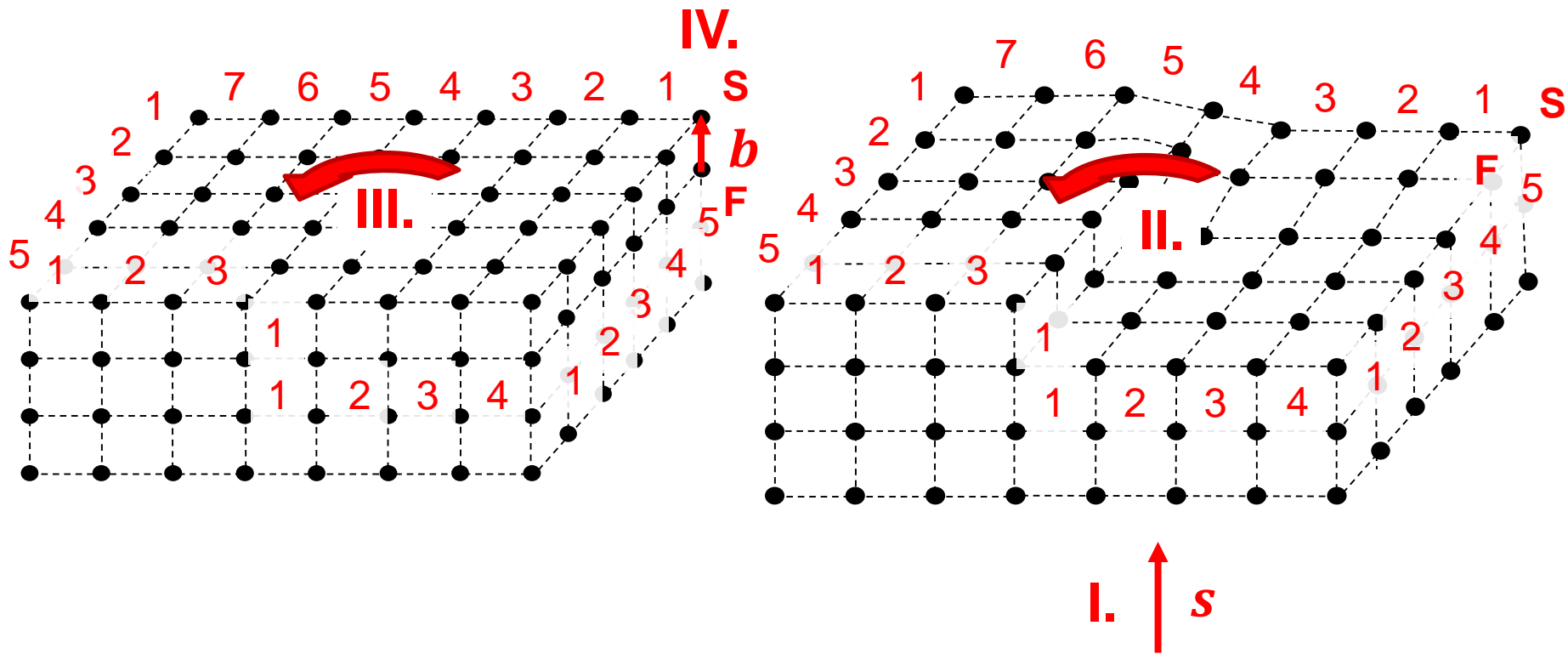


Burgers Circuit

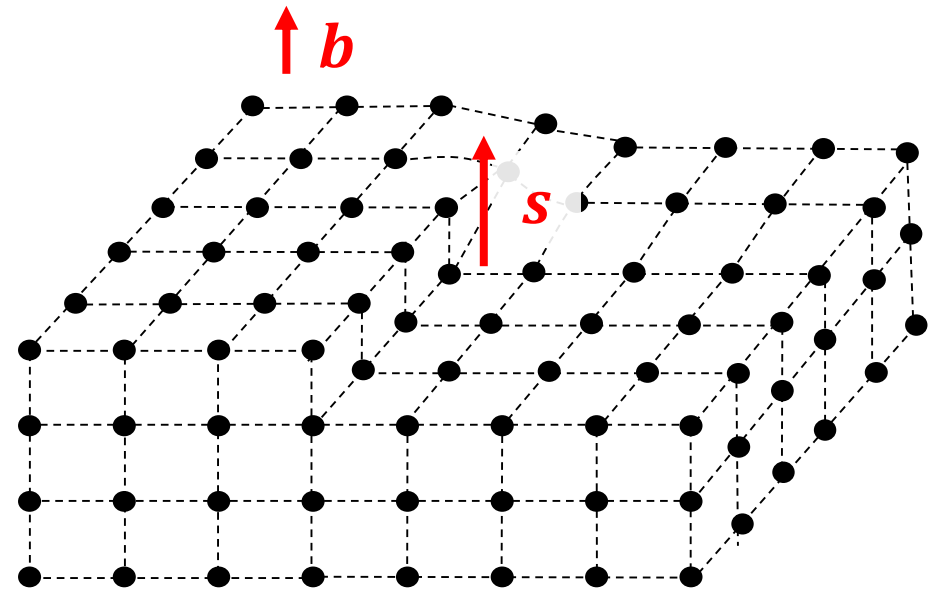
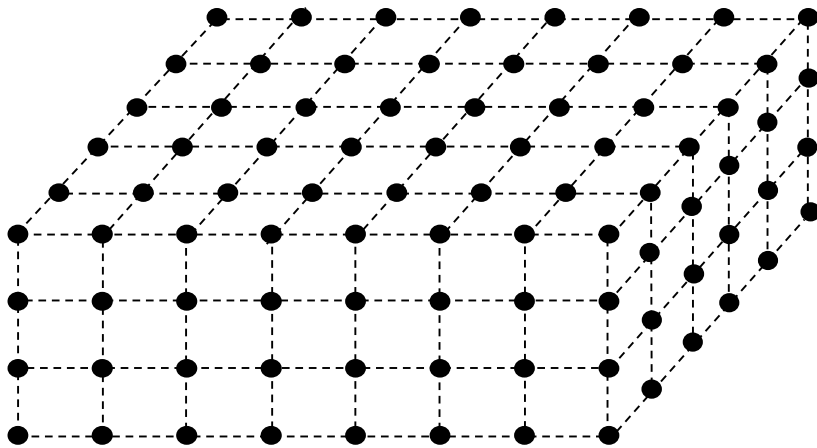


Close it in the perfect crystal with RH/FS!

