Crystal plasticity

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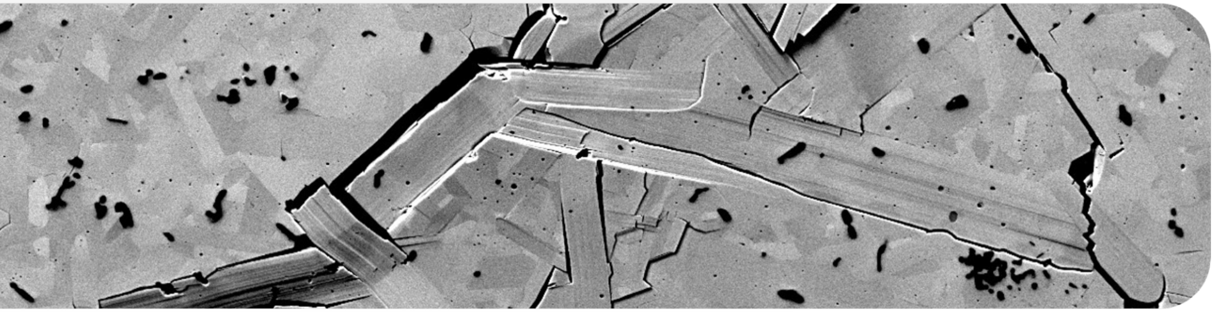

From craft to Science

Deformable / non-deformable

Solid

Non-deformable (Brittle)

Deformable / non-deformable

Solid

Non-deformable
(**Brittle**)

Deformable
(**Ductile**)

Deformable / non-deformable

Solid		Liquid
Non-deformable (**Brittle**)	Deformable (**Ductile**)	Too deformable

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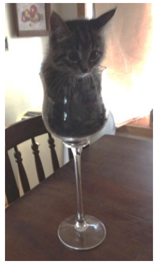

Ig-Nobel 2017, Marc-Antoine FARDIN (ENS Lyon)

What ancient metalworkers learned?

- From craft to knowledge
  - Long before science explained how materials behave, ancient people already knew how to shape metal.
  - Through practice and experience, they learned to control how metal responds to force, laying the foundation for what we now study as material behavior.

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- What they discovered?
  - Bronze Age (around 3000 BCE)
    - People used copper and bronze to make tools and ornaments
    - They noticed:
      - ✓ Hitting metal made it stronger
      - ✓ Heating metal made it softer and easier to shape again.
  - Iron Age (from around 1200 BCE)
    - Working with iron was harder, it needed more heat and stronger tools.
    - They learned:
      - ✓ Shaping hot iron helped make tools
      - ✓ Cooling quickly made them harder.
      - ✓ Reheating gently made them less fragile.

The so-called Mask of Agamemnon, discovered in Mycenae (Greece) in 1876, but crafted around the 16th century BCE. Made by cold-hammering a thin sheet of gold, it demonstrates early human control of irreversible metal deformation

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Forged iron obolo-s/-i (ὀβολό-ς/-ί) from ancient Sparta (c. 6th–4th century BCE). Heated, hammered, then quenched to induce brittleness, these rods illustrate early control of irreversible deformation and material properties for economic regulation.

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- What they knew without knowing?
  - Could tell the difference between:
    - Small changes that went back to normal
    - Bigger changes that stayed permanent
  - They got very good at controlling how metal behaved.

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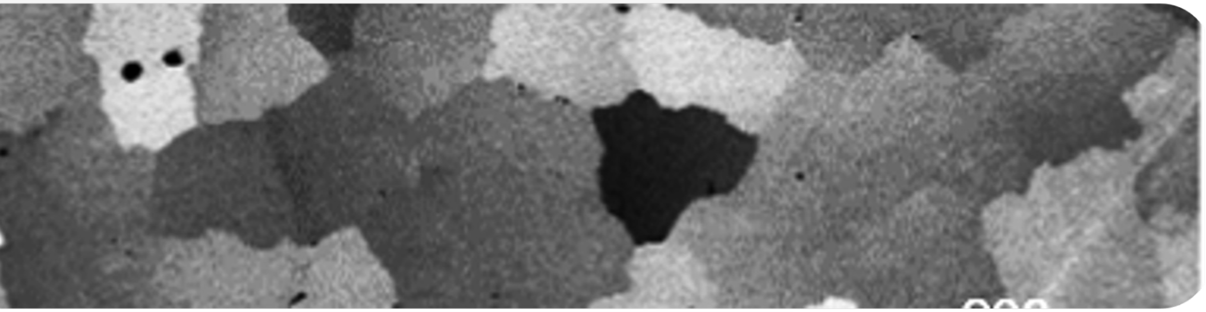

Macroscopic plasticity

The birth of elasticity (17th century)

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  - Antiquity: only observations
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      - ✓ But there were no theories or formulas. Only practical know-how.

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- **1800s: from words to equations**
  - In the early 19th century, researchers like Cauchy, Navier, and Poisson developed:
    - The concept of stress (σ)
    - The concept of strain (ε)
    - The framework of continuum mechanics
  - Around the same time, the elastic modulus became associated with the name Thomas Young (even though he didn't define it as we do today).

