One dimensional defects

Dislocations

"Introduction to dislocations"

By D. Hull and D.J. Bacon

Section 1.4, 3.1 to 3.6

One dimensional defects

Dislocations

"Solid State Chemistry and its Applications"

By A. R. West

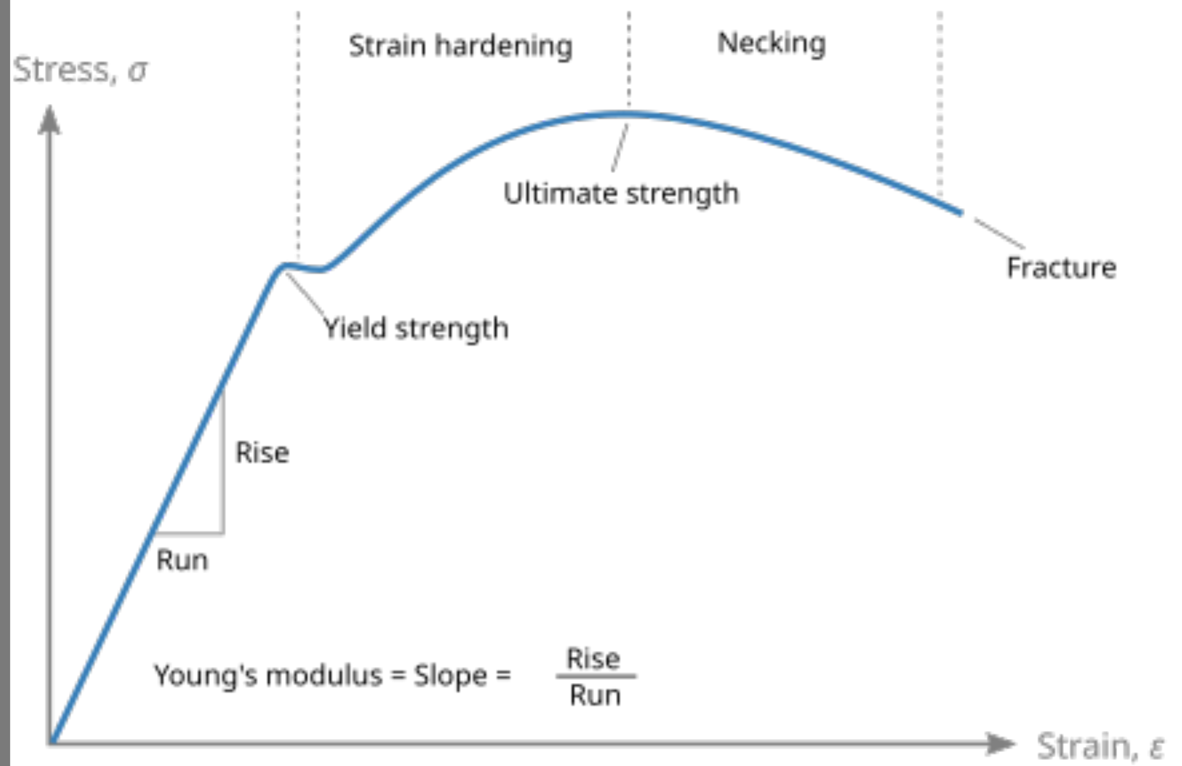
Section 2.5

"Introduction to dislocations"

By D. Hull and D.J. Bacon

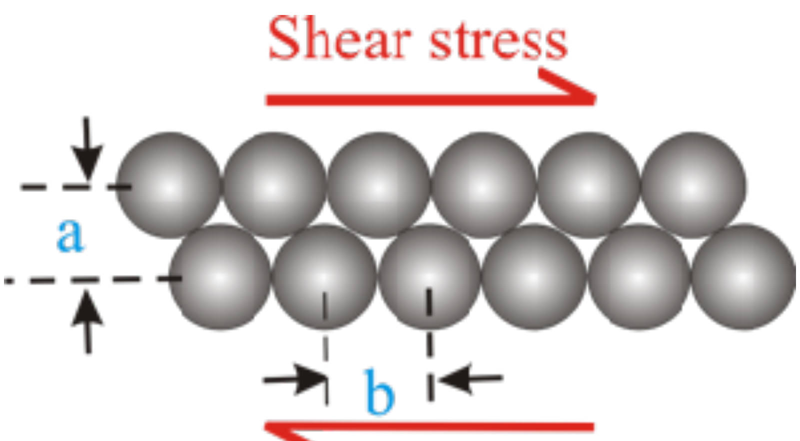
Section 1.4, 3.1 to 3.6

Mechanical response of materials



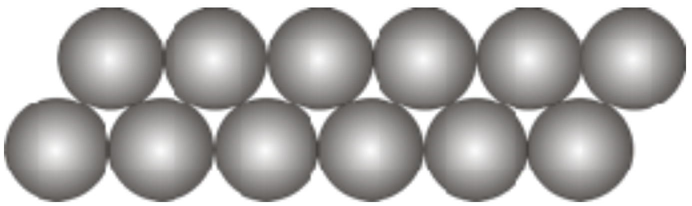
https://en.wikipedia.org/wiki/Stress–strain_curve, accessed on 30-09-2024

Extending elastic deformation concept

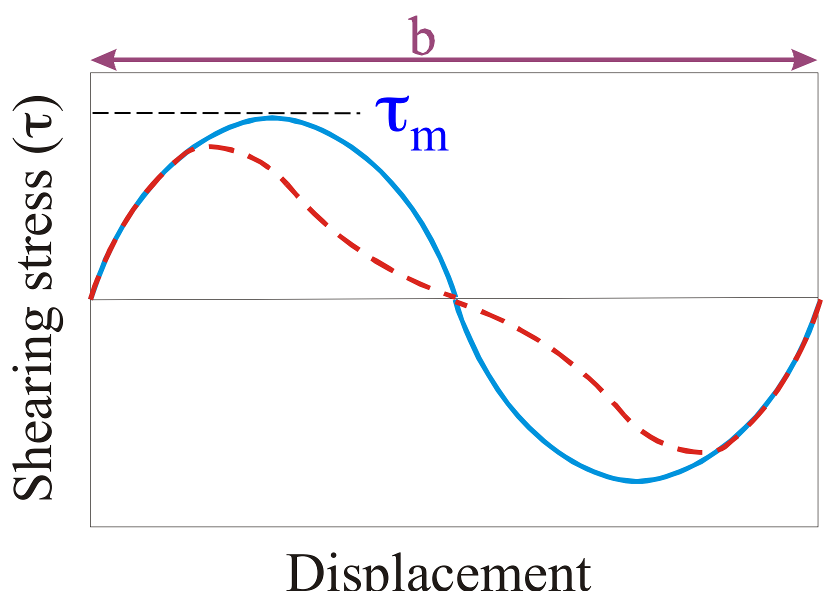


Starting configuration

Entire row of atoms sliding past another



Final configuration



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Maximum Shear stress

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Equating R.H.S

$$\therefore \frac{G}{a} = \frac{2\pi\tau_m}{b}$$

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$$\text{With } b \sim a,\ \tau_m = \frac{G}{2\pi}$$

The need for a different mechanism

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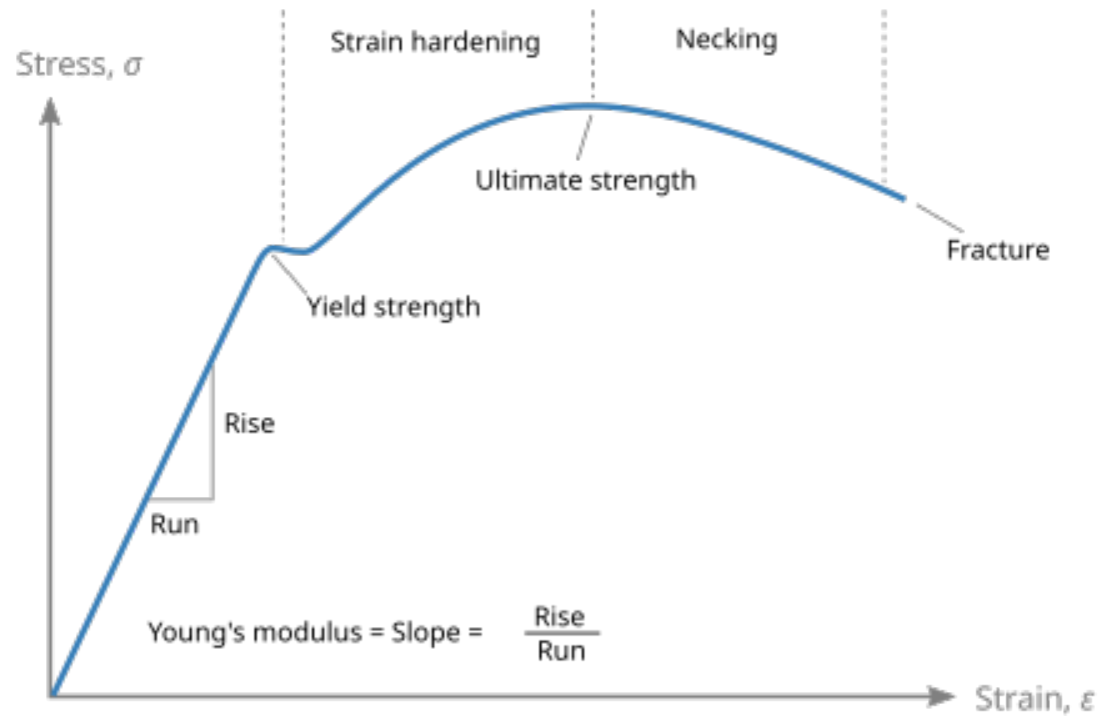