Burgers Circuit



Burgers Circuit



$$n = 0$$

Dislocation Character

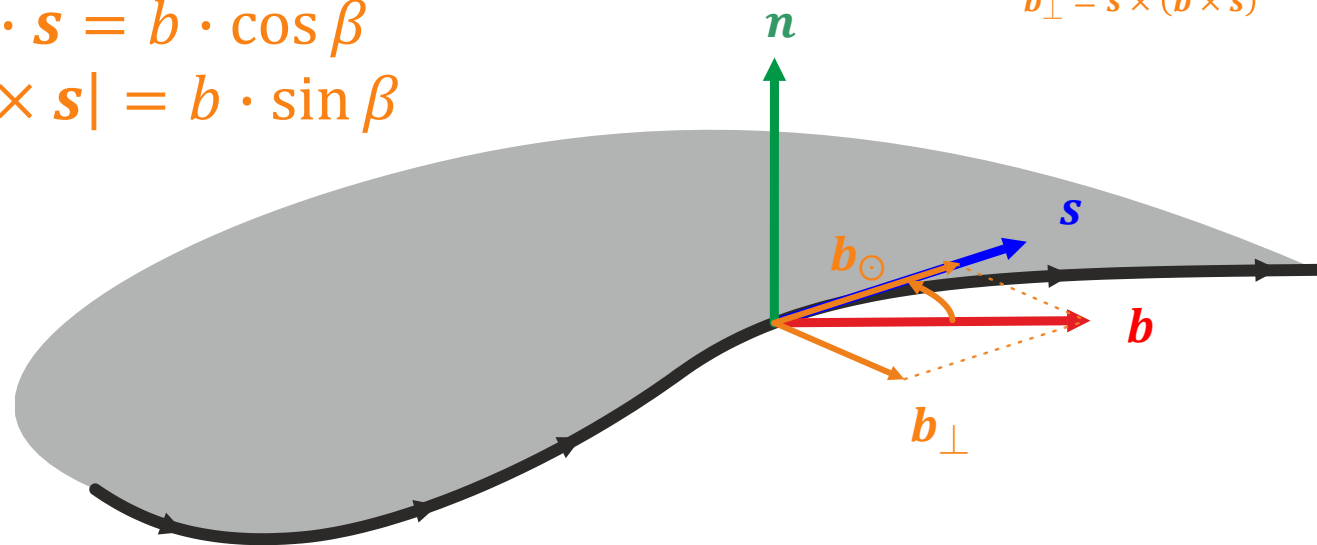
- An arbitrary dislocation can be described by the character $\beta = \angle(\mathbf{b}, \mathbf{s})$. The edge component of the dislocation is then:

$$b_{\odot} = \mathbf{b} \cdot \mathbf{s} = b \cdot \cos \beta$$

$$b_{\perp} = |\mathbf{b} \times \mathbf{s}| = b \cdot \sin \beta$$

$$b_{\odot} = (\mathbf{b} \cdot \mathbf{s}) \mathbf{s}$$

$$b_{\perp} = \mathbf{s} \times (\mathbf{b} \times \mathbf{s})$$

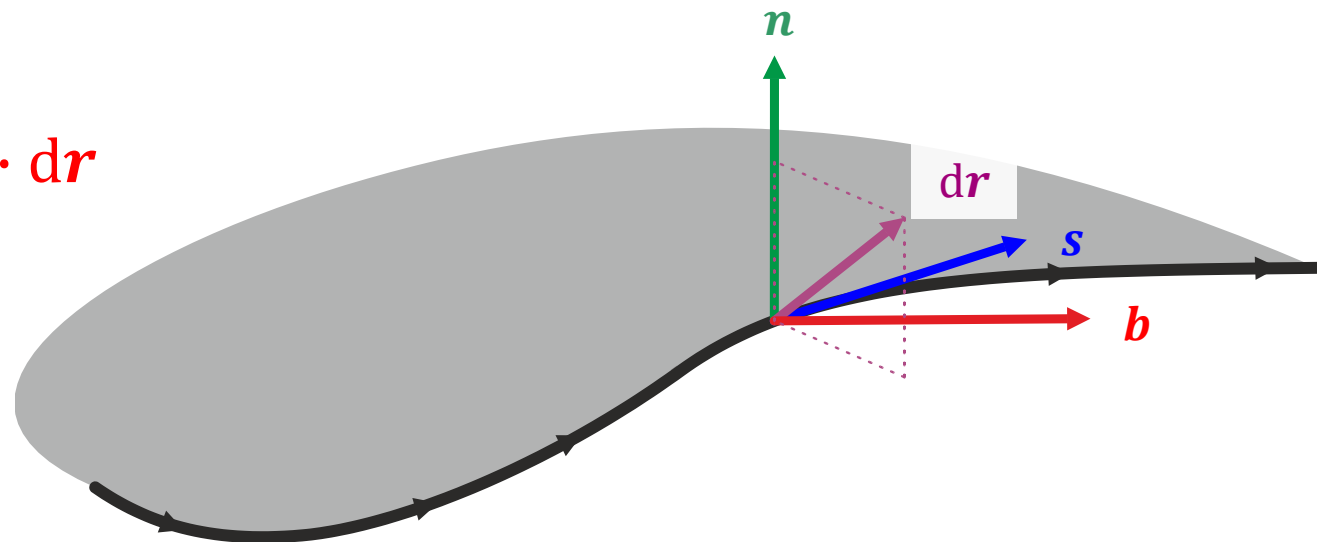


- $\beta = 0^\circ$ is pure screw, while $\beta = 90^\circ$ is pure edge.

Dislocation Character

- The volume consumption $\frac{dV}{L}$ for the motion of the line in the direction r is the following triple product:

$$\frac{dV}{L} = (\mathbf{b} \times \mathbf{s}) \cdot d\mathbf{r}$$



Dislocation Motion

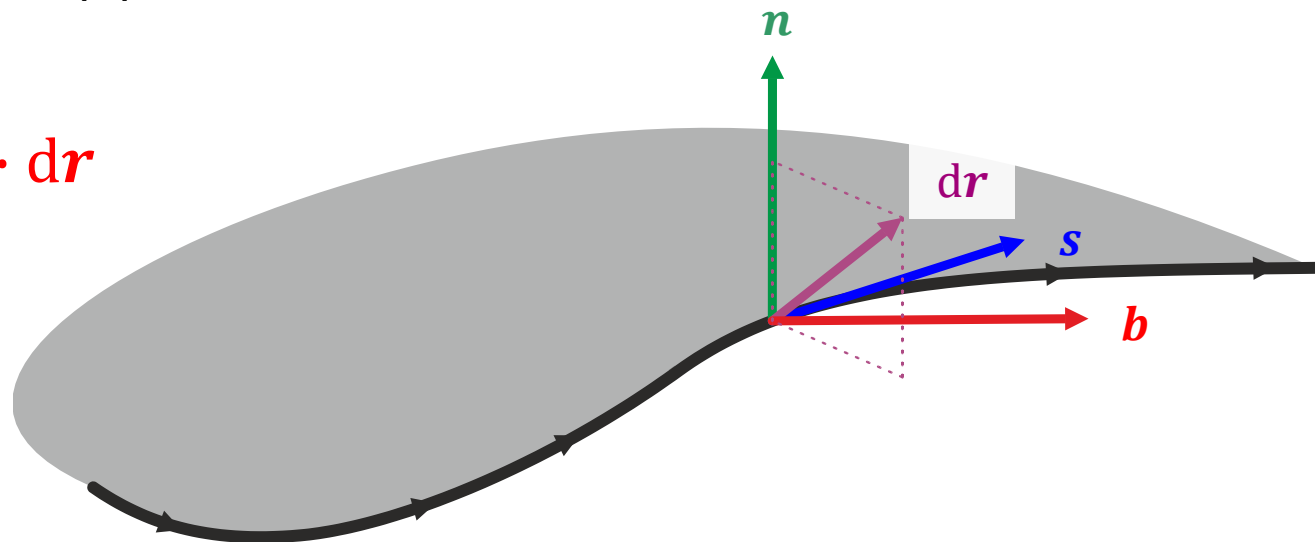
- We can distinguish different types of dislocation motion:

glide or slip

= motion within the slip plane $\angle(\mathbf{n}, d\mathbf{r}) = 90^\circ$

$$\frac{dV}{L} = (\mathbf{b} \times \mathbf{s}) \cdot d\mathbf{r}$$

$$= \mathbf{n} \cdot d\mathbf{r} = 0$$



Glide and slip of dislocations **is** (volume) **conservative**.

In old references, glide is used when single dislocations are considered while slip is the cooperative motion of many dislocations. In modern literature, both terms are used equally.