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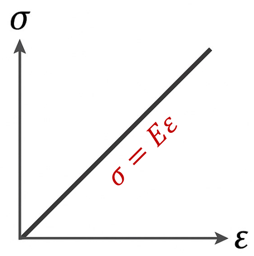
❖ **Late 19th century:**

$$\sigma = E\varepsilon$$

σ: stress; ε: strain; E: Young's modulus

Observations without theory



Elasticity becomes a law

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Essentials of elasticity

❖ **1D Hooke's law:**

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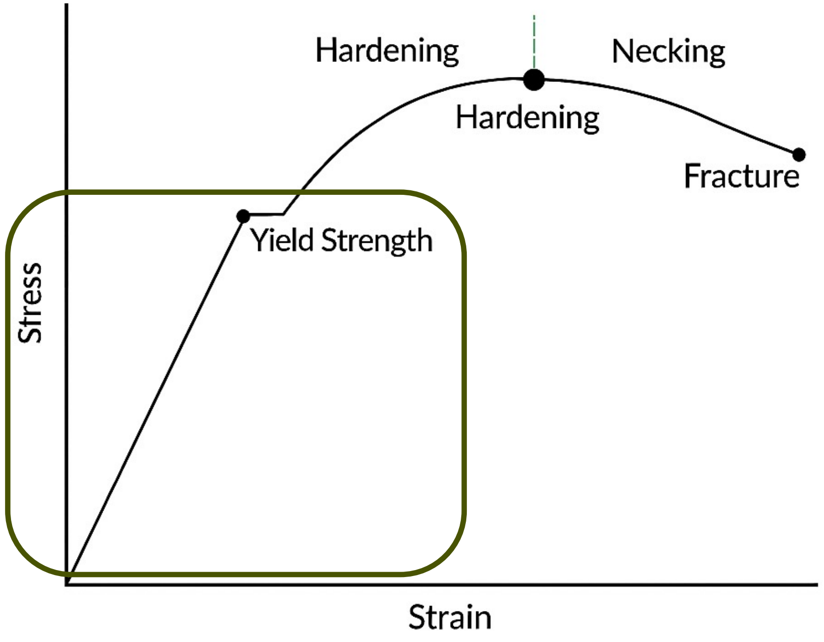

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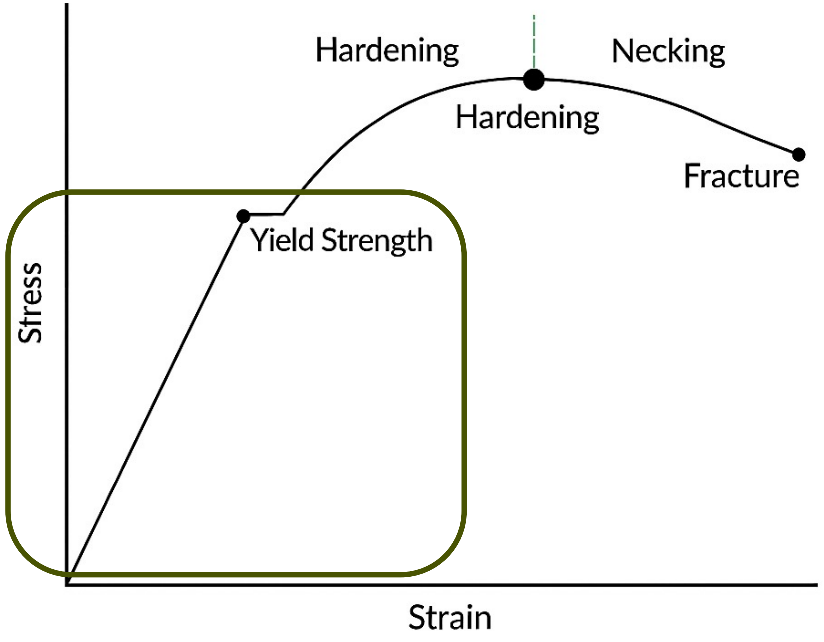

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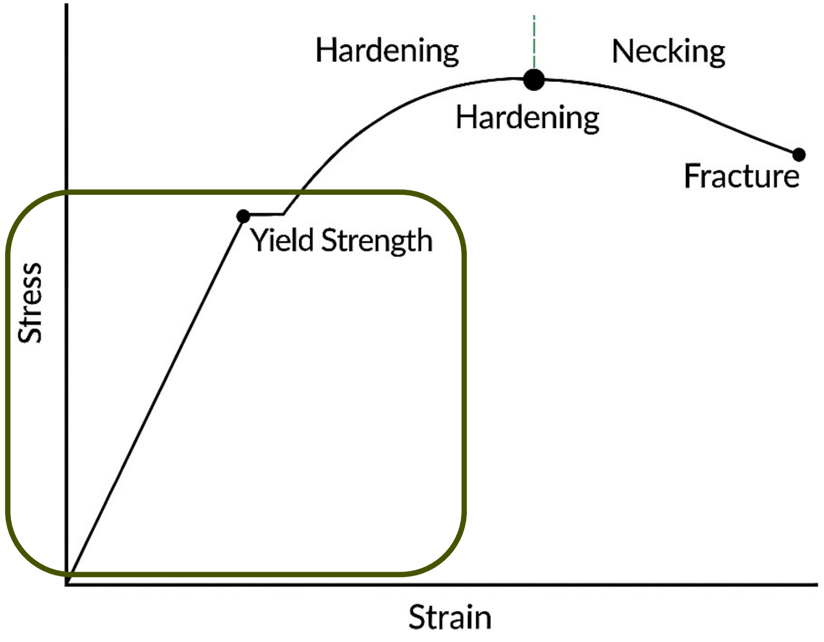
$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$; $\mu = \frac{E}{2(1+\nu)}$; σ_{ij}: stress tensor; ε_{ij}: strain tensor



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- **Strain tensor:**

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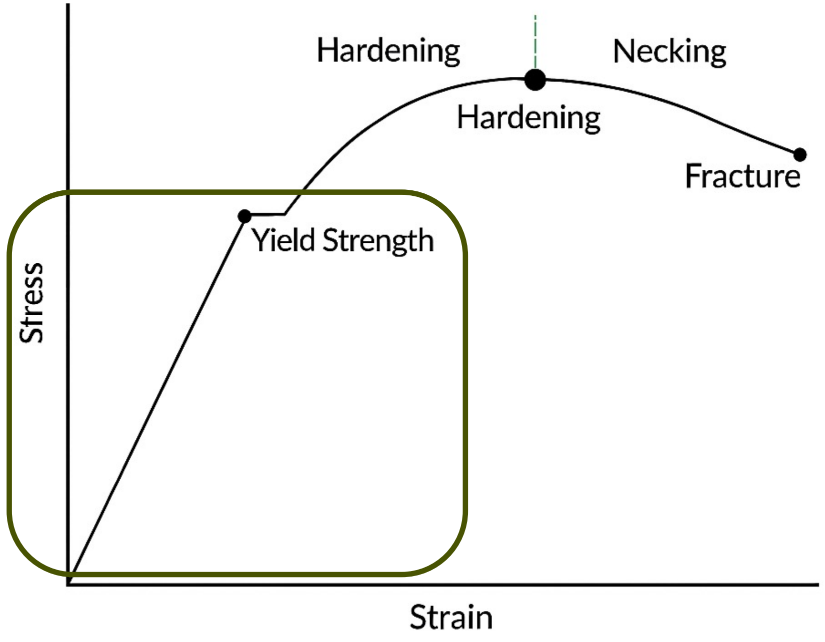
(u_i: displacement field)