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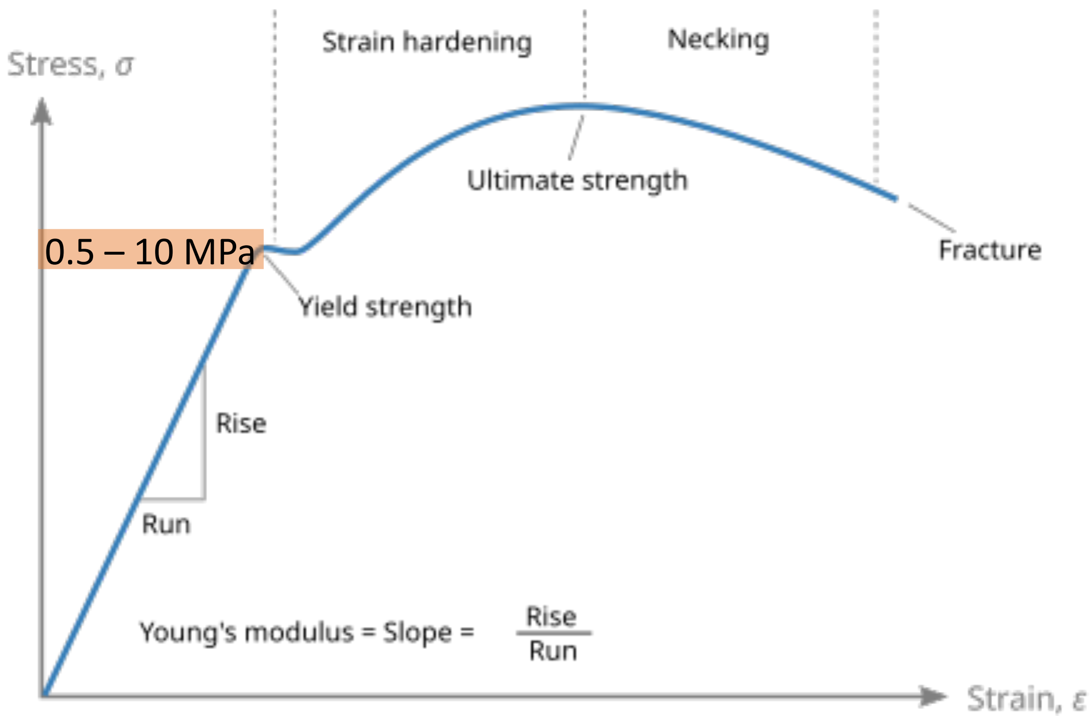

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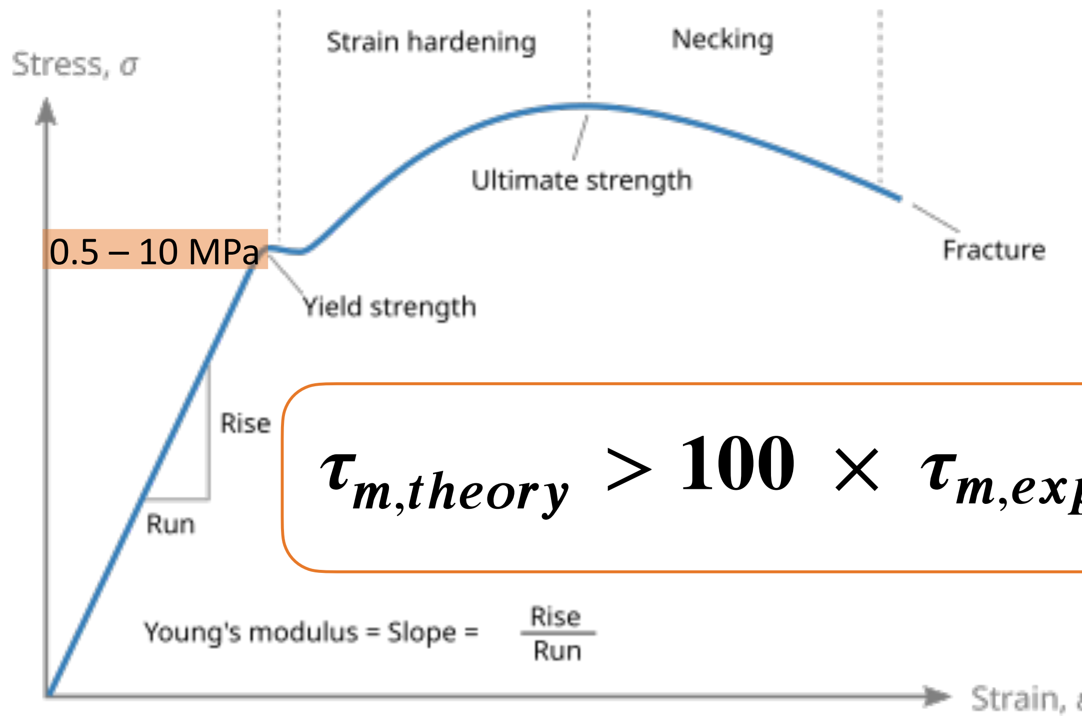
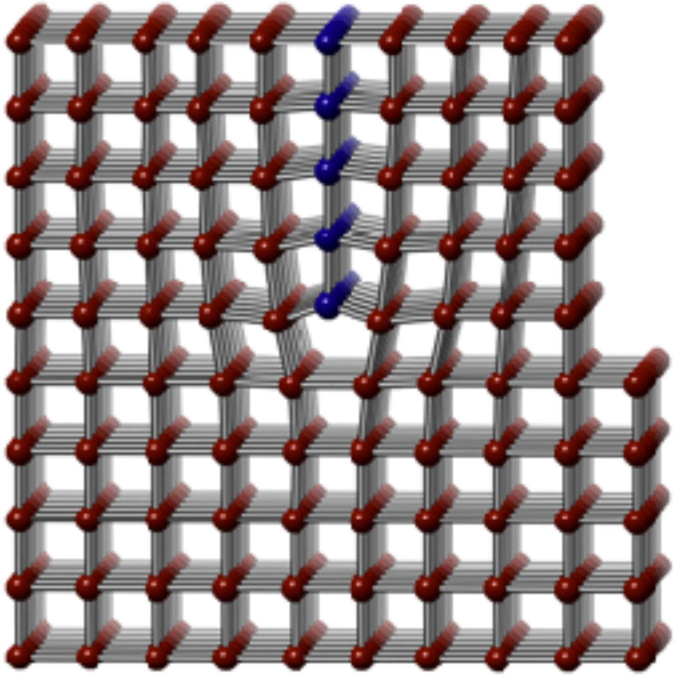


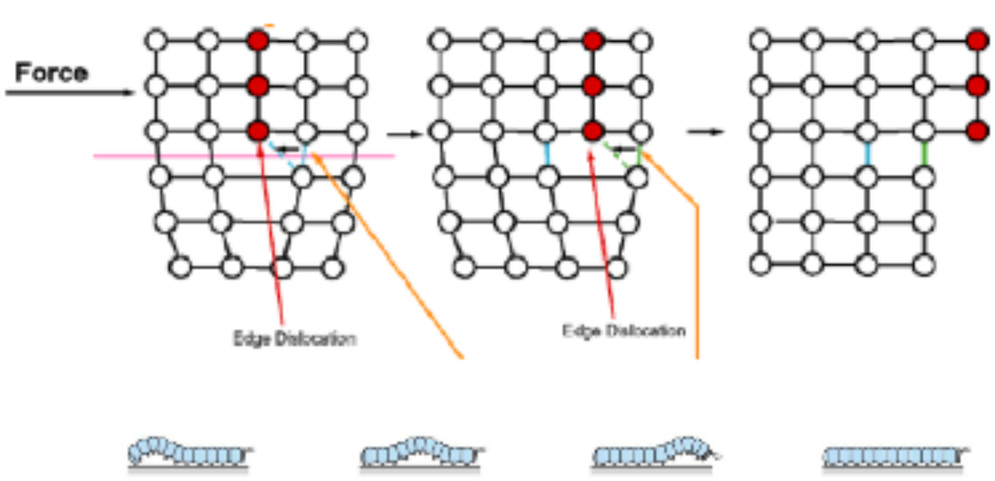
$$\boldsymbol{\tau_{m,theory} > 100 \times \tau_{m,expt}}$$