Dislocation motion

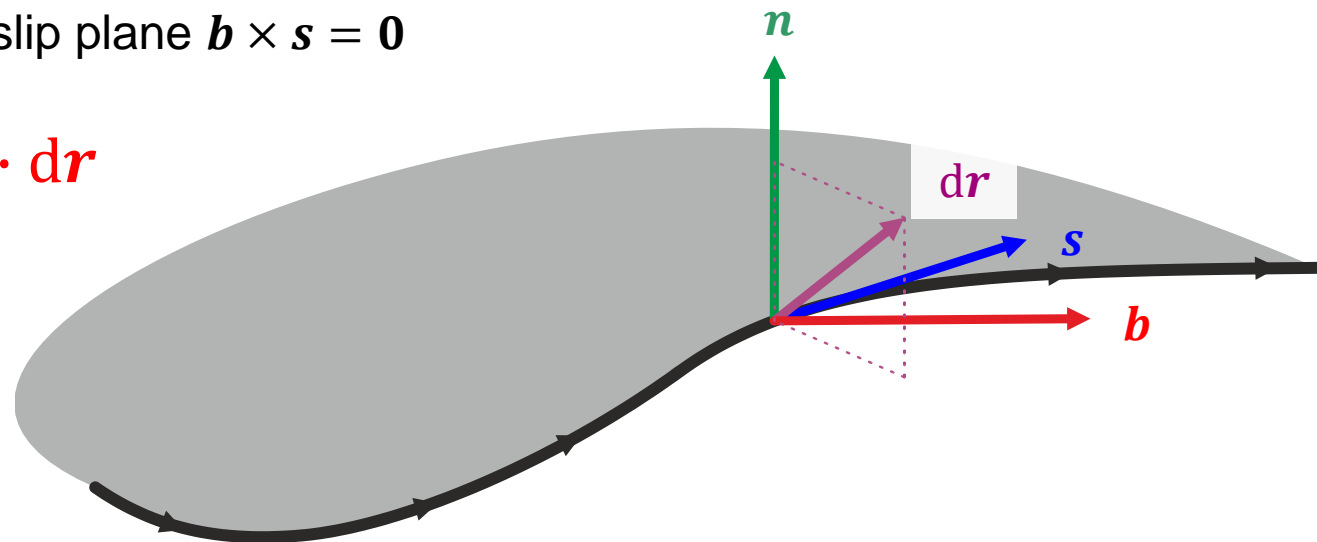
- We can distinguish different types of dislocation motion:

cross-slip

= motion of a screw dislocation
without a distinct slip plane $\mathbf{b} \times \mathbf{s} = \mathbf{0}$

$$\frac{dV}{L} = (\mathbf{b} \times \mathbf{s}) \cdot d\mathbf{r}$$

$$= \mathbf{0} \cdot d\mathbf{r} = 0$$

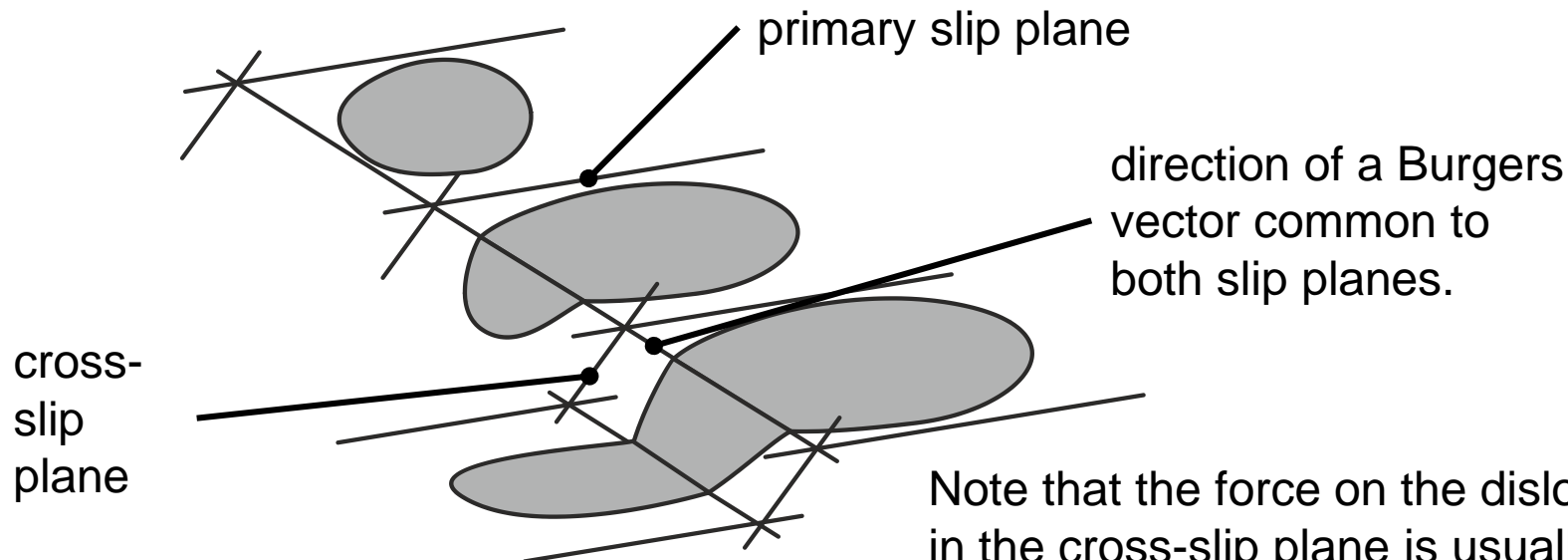


Cross-slip of screw dislocations **is** (volume) **conservative**.

Dislocation motion

- We can distinguish different types of dislocation motion:

The **discrete nature of crystals** causes the occurrence of distinct slip planes for screw dislocations. In case of **intersecting slip planes with slip directions along the intersection**, a change of the slip plane by cross-slip is possible.



Note that the force on the dislocation line in the cross-slip plane is usually lower.
Cross-slip is, therefore, thermally activated.

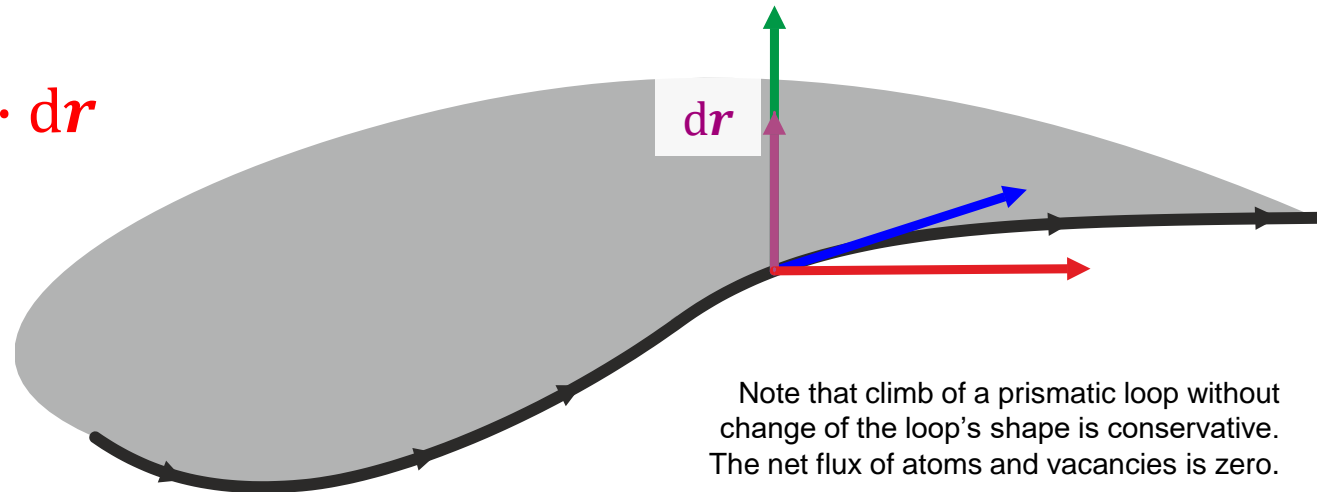
Dislocation motion

- We can distinguish different types of dislocation motion:

climb

= motion perpendicular to the slip plane

$$\frac{dV}{L} = (\mathbf{b} \times \mathbf{s}) \cdot d\mathbf{r}$$

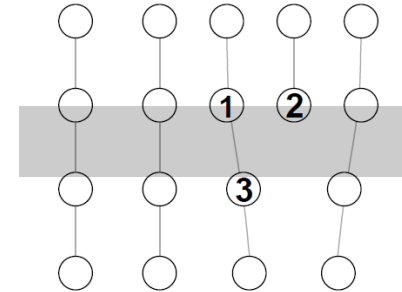
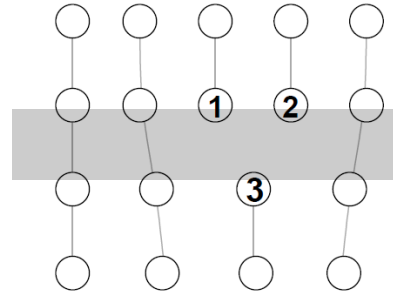
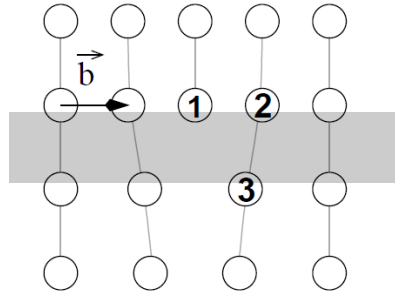


Climb of dislocations **is non-conservative**. Depending on the sign of the volume change associated with it, atoms or vacancies have to diffuse to the dislocation line.

Dislocation motion

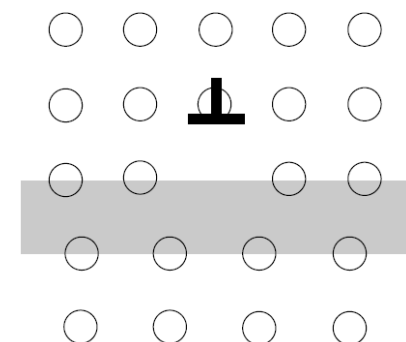
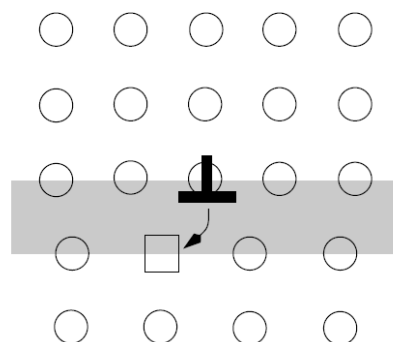
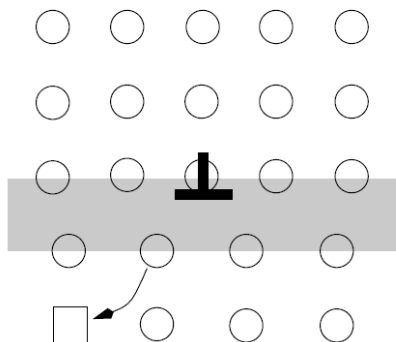
■ Glide, slip