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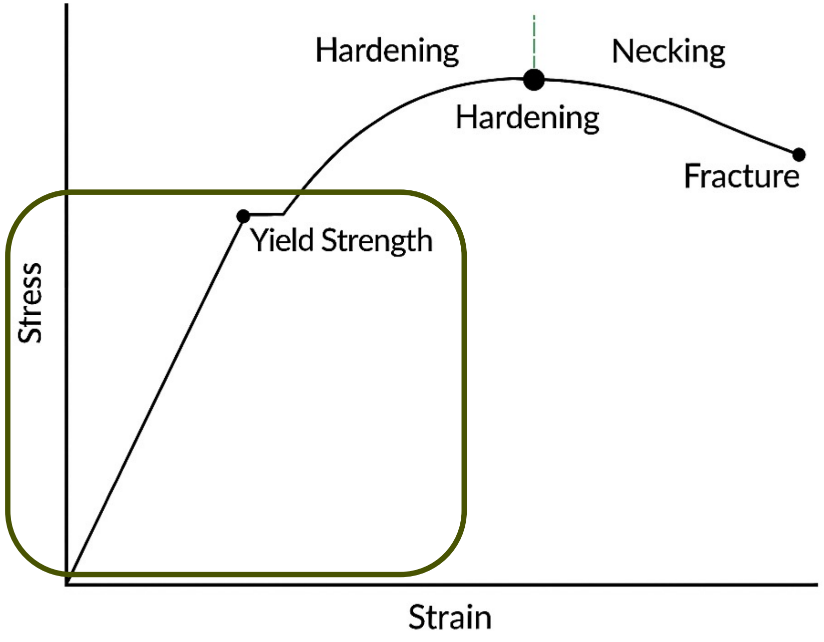
- **3D generalization for anisotropic materials:**

$$\boldsymbol{\sigma} = \mathbb{C}:\boldsymbol{\varepsilon} \Leftrightarrow \sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

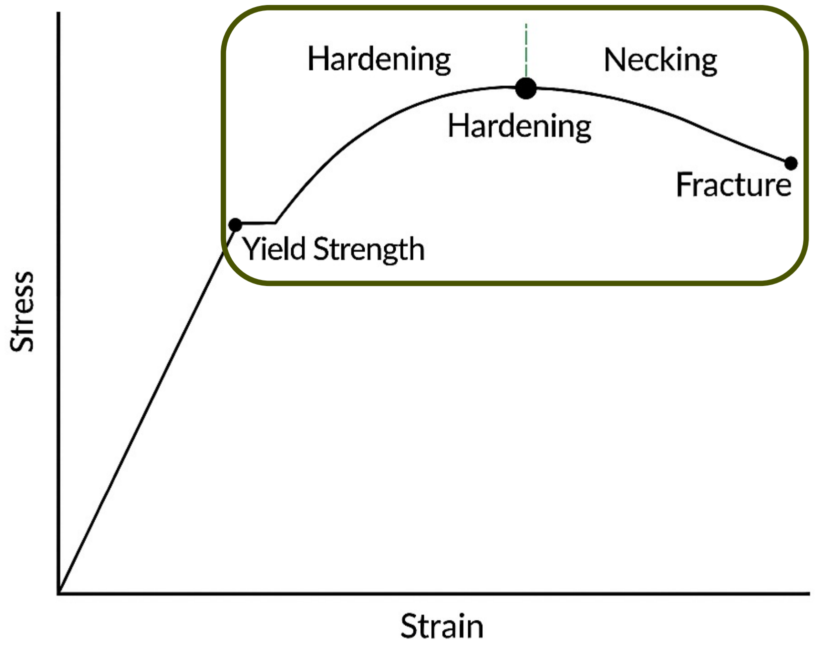
$\mathbb{C}, C_{ijkl}$: stiffness tensor



First empirical law of strain hardening

❖ Historical context:

- 1909: Paul Ludwik introduced the first empirical law describing the plastic behavior of ductile metals.
- At the time, most materials science focused on elasticity; Ludwik was among the first to address permanent deformation quantitatively.



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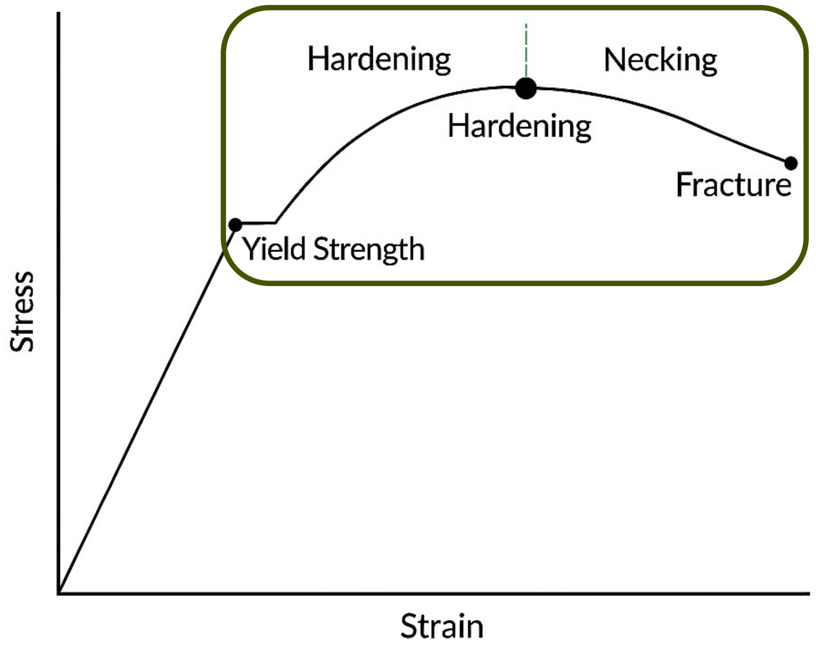