Dislocations – 1-D defects

Line defects are called dislocations



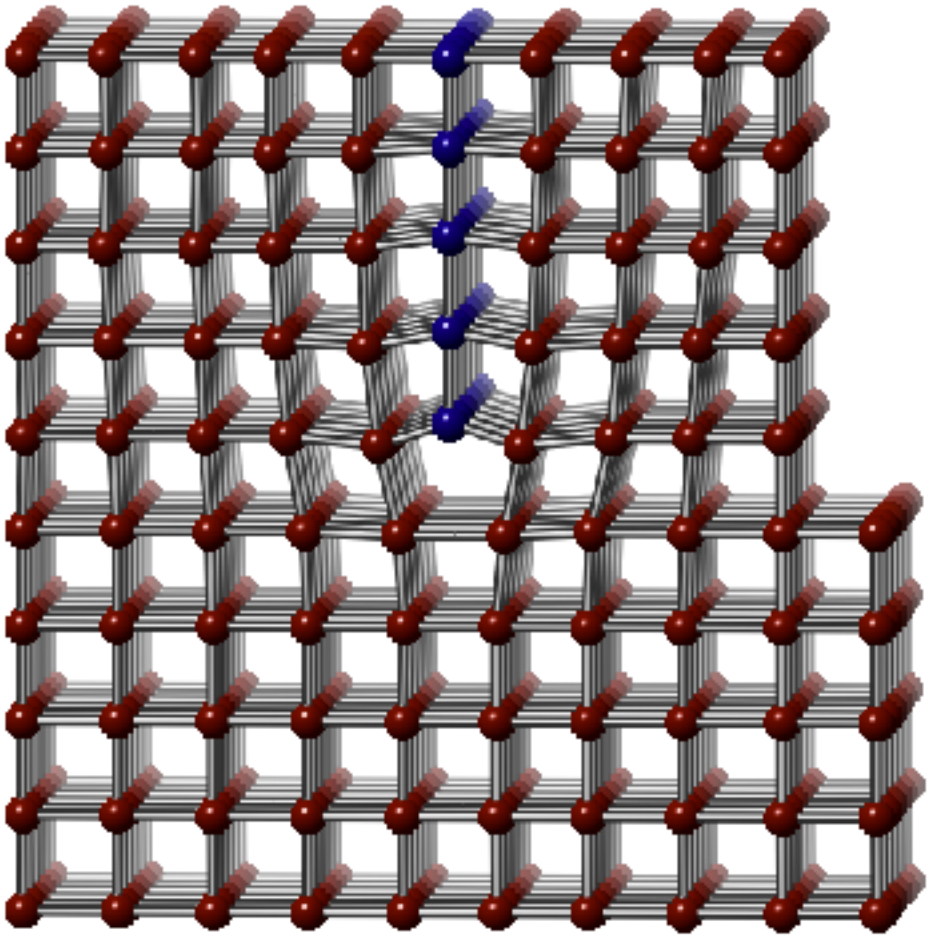
- Lower stress to plastic deformation



G.I. Taylor, Proceedings of the Royal Society A, 145 (1934) 362. E. Orowan, Zeit. Physics, 89 (1934) 605. N. Polanyi, Zeit. Phys. 89 (1934) 660. Vito Volterra, 1905.

Geometry of dislocations

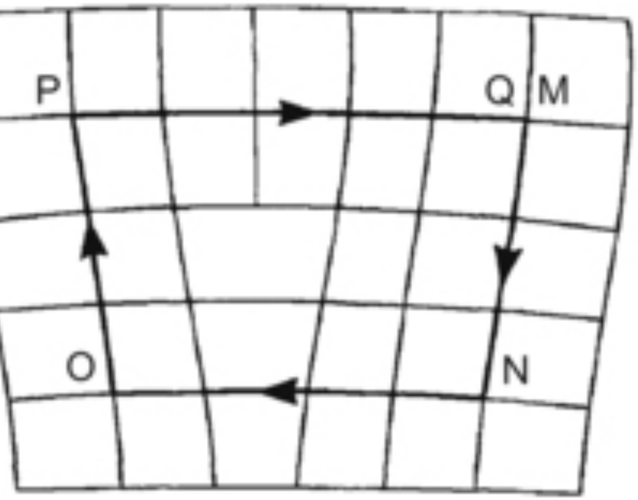
- Two vectors define a dislocation
  - Line Vector
  - Burgers vector
- Angle between these vectors characterizes it
  - Always 90° - Edge dislocation
  - Always 0° - Screw dislocation
  - Any other - Mixed dislocation

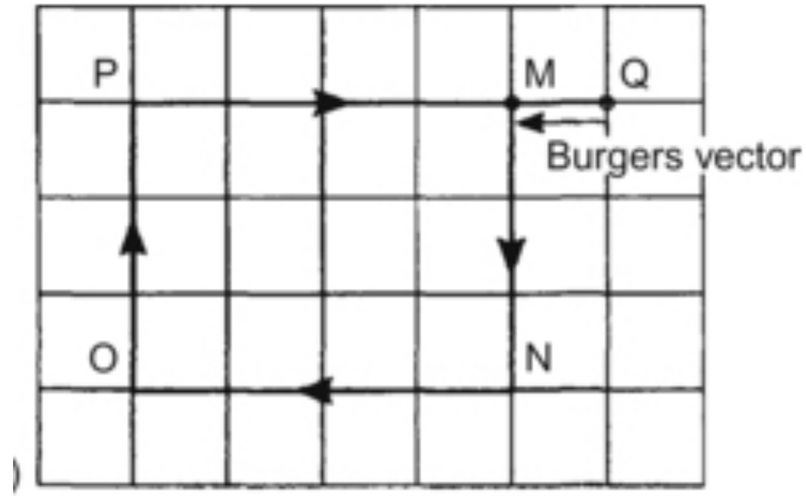


- extra half-plane of atoms
- distortion concentrated around the bounding line
- deflection and distortion of the interatomic bonds decrease with increasing distance from the line
- line sense taken as positive going in to the plane of the paper

Edge Dislocations – Line vector

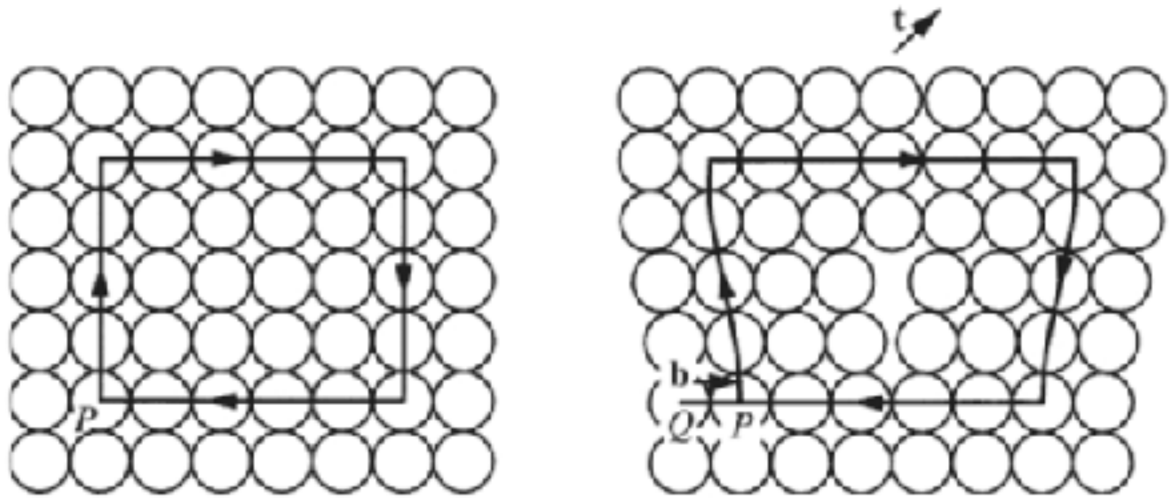
(a)





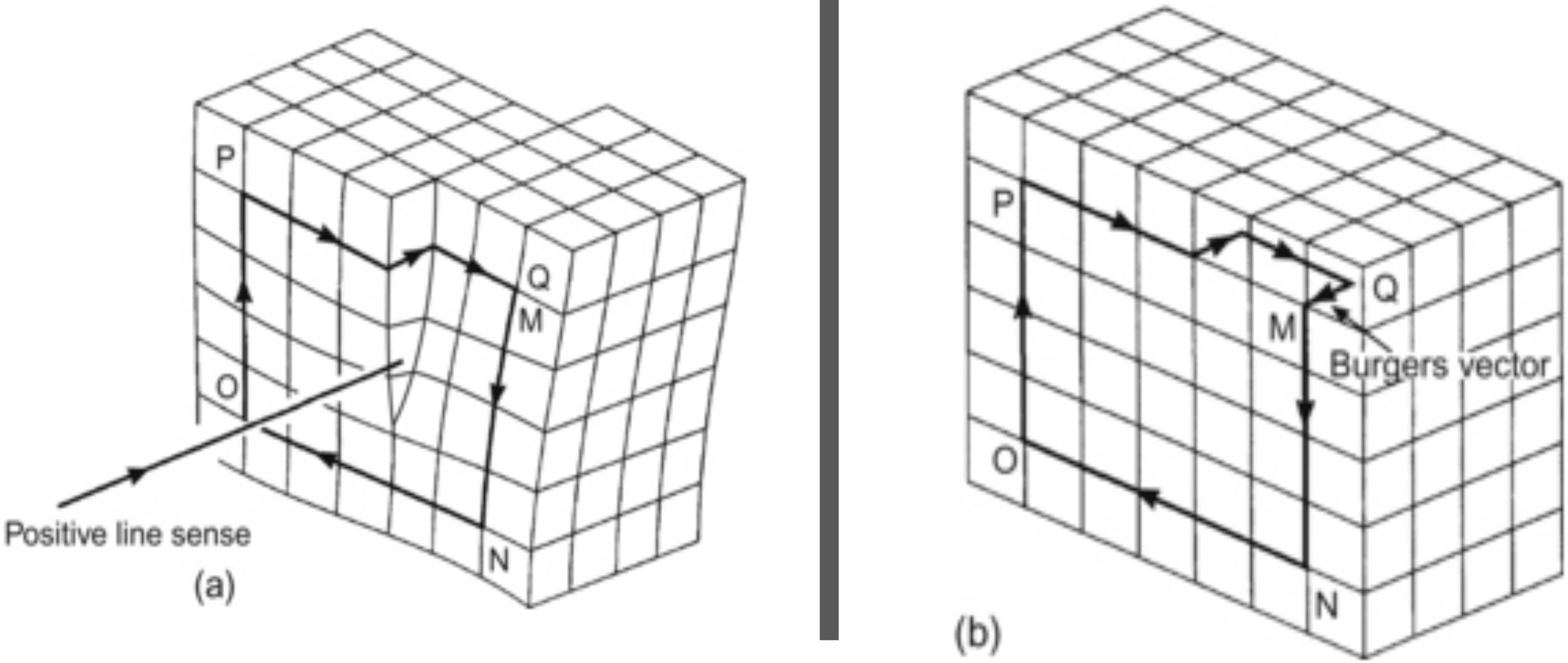
- Circuit MNOPQ with Ds. inside : 3 ↓ , 4 ← , 3 ↑ , 5 → (*Right Handed, **RH***)
- Follow the same steps in the perfect crystal
- The ‘missing link’ (*Finish to Start, **FS***) in the ***perfect crystal*** is the **Burgers vector**
- In this case, $\overrightarrow{\mathbf{QM}}$ is the Burgers vector, $\overrightarrow{\mathbf{b}}$