motion ↔



■ Climb

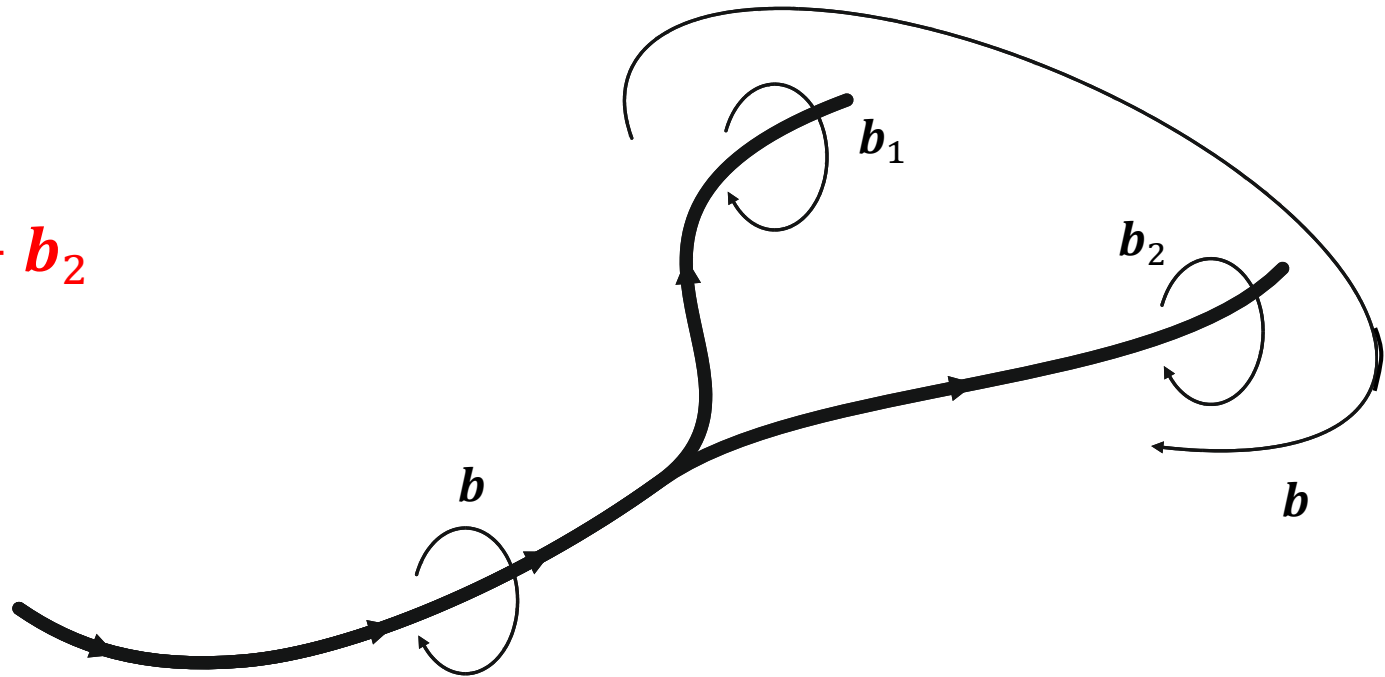
motion ↑↓



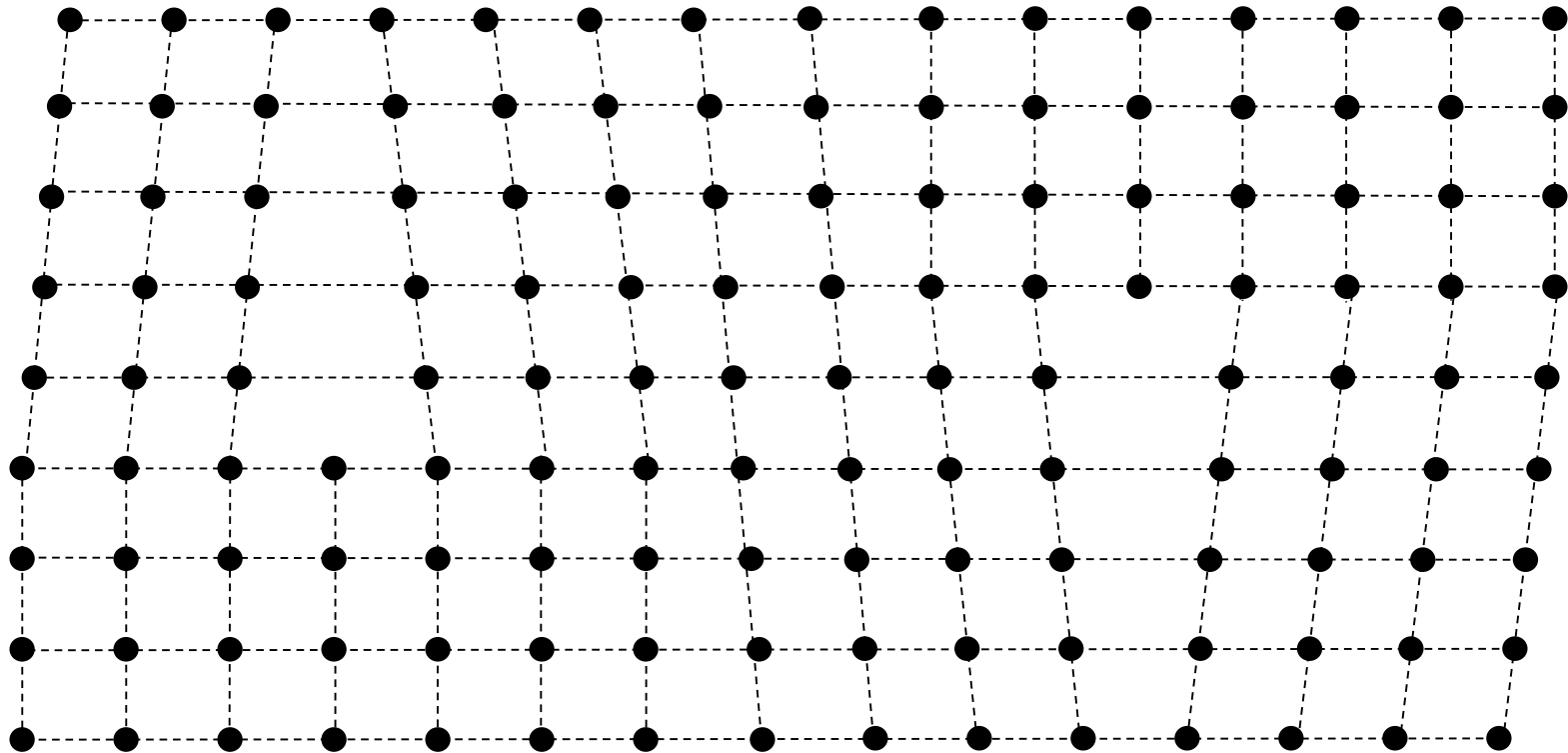
Dislocation nodes

- **Burgers vectors are added** during reactions of dislocations and at nodes:

$$b = b_1 + b_2$$

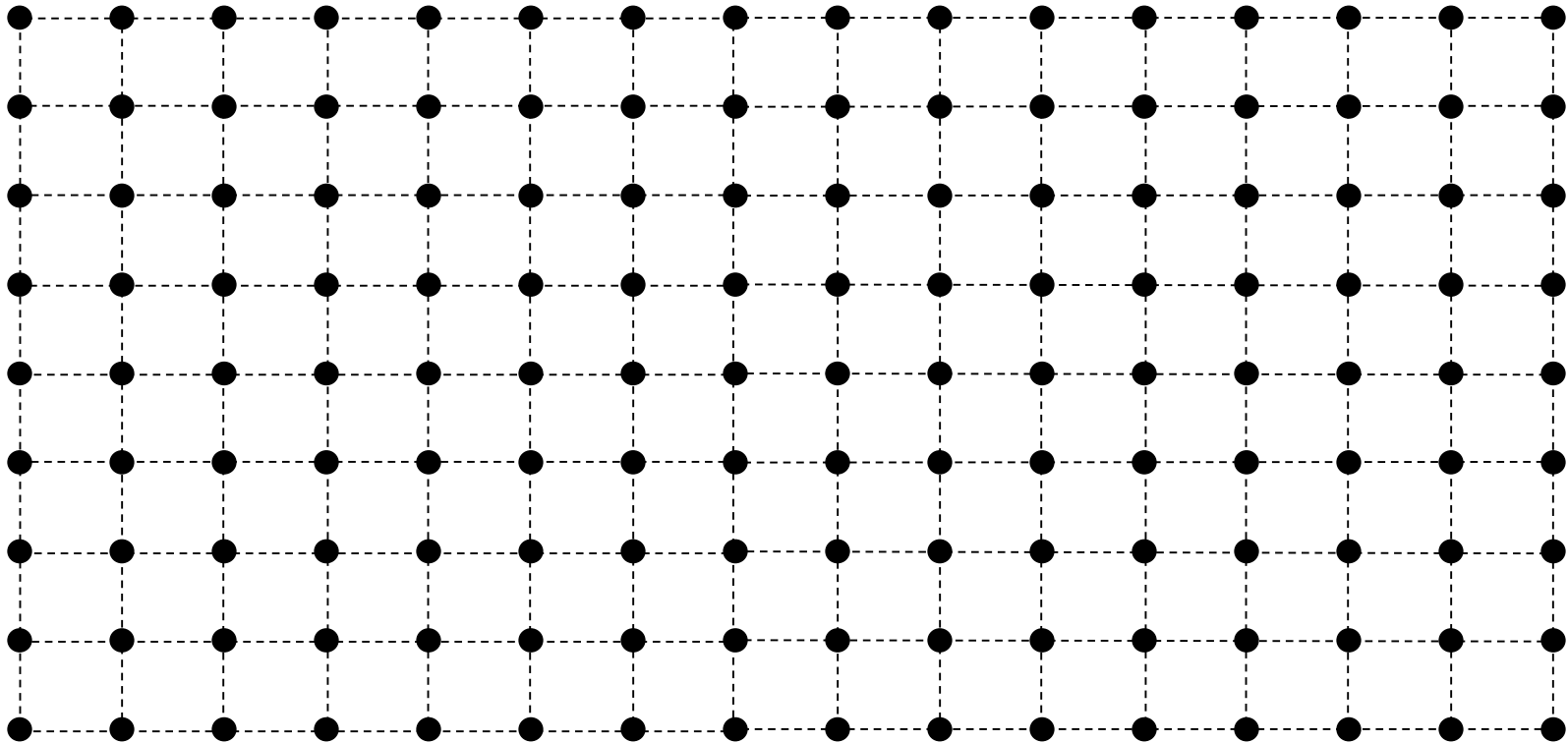


Burgers Circuit



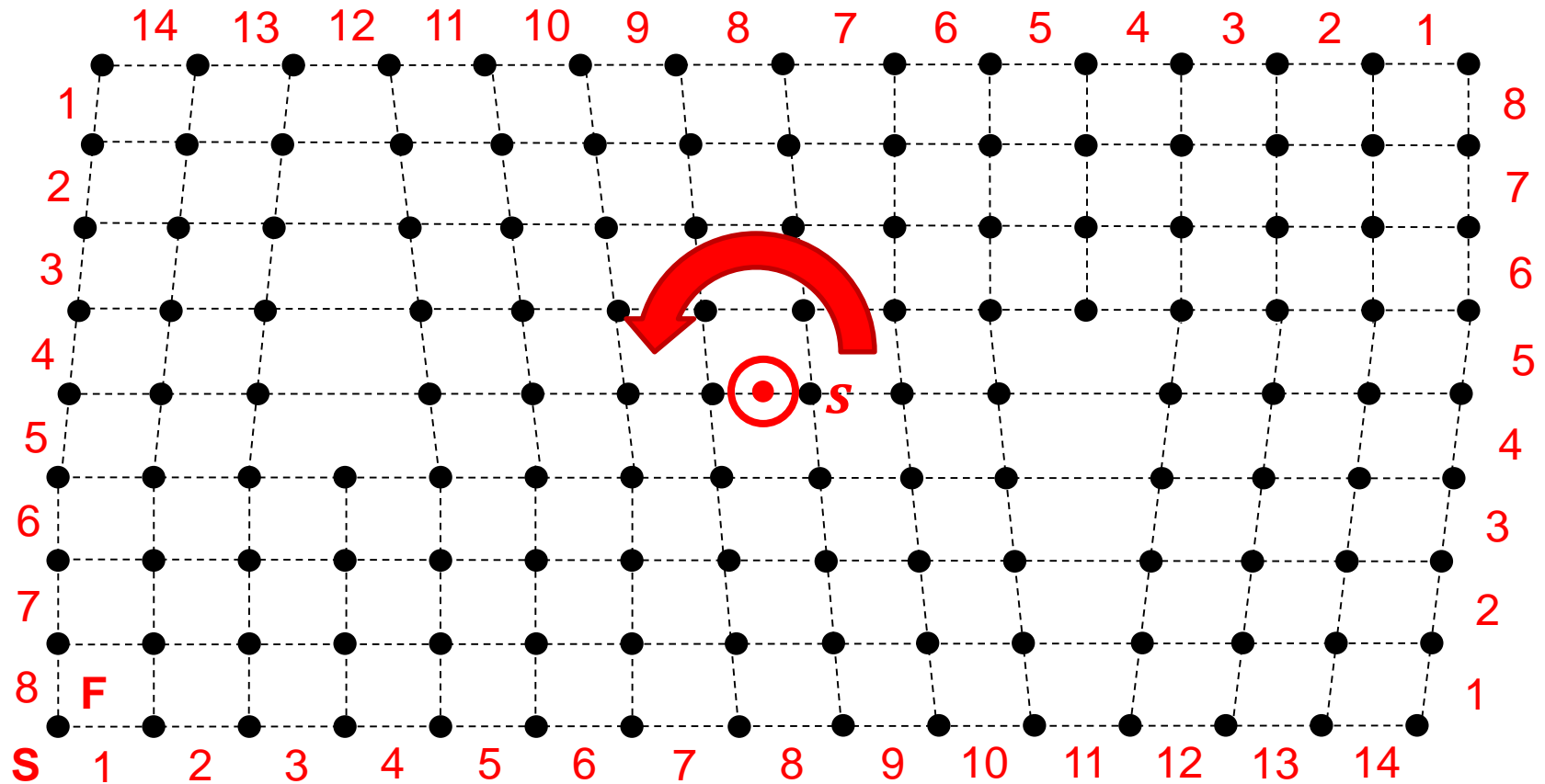
Close it in the perfect crystal with RH/FS!

Burgers Circuit

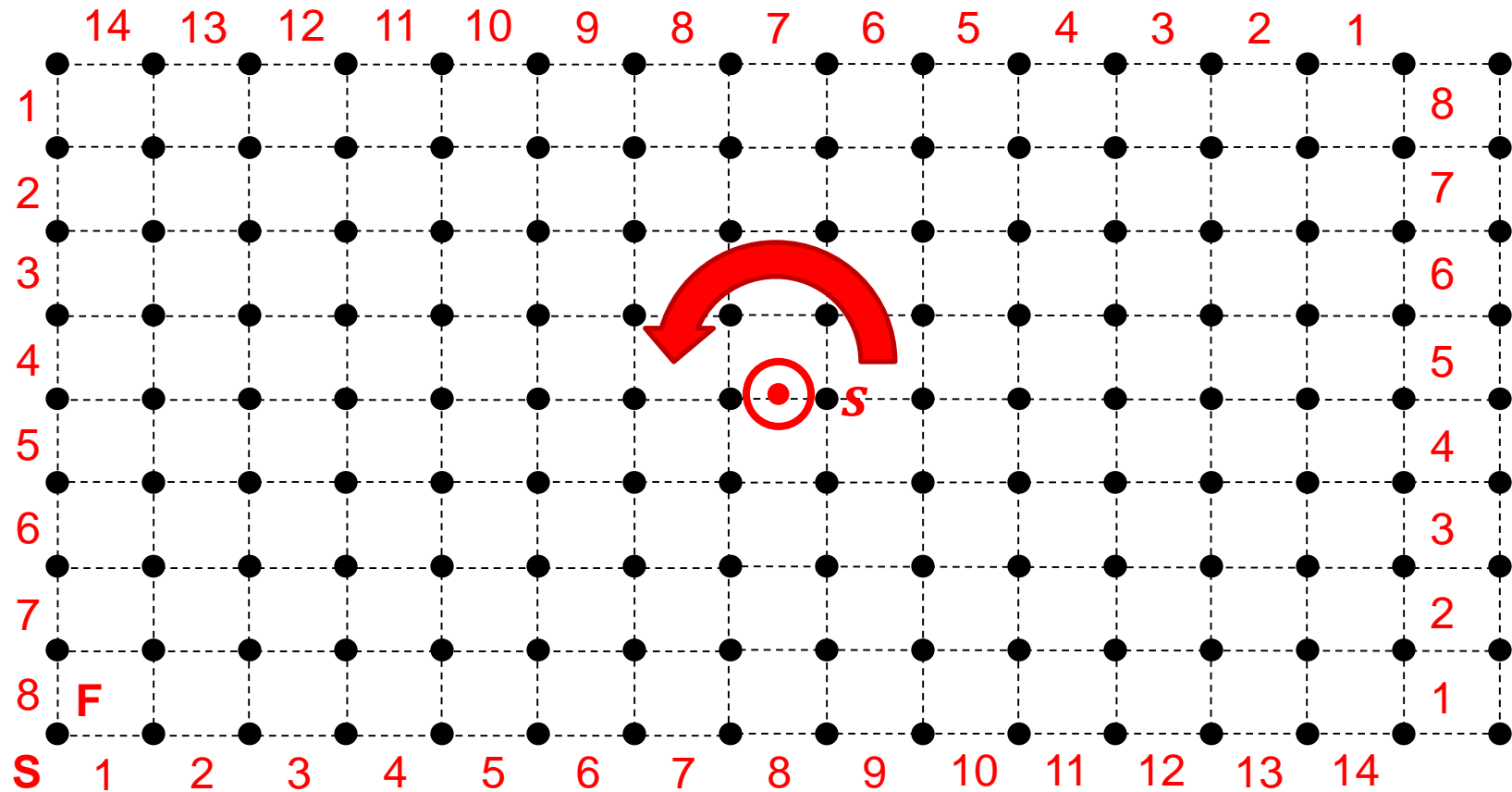


Close it in the perfect crystal with RH/FS!