❖ Ludwik's law (1909):

$$\sigma_T = \sigma_0 + K\varepsilon_T^n$$

$\sigma_T = \frac{F}{A_{inst}}$: true stress; $\varepsilon_T = \int_{L_0}^{L} \frac{\mathrm{d}L}{L} - \varepsilon_e$: true plastic strain;
K: strength coefficient; n: strain hardening exponent;
σ_0: yield stress (threshold for plastic flow)

- If $\sigma_0 = 0 \Rightarrow \sigma_T = K\varepsilon_T^n$ (Hollomon's law)

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Visual evidence of crystal plasticity

- **Late 19th – early 20th century:**
  - Mechanical testing of annealed polycrystalline metals (e.g., copper, brass) revealed surface markings after plastic deformation.

J.C. Ewing, W. Rosenhain, The crystalline structure of metals, *Philos. Trans. R. Soc. A*, 194, 279–300 (1900)

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- **Slip lines observed:**
  - Appeared as parallel, planar markings in individual grains.
  - Visible under optical microscopy or oblique lighting.
  - Aligned with specific crystallographic directions.
  - Not cracks: they result from localized shear revealing slip planes.

FIG. 1.—Soft Sheet Iron strained by tension. 400 diameters.

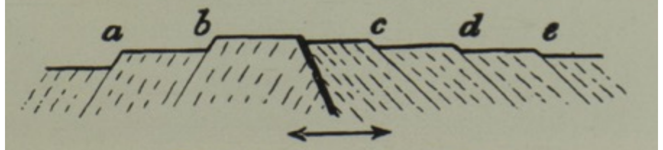

Fig. 3. After straining

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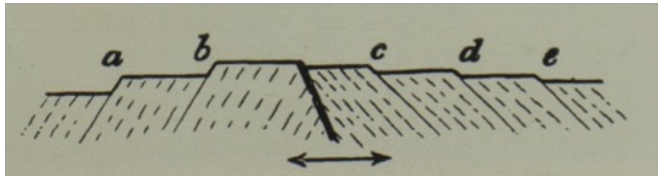

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    - Used in situ optical microscopy with a tensile device.
    - Provided early support for localized, anisotropic plastic deformation.
- **Main interpretation:**
  - Plastic deformation occurs by shear along discrete crystallographic planes, not homogeneously.
  - Slip is localized and planar, consistent with the anisotropy of crystal structures.

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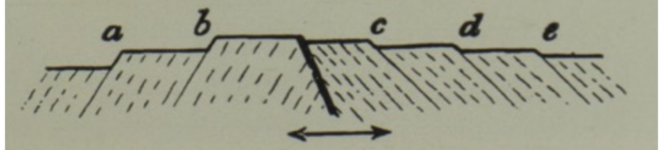

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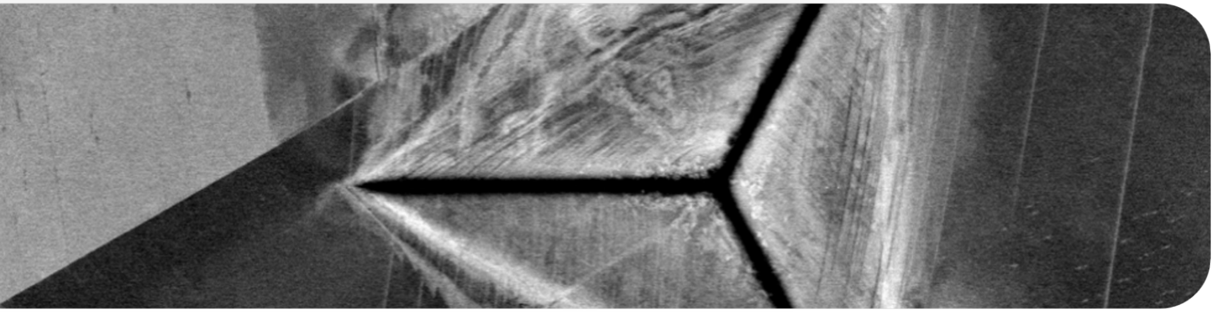
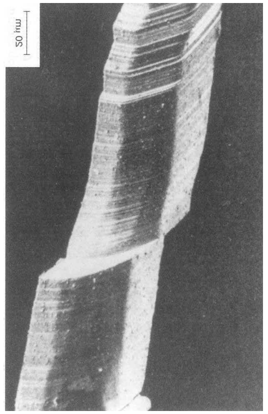


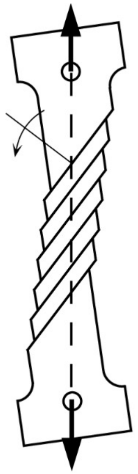
Crystal structure and slip systems

Explaining slip lines: the Schmid-Boas law

❖ Observations & hypotheses:

- Plastic deformation in single crystals occurs by slip along specific crystallographic planes and directions.
- The driving force for slip is the resolved shear stress acting on a given slip system.
- Slip initiates only when this resolved shear stress reaches a critical value, characteristic of the material.
- The normal stress on the slip plane has no effect on the onset of slip.
- Among all possible slip systems, the one with the highest resolved shear stress will be activated first.