Edge Dislocations – Burgers vector



- Circuit P → P in perfect crystal: 4 ↑ , 5 → , 4 ↓ , 5 ← (*Right Handed, **RH***)
- Follow the same steps in the defected crystal, the circuit will end at Q
- The 'missing link' (*Finish to Start, **FS***) in the ***defected crystal*** is the **Burgers vector**
- In this case, $\overrightarrow{\mathbf{QP}}$ is the Burgers vector, $\vec{\mathbf{b}}$

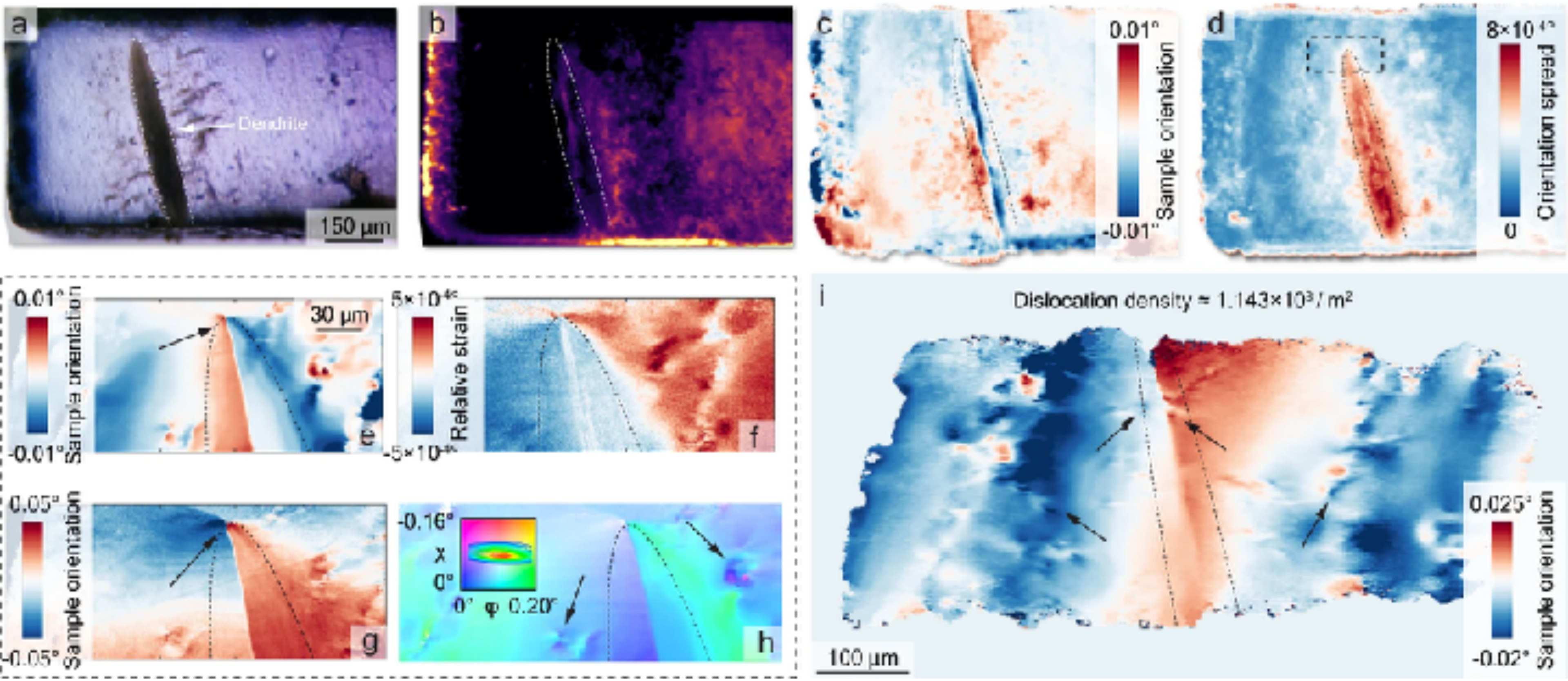
Alternate conventions



Screw dislocations

Line and Burgers vector

Dislocation density



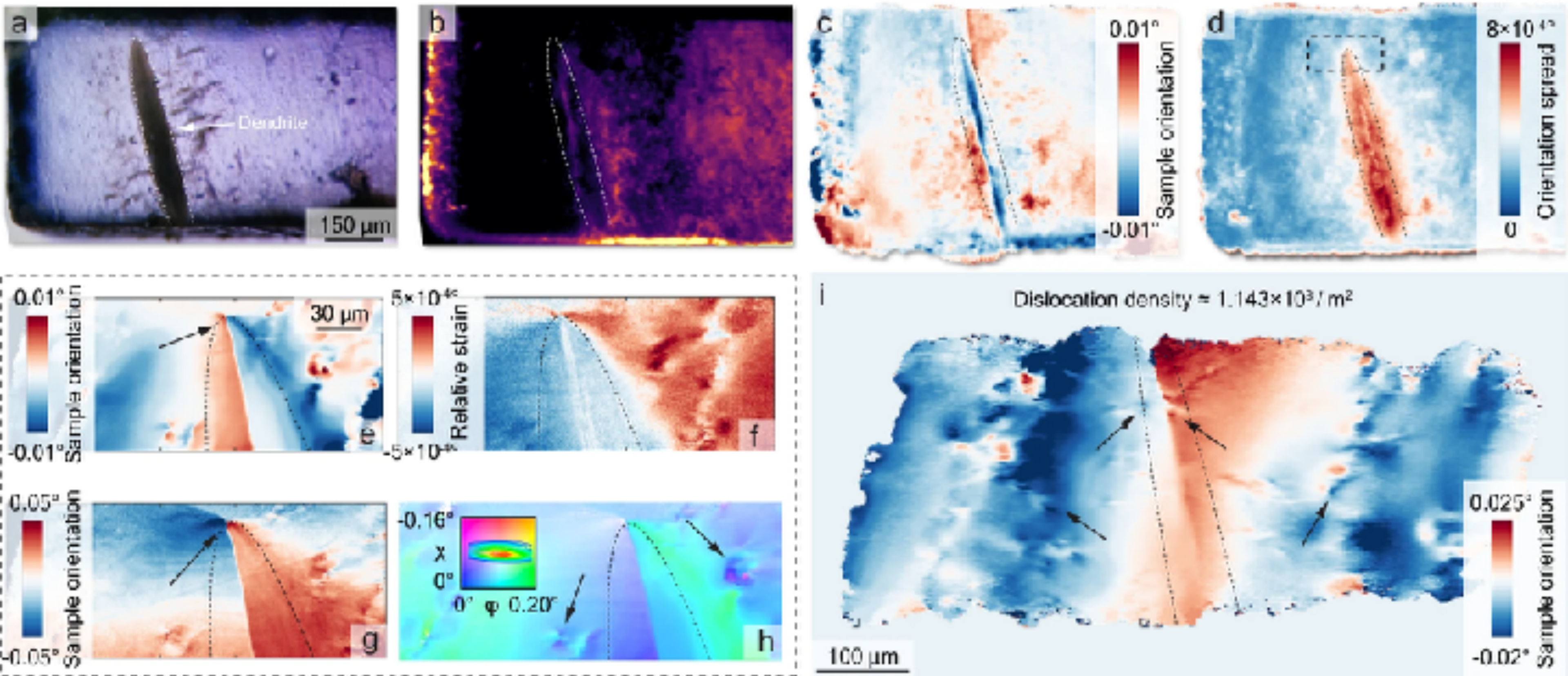
Dislocation density, $\rho :=$

Length of dislocations per unit volume

Number of dislocations intersecting unit area

Yildirim, C., Flatscher, F., Ganschow, S. *et al.* Understanding the origin of lithium dendrite branching in Li6.5La3Zr1.5Ta0.5O12 solid-state electrolyte via microscopy measurements. *Nat Commun* **15**, 8207 (2024).