Burgers Circuit

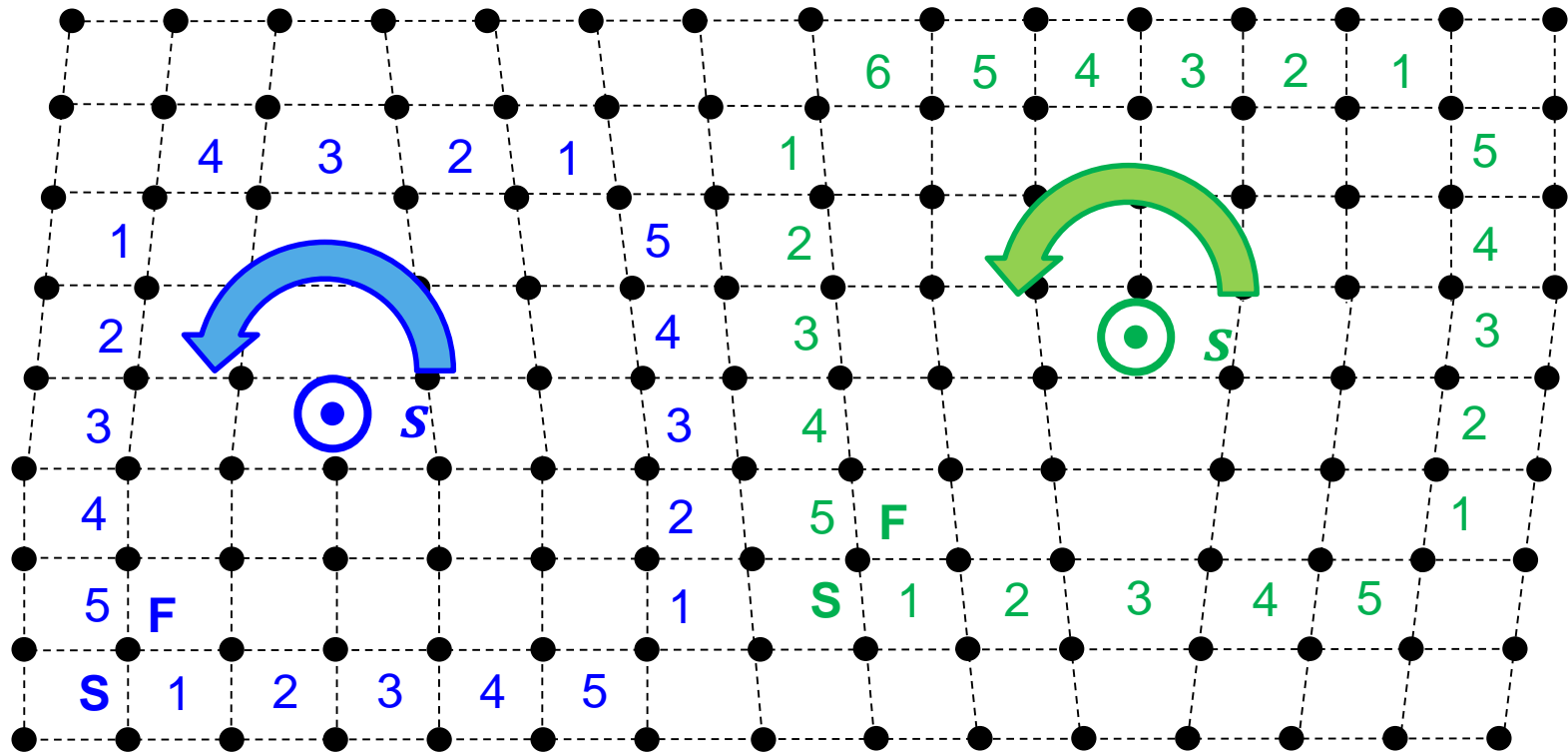


Burgers Circuit

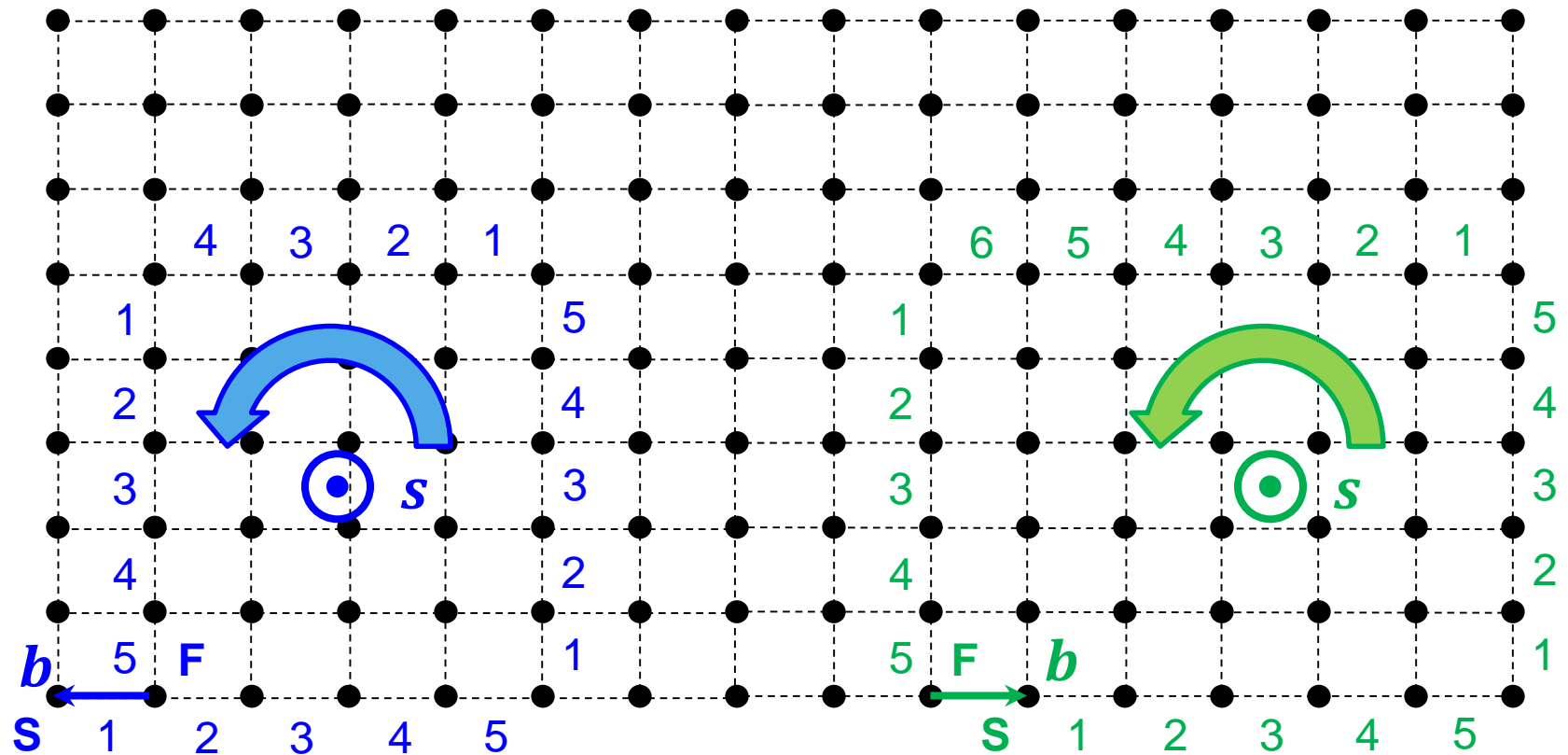


No net Burgers vector!

Burgers Circuit



Burgers Circuit



The Burgers vectors are antiparallel.

Dislocation Density

- The dislocation density quantifies the amount of dislocations in a volume. It corresponds to the total length of dislocations per volume:

$$\rho = \frac{L}{V}, [\rho] = \frac{\text{m}}{\text{m}^3} = \frac{1}{\text{m}^2}$$

- The lowest dislocation densities are found in „dislocation-free“ Si or Ge crystals. During the Czochalski procedure, the size of the crystal remains small in the beginning in order to allow growth dislocations to leave the crystal. Otherwise, growth dislocations remain in the crystal and allow for faster crystal growth. For more details, see the lecture “Phase Transformations in Materials”.
- As rough estimates:
 - dislocation-free: $\rho \approx 0 \text{ m}^{-2}$
 - common lab crystals: $\rho \approx (10^7 \dots 10^9) \text{ m}^{-2}$
 - polycrystalline, recrystallized: $\rho \approx (10^9 \dots 10^{13}) \text{ m}^{-2}$
 - deformed metals and alloys: $\rho \lesssim 10^{16} \text{ m}^{-2}$

Dislocation Density

- As we have seen, there are dislocation arrangements **without net Burgers vector** (dipoles). Hence, there is no (significant) net deformation of the body. The according dislocations are called “**statistically stored**” and are associated with a respective density of statistically stored dislocations.
- Dislocation arrangements with **net Burgers vector**, result in a significant deformation of the body. These dislocations are called “**geometrically necessary**”. The deformation of the body depends on the density of geometrically necessary dislocations.