E. Schmid, *Proc. Internat. Congr. Appl. Mech.*, Delft (1924)
E. Schmid, & W. Boas, Kristallplastizität: Mit besonderer Berücksichtigung der Metalle. Springer (1935)

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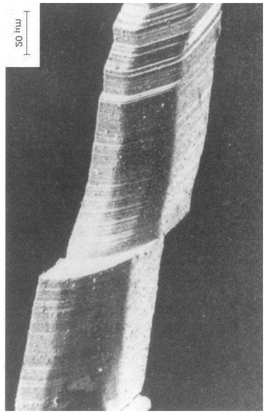

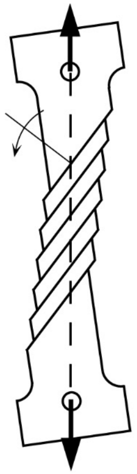

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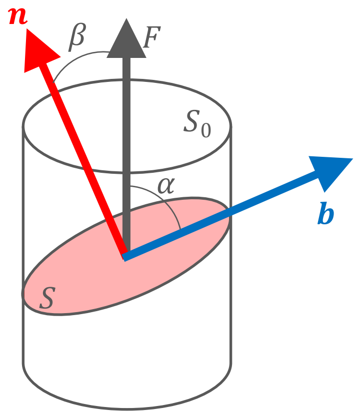

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Explaining slip lines: the Schmid-Boas law

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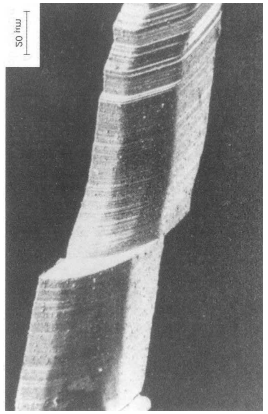

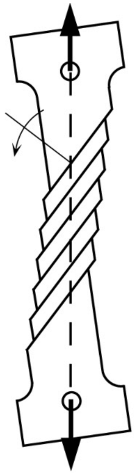

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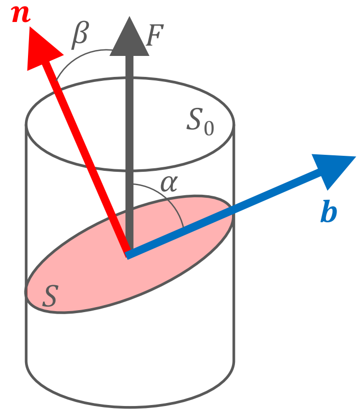

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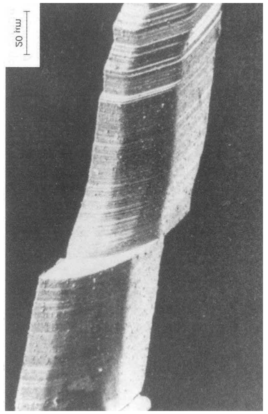

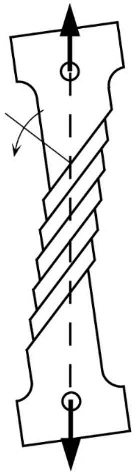

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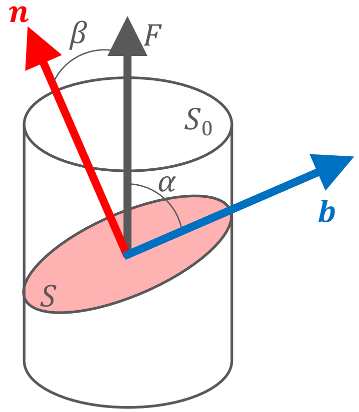

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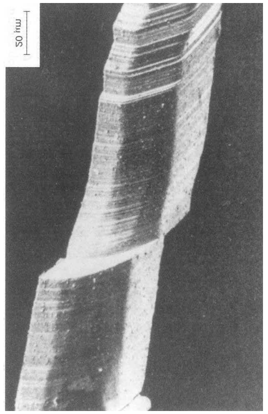

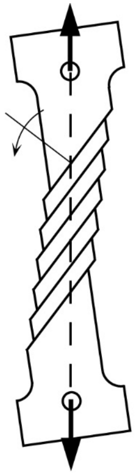

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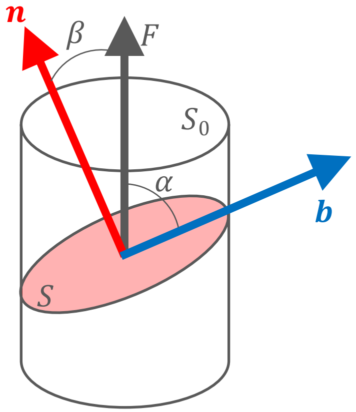

- The projected shear stress (resolved shear stress) τ_{RSS} on the surface S is:

$$\tau_{RSS}^{s} = \frac{F_b}{S} = \frac{F\cos\alpha}{\frac{S_0}{\cos\beta}} = \frac{F}{S_0}\cos\alpha\cos\beta = \sigma\cos\alpha\cos\beta$$

$$\tau_{RSS}^{s} = \boldsymbol{\sigma} : \boldsymbol{b_s} \otimes \boldsymbol{n_s}$$

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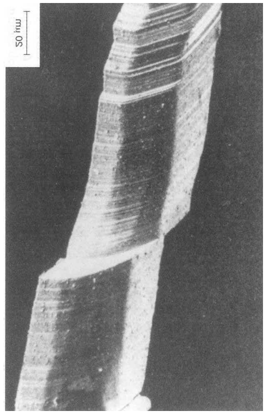

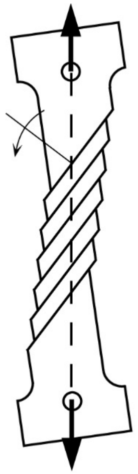

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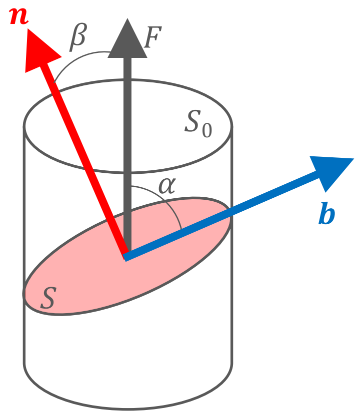

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❖ The Schmid-Boas law:

> ↳ The $s = (\boldsymbol{b}, \boldsymbol{n})$ slip system is active $\Rightarrow$ $\tau_{RSS}^{s} > \tau_{CRSS}^{s}$
> (τ_{CRSS}^{s}: critical resolved shear stress for the slip system s)

- Numerous materials do not follow the Schmid-Boas law...