Dislocation density



- Units of / m^2
- High in metallic materials $\left(10^{12} - 10^{14}\right)$
- Increases with plastic deformation to 10^{15}
- Low in non-metallic crystals, as low as 10^{5}

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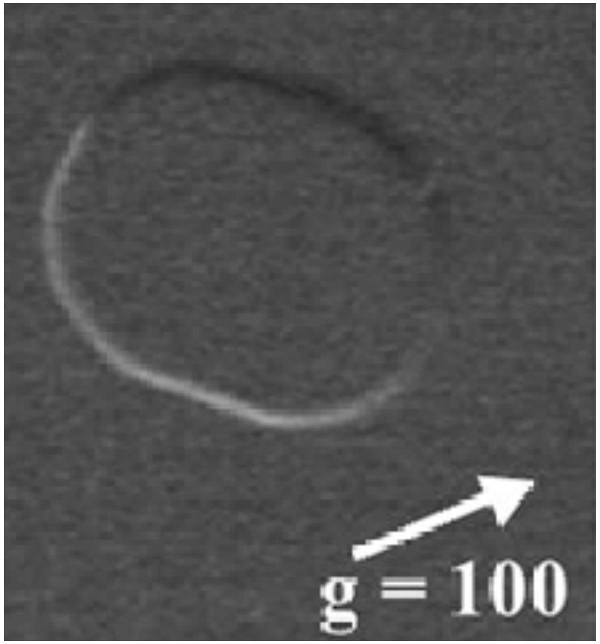
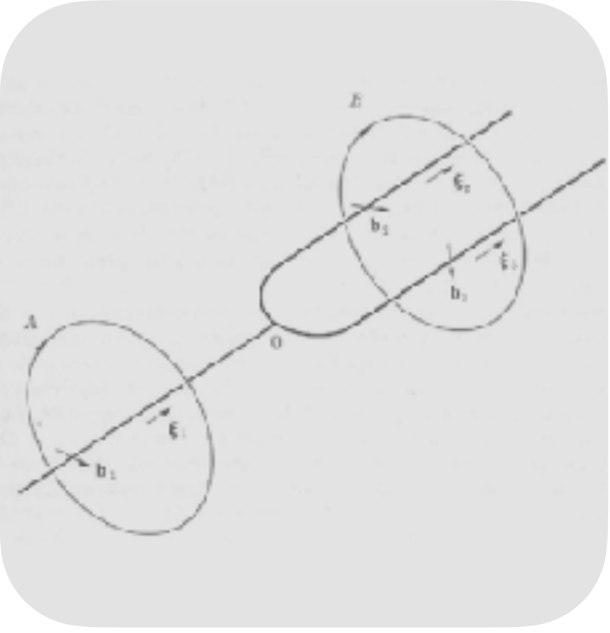
Dislocation loops and branches

- Dislocation lines can end at the surface of a crystal and at grain boundaries
  - never inside a crystal
  - form closed loops
  - branch into other dislocations

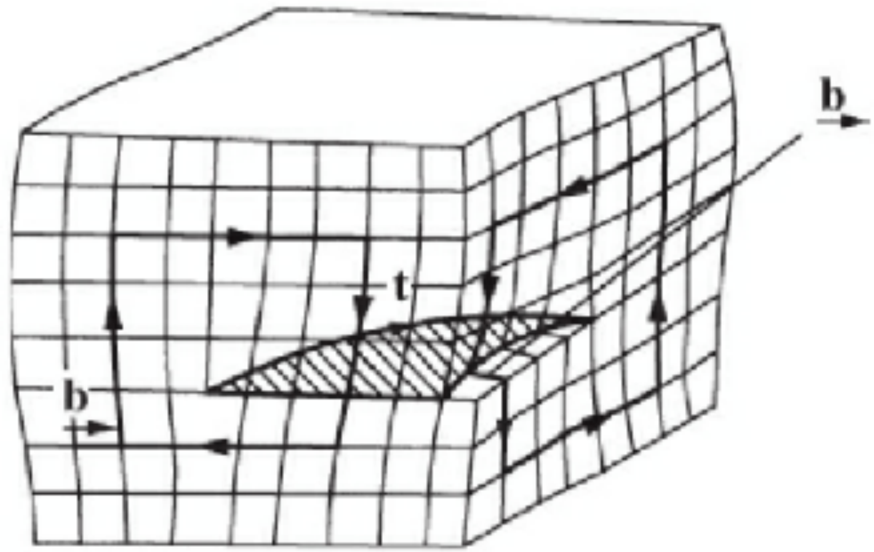
- When three or more dislocations meet at a point, or node
  - Burgers vector is conserved
  - vector total in equals vector total out

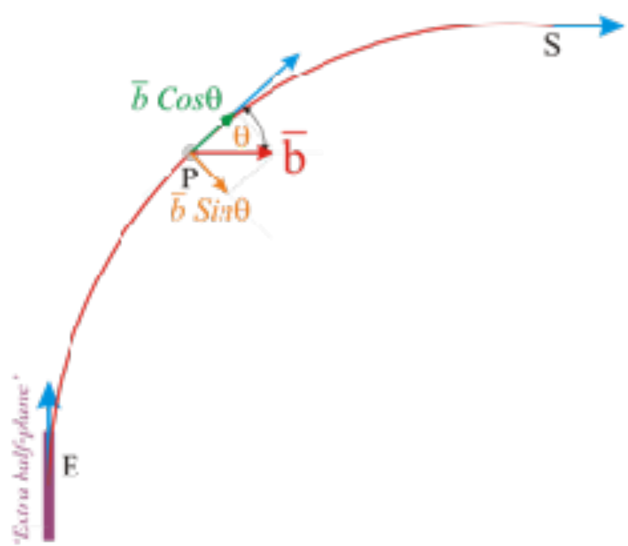
Kamaladasa, Ranga & Jiang, Wenkan & Picard, Yoosuf. (2011). Imaging Dislocations in Single-Crystal SrTiO3 Substrates by Electron Channeling. Journal of Electronic Materials - J ELECTRON MATER. 40. 2222-2227. 10.1007/s11664-011-1723-9.





Mixed Dislocation Loop





Problem

- Cubic crystal
- Mixed dislocation straight line
  - Along [112] direction
  - Burgers vector is ½[110]

What are the edge and screw vector components of the Burgers vector

Dislocation motion

Dislocation motion

- Two types of movement of dislocations

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  - Glide or conservative motion

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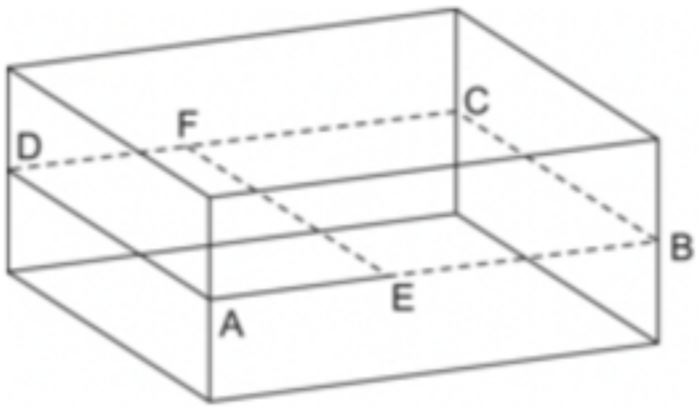
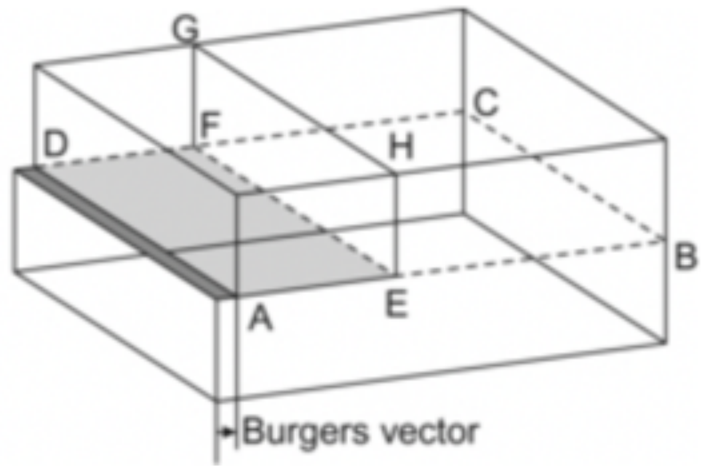
- Glide of many dislocations results in slip: most common manifestation of plastic deformation in crystalline solids