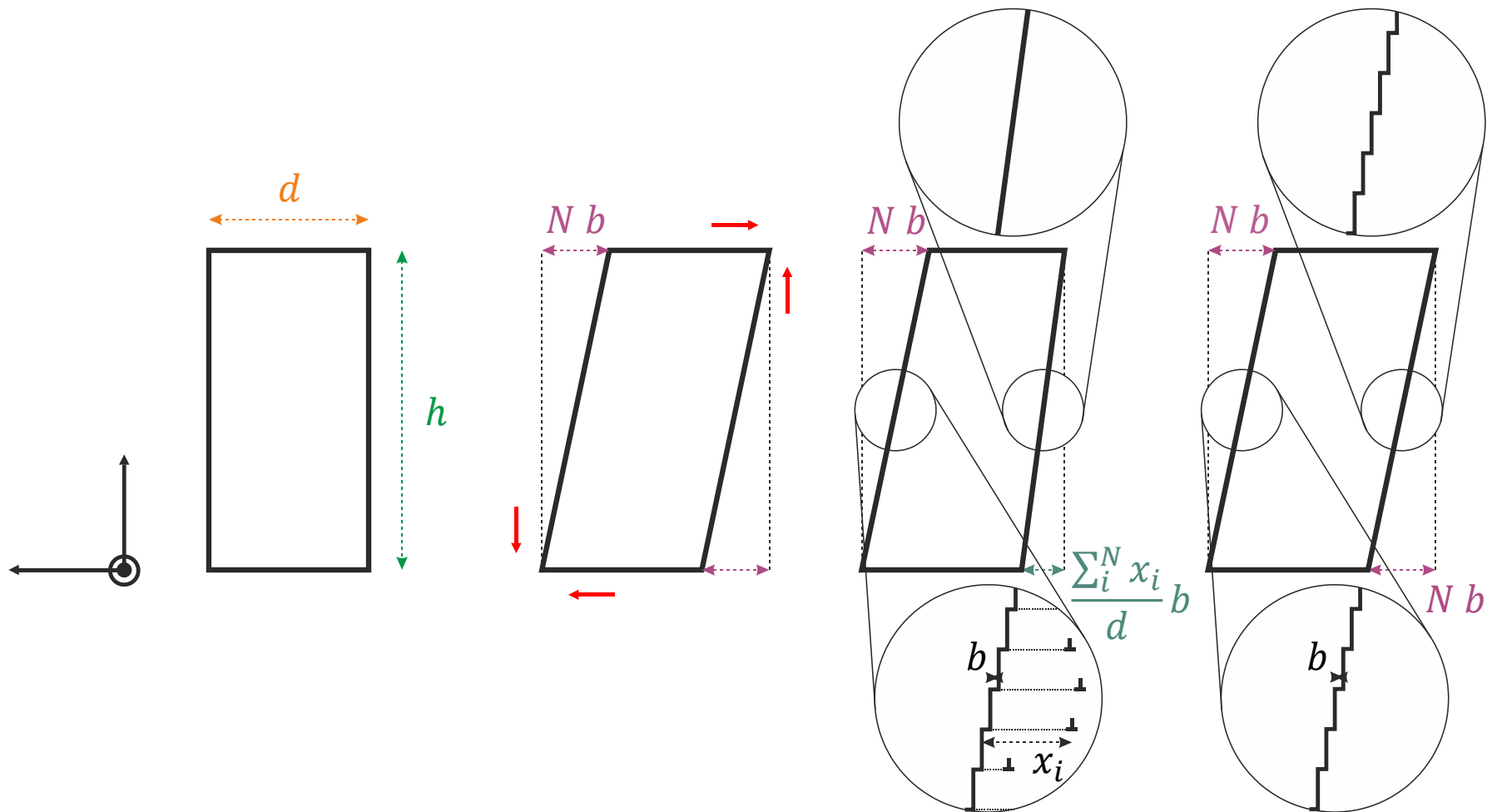
Note that strictly speaking, the orientation change within a crystal depends on the density of geometrically necessary dislocations. Once dislocations have left the crystal through the surface, there is no dislocation anymore but the body is deformed plastic due to completion of the slip process.

Plastic Deformation by Slip

- Complete slip of a body of h in height by N dislocations with Burgers vectors of length b yields a shear of $\gamma \approx \frac{N b}{h}$.
- In case, the slip process is not complete, a partial slip distance x_i specific to every dislocation and smaller than the maximum slip distance $x_i < d$ can be used: $\gamma \approx \frac{b \sum_i^N x_i}{h d}$.
- The shear can then be described using the density of glissile dislocations: $\rho \approx \frac{N l}{h d l} = \frac{N}{h d}$ (total length of the glissile dislocations divided by the volume of the body, with l being the depth of the body). If $\bar{x} = 1/N \sum_i^N x_i$ is the average slip distance of the dislocations, we obtain:

$$\gamma = b \rho \bar{x}$$

Plastic Deformation by Slip



Plastic Deformation by Slip

- If we consider an initial dislocation density of $\rho \gtrsim 10^9 \text{ m}^{-2}$ at a crystallite size of about $\bar{x} \approx 500 \text{ }\mu\text{m}$ and Burgers vectors of $b \approx 2.5 \text{ }\text{\AA}$, this yields:

$$\gamma = b \rho \bar{x} \approx 1.25 \cdot 10^{-4}$$

- This is orders of magnitude lower than the strains achieved in metallic and intermetallic materials, see Ch. 2!
- Obviously, the dislocation density must increase during plastic deformation since the other quantities remain (approx.) constant; dislocation multiplication must take place.

Plastic Deformation by Slip

- The plastic strain rate by dislocation slip is then (“Orowan equation”):

$$\dot{\gamma} = b \dot{\rho} \bar{x} + b \rho v$$

$$\approx b \rho v$$

- The slip of dislocations leads to instantaneous plastic deformation:

$$b \approx 2.5 \text{ \AA}, \rho \gtrsim 10^9 \text{ m}^{-2}, v \lesssim 3800 \text{ m/s}$$

$$\dot{\gamma} \approx 950 \text{ s}^{-1}$$

More details on the speed of dislocations are provided in Ch. 4e.

Historical Evolution

- In order to provide an impression of how revolutionary the introduction of the slip and dislocation concept is (not was), some fundamental questions from the time might be recapped:
 - **How can crystalline solids deform plastic without losing their crystal structure?**
(That metallic materials are crystalline was known for a long time and proven by X-ray diffraction after 1911.) ✓
 - **Why is the onset of plastic deformation obtained at low shear stresses?**
(That plastic deformation is mainly triggered by shear stress was already clear for a long time; note that Tresca passed away in 1885.) ✓
 - **Why is plastic deformation instantaneous** and becomes time-dependent at high temperatures? ✓
 - Even though defects might mediate plastic deformation, **why are the obtained strains are so high?** ✓

Summary

- **Plastic deformation of most crystalline materials is controlled by shear stresses and mediated by dislocation motion.**
- Dislocations are **line defects**, the **strength** of which is described by the **Burgers vector**. **The Burgers vector determines the macroscopic deformation of the body after complete slip.**
- **The Burgers vector is constant along the dislocation line.** Burgers vectors are added during dislocation reactions and at dislocation nodes.
- **Dislocations do not terminate within crystals. Dislocation loops exist.**
- Dislocations can move volume **conservative by slip and cross-slip** or **non-conservative by climb.**