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How many slip systems does it take to make a crystal ductile?

- What we means
  - A homogenous plastic deformation, *i.e.* a macroscopic plastic deformation that is continuous and compatible:
    - Homogeneous: the deformation is assumed to be uniform at the scale of the crystal (no local gradients of strain, no discontinuities between regions).
    - Plastic: it is produced solely by slip on slip systems, hence it is isochoric.
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$\Rightarrow$ which provides one scalar constraint.

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At least 5 linearly independent slip systems are required.

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Slip systems and crystallographic structures

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- ❖ Slip occurs most easily in dense planes (highest atomic packing).

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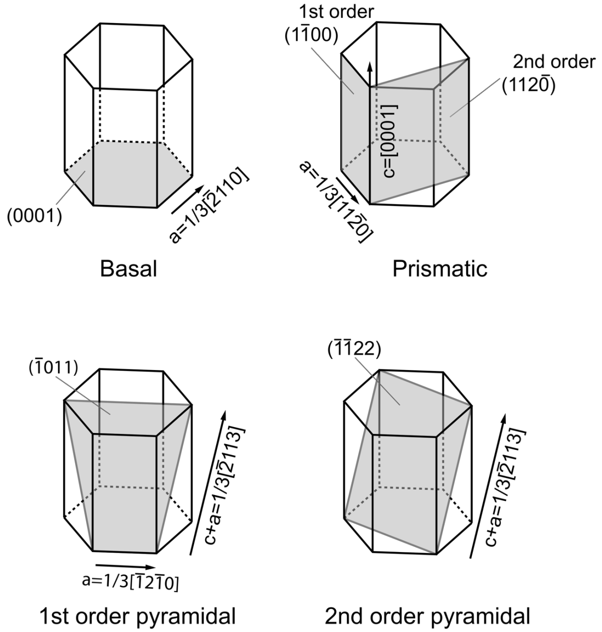
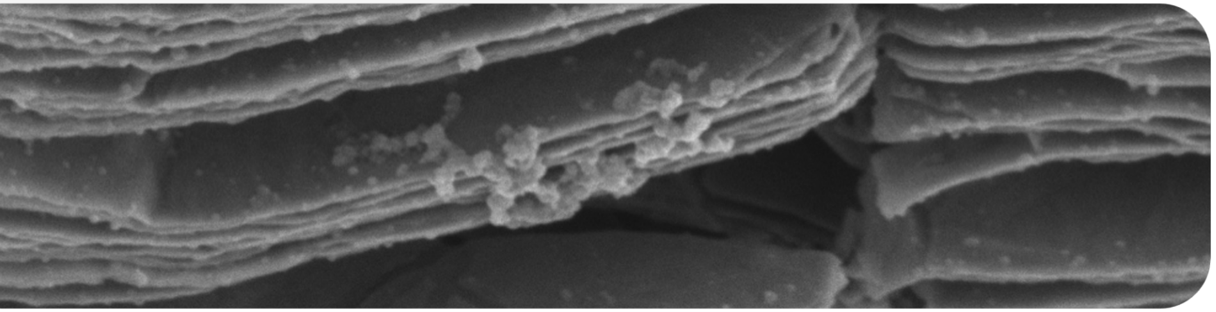
Structure	Slip direction (m_s)	Slip plane	Number of systems
FCC	$\langle 110 \rangle$	$\{111\}$	12
BCC	$\langle 111 \rangle$	$\{110\}$ $\{112\}$ $\{123\}$	12 12 24
HCP	$\langle 11\bar{2}0 \rangle = \langle a \rangle$ $\langle 11\bar{2}0 \rangle = \langle a \rangle$ $\langle 11\bar{2}0 \rangle = \langle a \rangle$ $\langle 11\bar{2}3 \rangle = \langle a + c \rangle$ $[0001] = \langle c \rangle$ $[0001] = \langle c \rangle$	(0001) $\{1\bar{1}00\}$ $\{\bar{1}01l\}$ $\{hkil\}$ $\{1\bar{1}00\}$ $\{11\bar{2}0\}$	3 3 6 12 3 3





The atomic model and dislocations

The atomic model

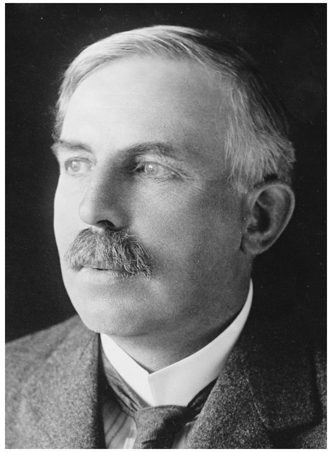
From the "plum pudding" model to Rutherford's atom

- **Before 1911:**
  - The dominant atomic model was the "plum pudding" model (J.J. Thomson, 1904):
    - Atoms were seen as a positively charged "pudding",
    - with electrons embedded like "plums" inside —

      ⇒ No structured nucleus, no empty space, no concept of atomic lattice.
- **1911: Rutherford's gold foil experiment overturned this view:**
  - Most α-particles passed through gold foil, but a few were deflected at large angles.

    ⇒ Atoms are mostly empty space with a dense central nucleus.

    "It was as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you." (apocryphal)
  - New atomic model:
    - Tiny, positively charged nucleus at the center,
    - Electrons orbiting at large distances.
    - Matter is composed of discrete, organized atoms



Ernest RUTHERFORD
(1871 – 1937) 🇳🇿
1 Nobel Prize (1908)

↳The idea of a regular atomic lattice became physically meaningful only after Rutherford's atomic model and was firmly established through the development of X-ray crystallography. (Laue, 1912; Bragg, 1913)

E. Rutherford, Philos. Mag. 21, 669 (1911)

First atomic model for the plasticity

- **Observations & hypotheses:**
  - Crystals were known to deform plastically.
  - Slip was observed to occur along specific crystallographic planes (slip planes).
  - The atomic theory of matter is established, and crystals are described as periodic arrangements of atoms.