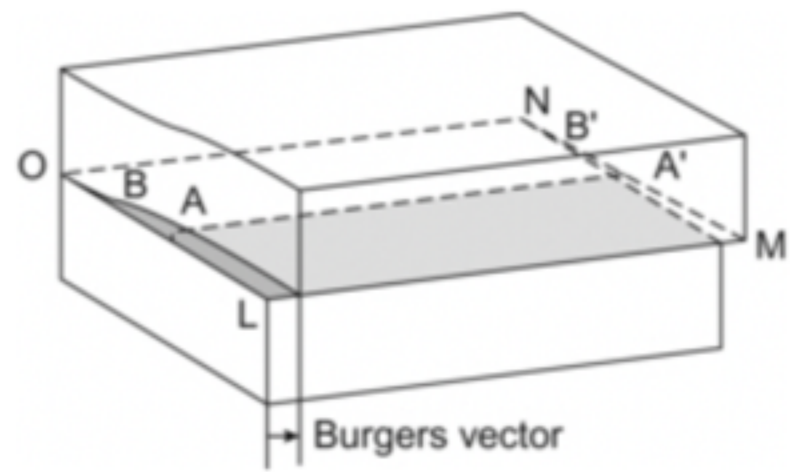
Dislocation - alternative definition



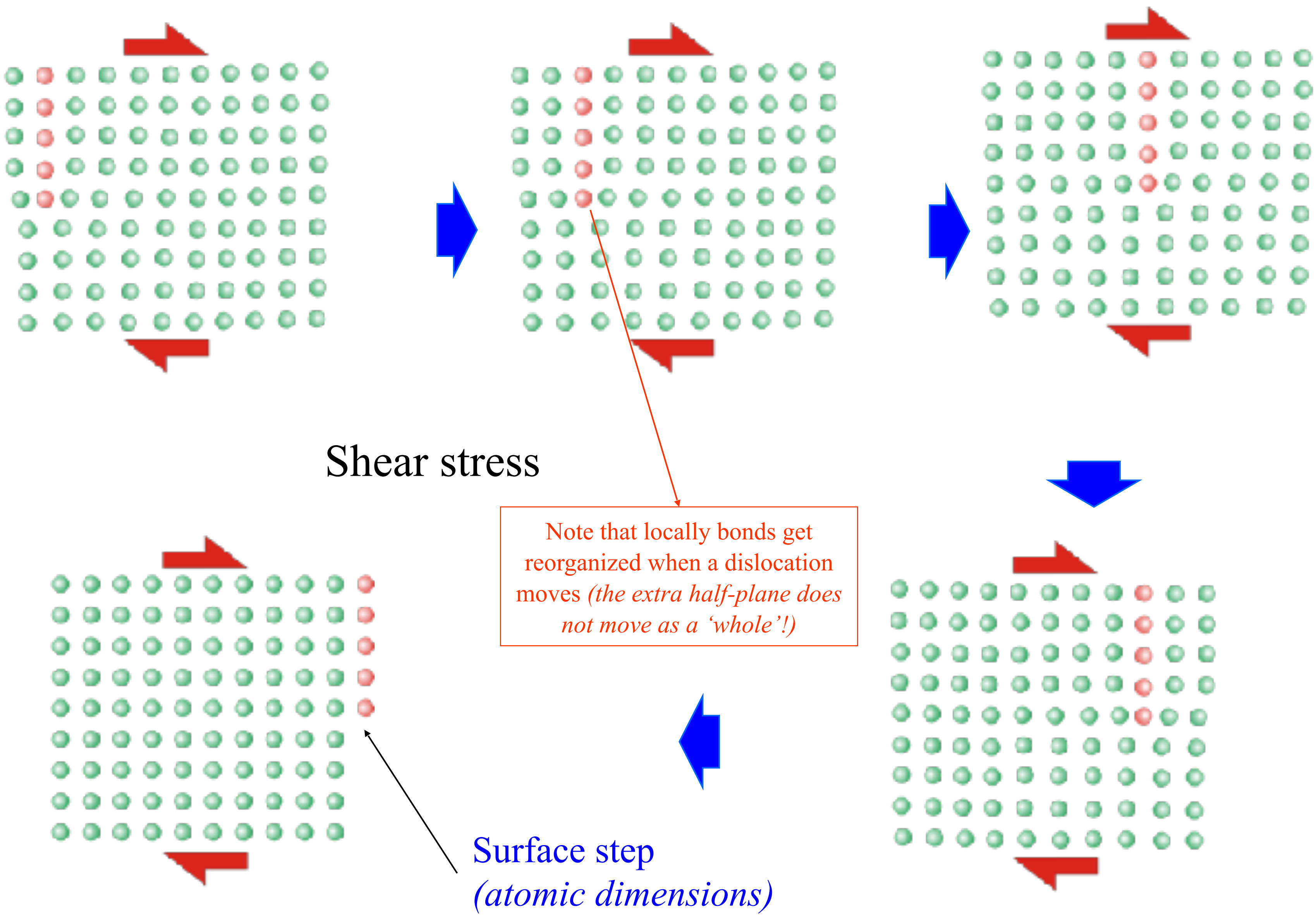


- Boundary between ***slipped and the un-slipped*** parts of the crystal

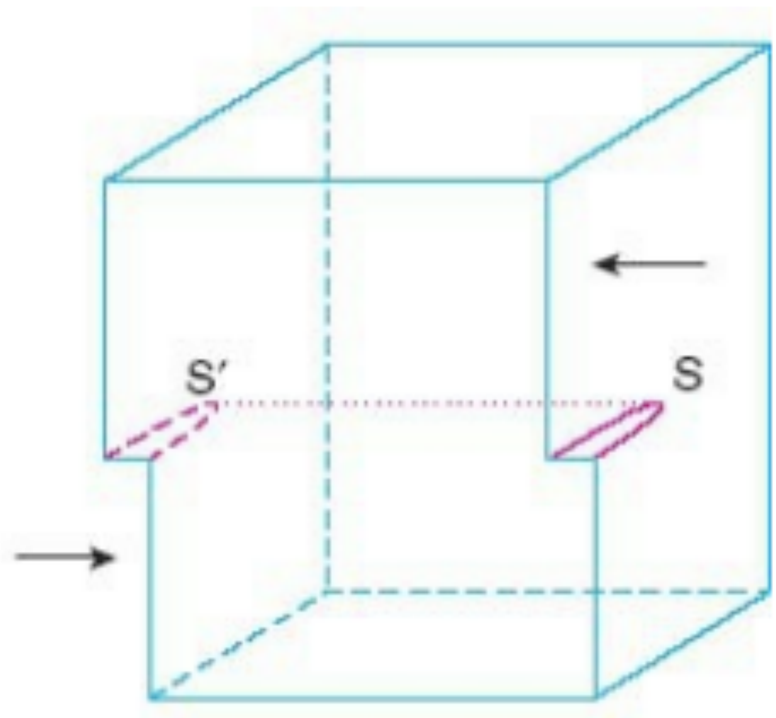
- Plane containing the line and Burgers vector defines a ***slip plane***

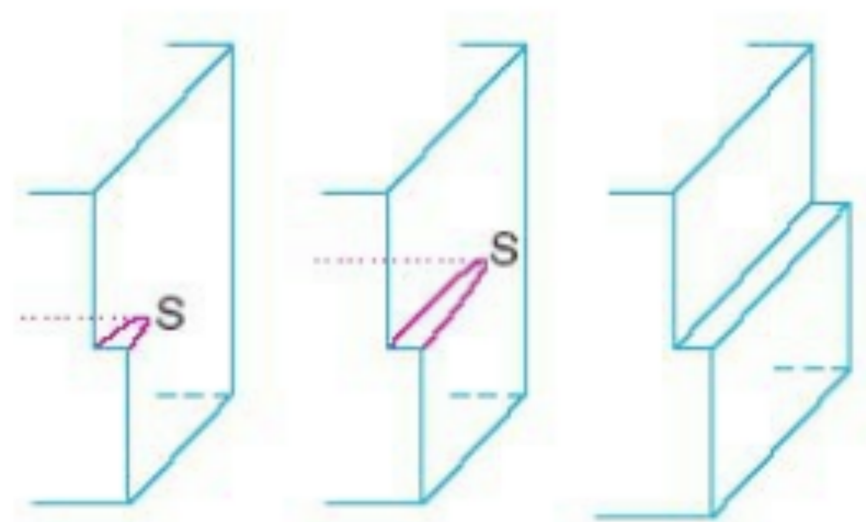


Dislocation Glide or Slip - Edge Ds



Dislocation Glide or Slip - Screw Ds.





Slip in Crystals

Slip occurs in that crystallographic plane that contains both line vector and Burgers vector

Burgers vector is the slip direction

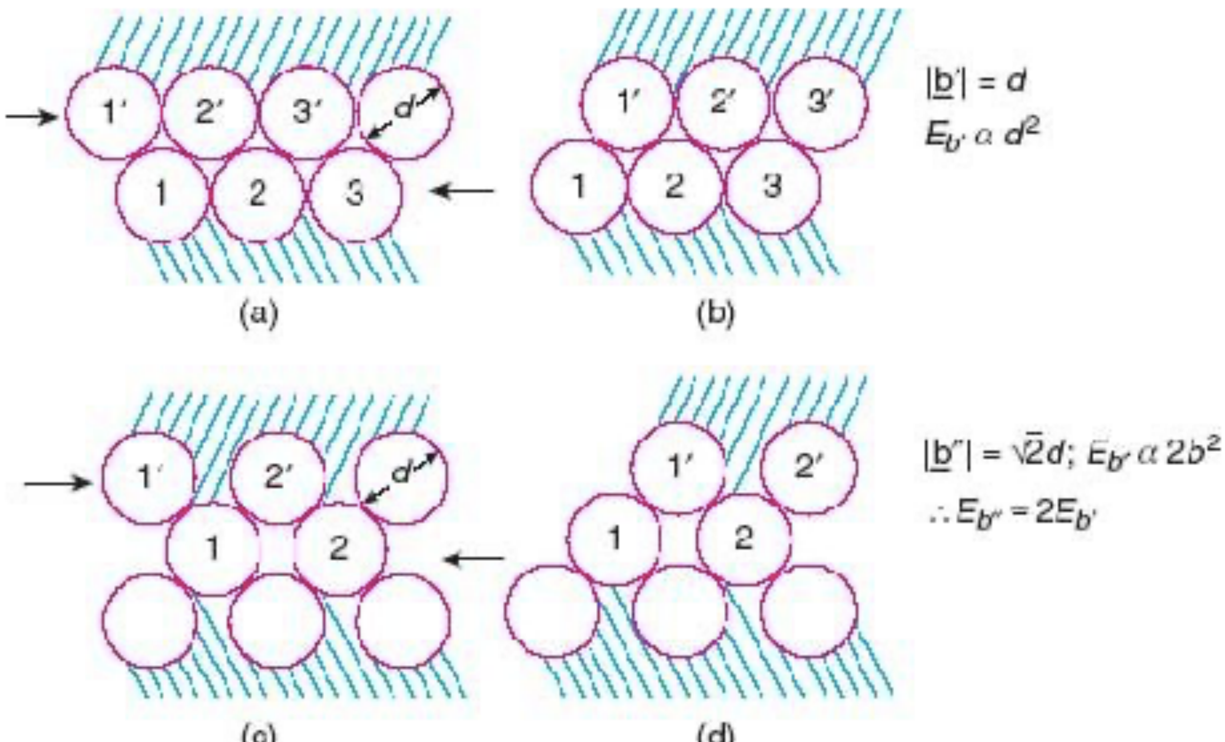
The plane and direction constitute a slip system

High planar density

High linear density in that plane

Why does a slip system exist?