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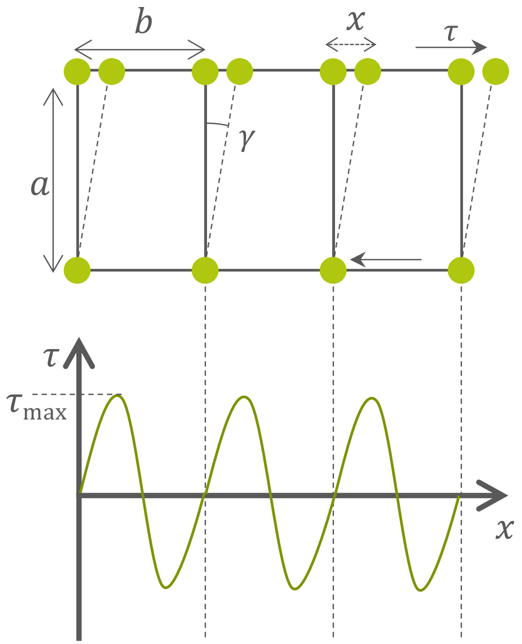

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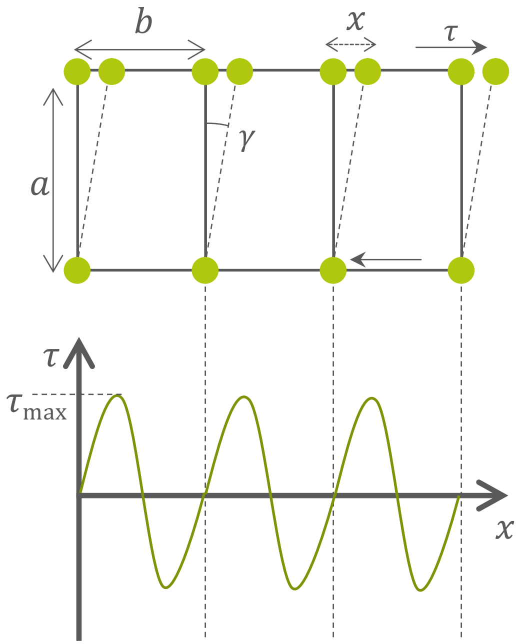

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But $\tau = G\gamma$ (G: shear modulus)

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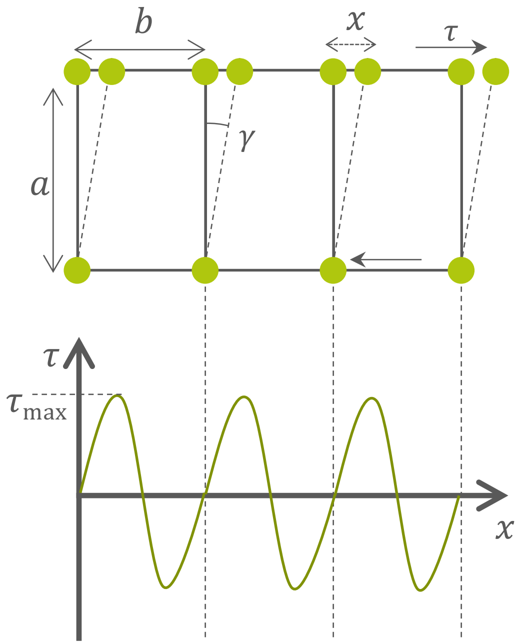

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$$\Rightarrow \tau_{max} = \frac{G}{2\pi}\frac{b}{a} = \frac{G}{2\pi} \text{ (if } a = b) \Rightarrow \tau_{max} \sim \frac{G}{6}$$

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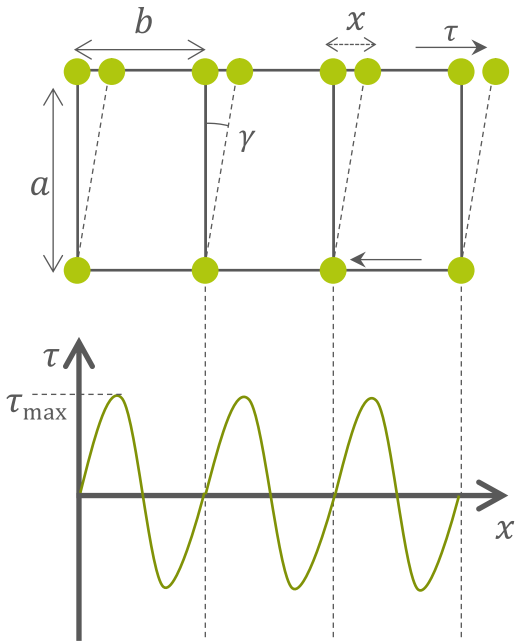

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- To compare with R_e, τ_{max} must be converted to an equivalent one using plasticity criteria: (Tresca: $\tau^{Tr} = \frac{R_e}{2}$ or Von Mises: $\tau^{VM} = \frac{R_e}{\sqrt{3}}$)

Materials	R_e (MPa)	τ^{Tr} (MPa)	τ^{VM} (MPa)	τ_{max} (MPa)
Al (FFC)	10	5	5.8	26000
W (BCC)	750	375	433	160000
Mg (HCP)	25	12.5	14.4	16000

↳In strong disagreement with experiments! **Plasticity cannot be explained by homogeneous shear.**

J. Frenkel, *Z. Phys.* 37, 572 (1926)

From Frenkel's paradox to dislocations

❖ G. I. Taylor (1934)