$$E \propto b^2$$



Burgers vector is along a close packed direction

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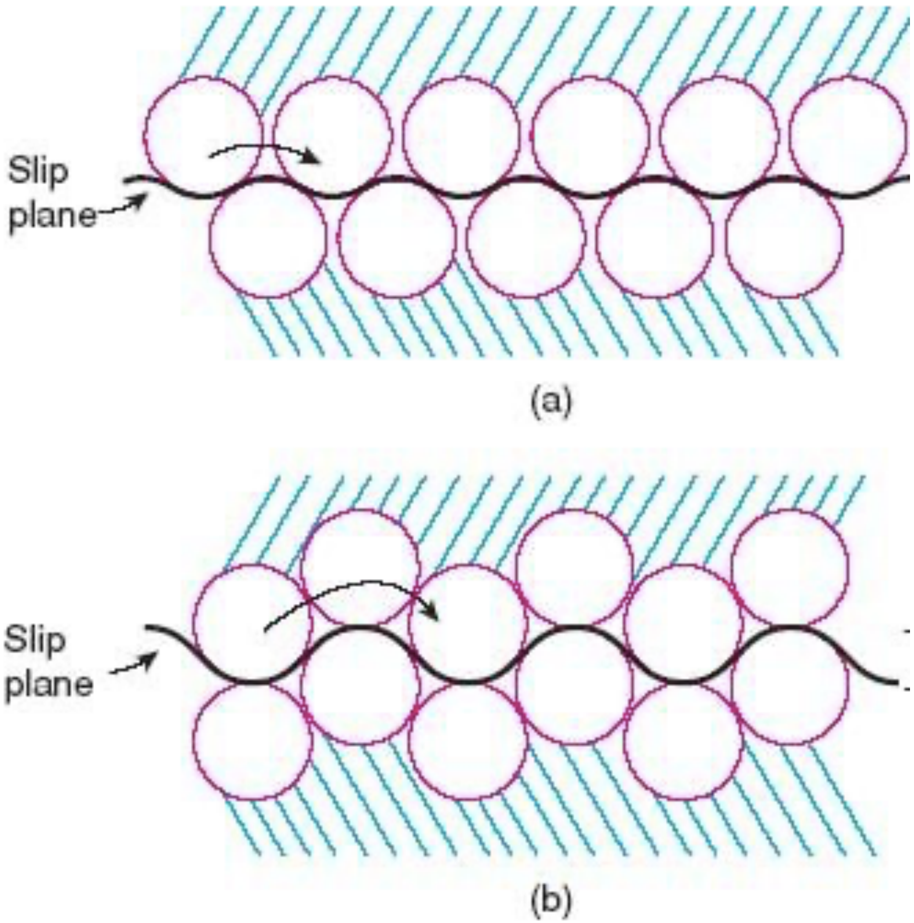


Lower energy barrier for atom movement

Slip occurs on a close packed plane

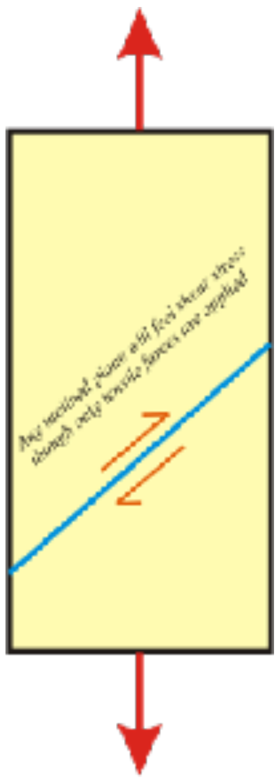
Slip systems

Crystal system	Slip Plane	Slip direction	Degeneracy
FCC	{111}	$\langle 1\bar{1}0 \rangle$	12
BCC	{110}	$\langle \bar{1}11 \rangle$	12
	{211}		12
	{321}		24
HCP	{001}	$\langle 01\bar{1} \rangle$	3
	{100}		3
	{101}		6

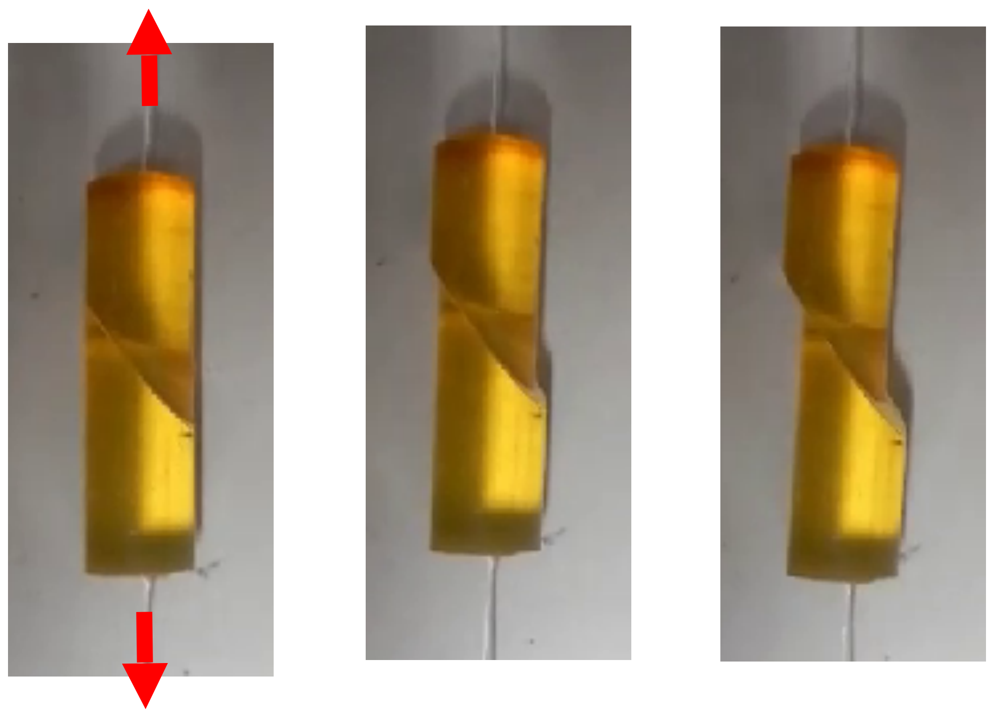
Glide and Deformation

- Uniaxial tensile test – shear stress on all planes
- shear stress > stress needed to move dislocation

Resolved shear stress



Critical Resolved shear stress



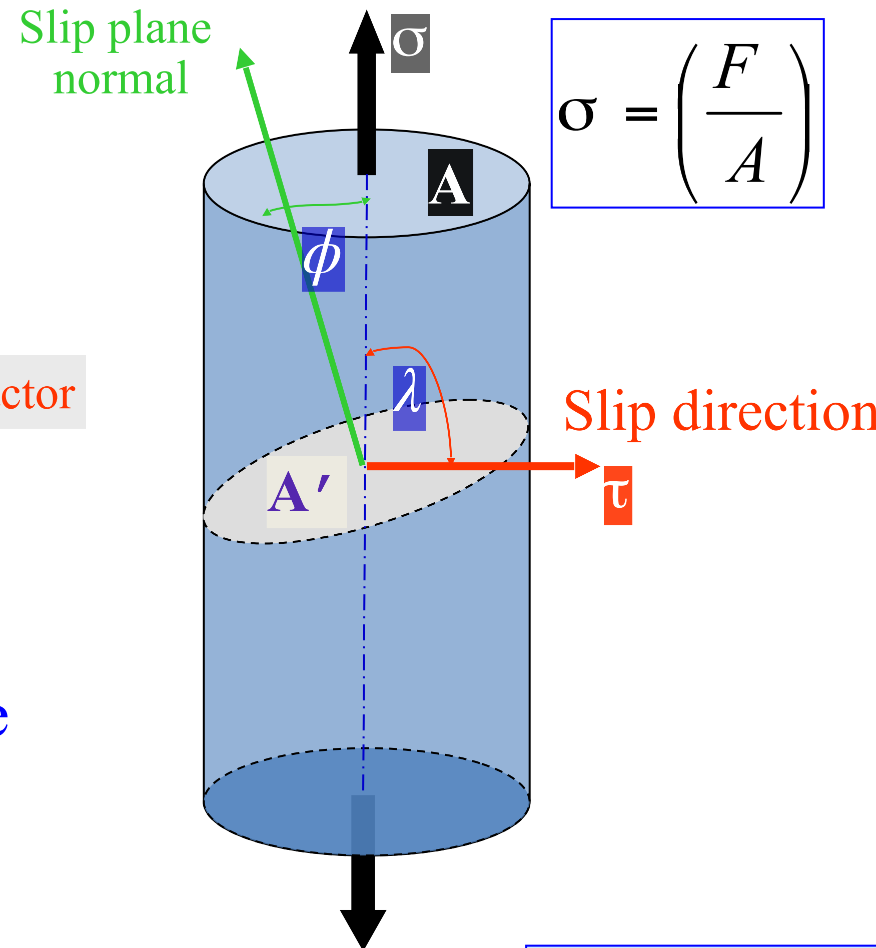
Resolved shear stress

$$Stress = \left(\frac{Force}{Area}\right)_{1D}$$

$$\tau_{\mathrm{RSS}} = \frac{F\cos\lambda}{\frac{A}{\cos\phi}}$$

$$\tau_{RSS} = \sigma \cos\phi \cos\lambda$$

Schmid factor

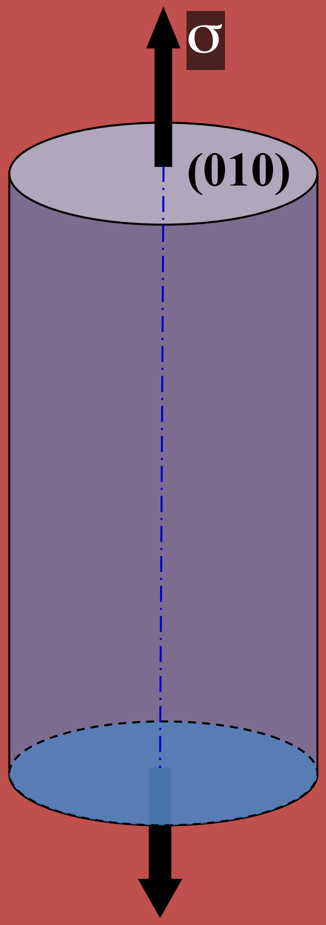


$$\sigma = \left(\frac{F}{A}\right)$$

- Maximum shear stress is in a plane inclined at (θ =) 45°.
- The vertical (90°) and horizontal plane (0°) feel no shear stresses.

Slip is initiated when $\tau_{RSS} \geq \tau_{CRSS}$

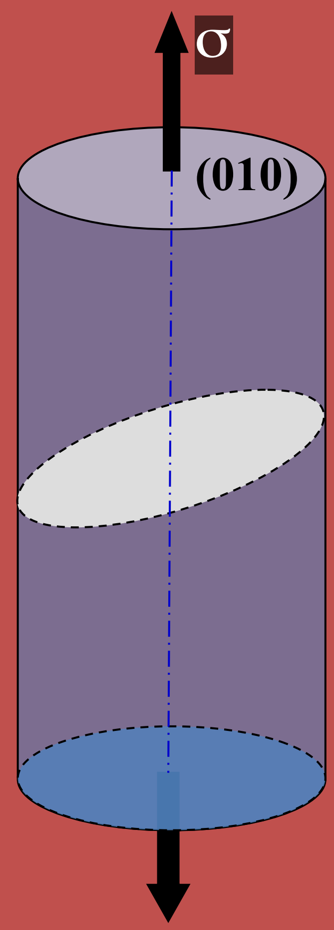
Problem



- Single crystal bcc Fe
- Tensile stress on (010)
- Slip initiated in a slip system
- $\tau_{CRSS} = 30\ MPa$

1. Compute resolved shear stress when a tensile stress of 52 MPa is applied
2. Compute the yield strength

Problem



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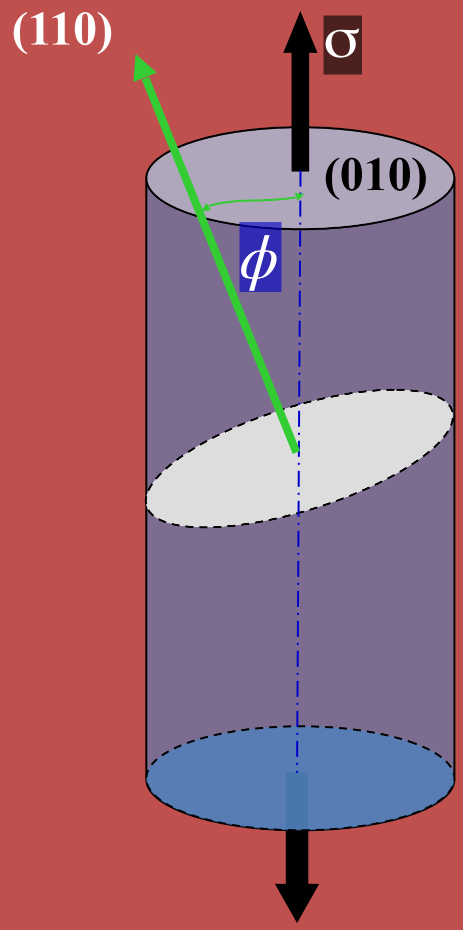

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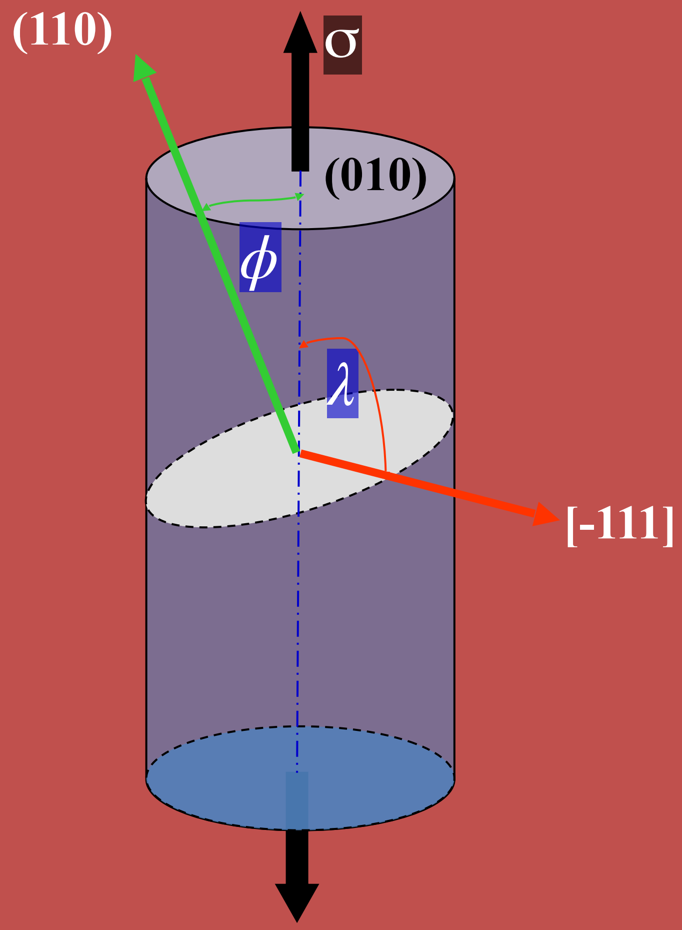

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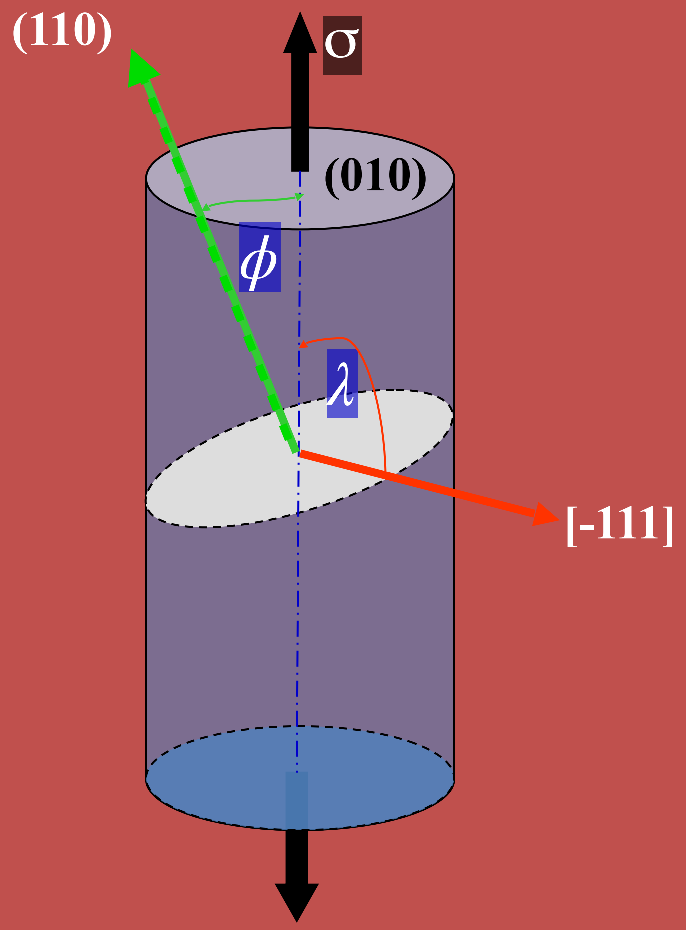

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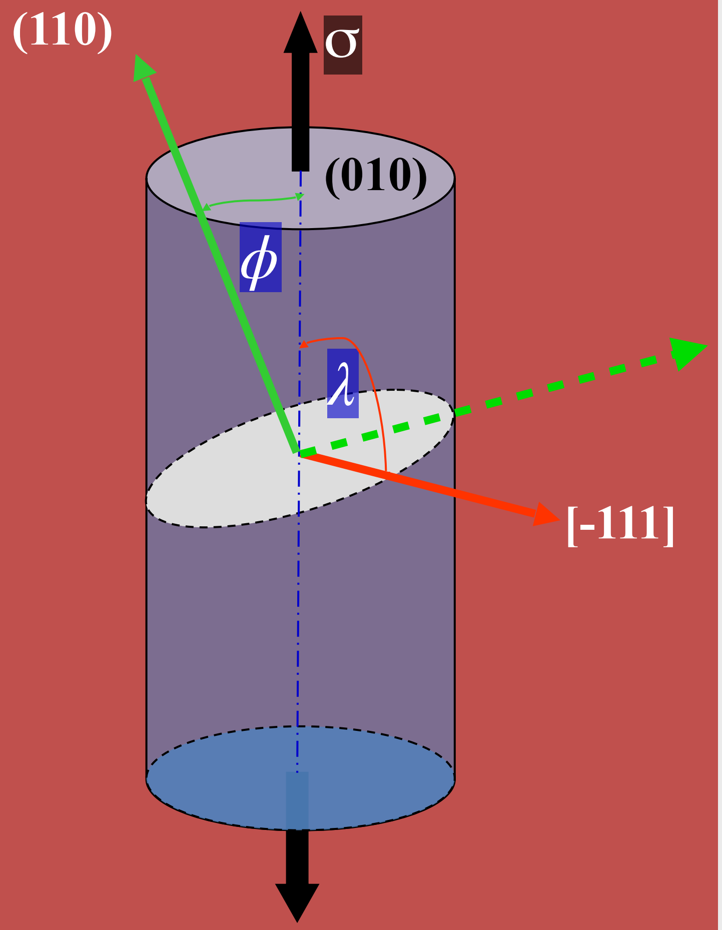

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