- Proposed that plastic shear could be explained by the motion of line defects in the crystal.
- Highlighted that such defects would allow slip at stresses far lower than Frenkel's homogeneous shear stress.
- Interpreted macroscopic plastic strain as the cumulative effect of many moving defects.
- Proposed a relation of the form:

$$\tau_C \propto G\delta\sqrt{\rho}$$

(τ_C: shearing stress required to produce slip; ρ: defect density; δ: slip per line, later recognized as the Burgers vector; G: shear modulus)

G. I. Taylor, *Proc. R. Soc. A* 145, 362 (1934); E. Orowan, *Z. Phys*. 89, 605 (1934); M. Polanyi, *Z. Phys*. 89, 660 (1934)
J. M. Burgers, *Proc. Kon. Ned. Akad. Wetensch*. 42, 293 (1939)

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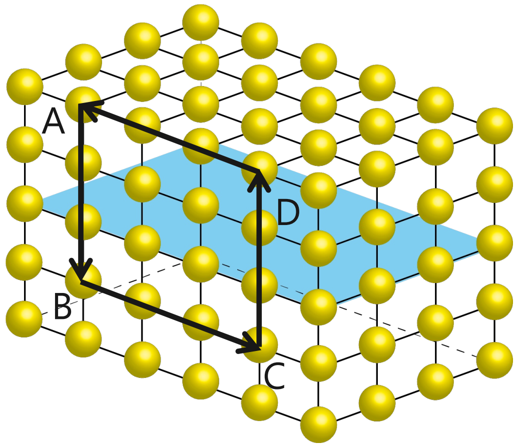

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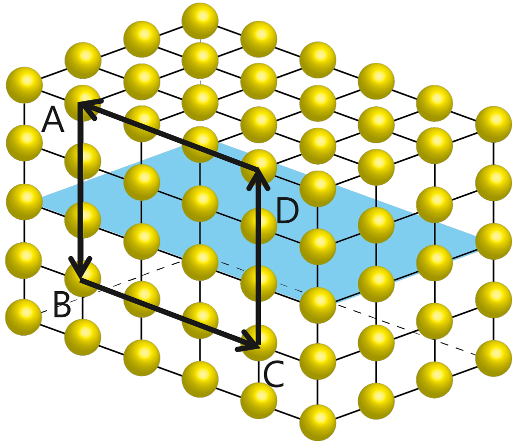

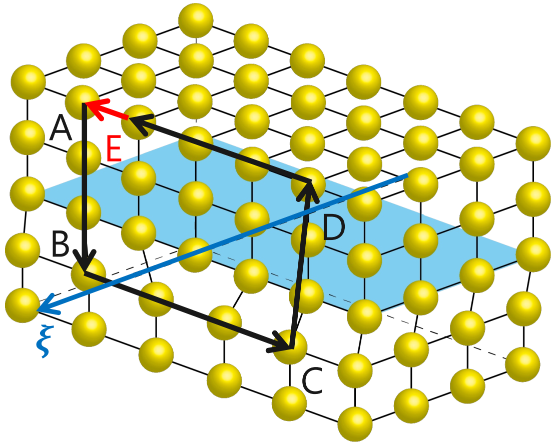

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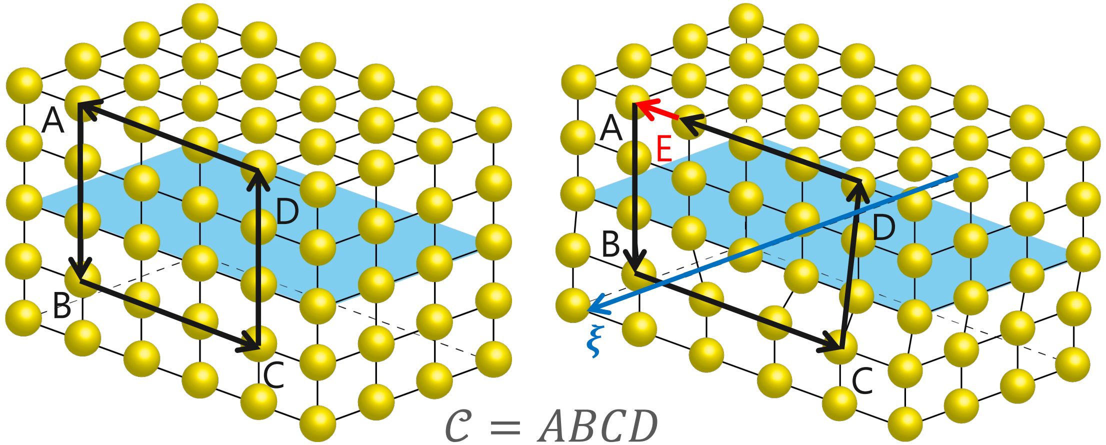

$$\mathcal{C} = ABCD$$

$$\boldsymbol{EA} = \boldsymbol{d} = \boldsymbol{b} = \oint_{\mathcal{C}} \boldsymbol{U^e}\mathrm{d}\boldsymbol{r} \Rightarrow b_i = \oint_{\mathcal{C}} \frac{\partial u_i}{\partial x_j} dx_j$$

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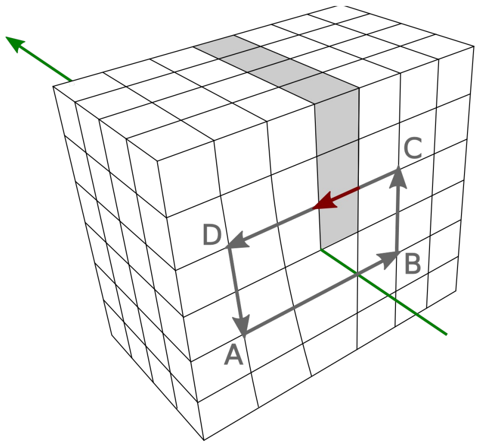
Dislocation types

Edge

Characterized by an extra half-plane of atoms inserted into the lattice ($\boldsymbol{b} \perp \boldsymbol{\xi}$).



Symbol: ⊥

F. C. Frank, *Proc. Phys. Soc. A*, 62, 131–134 (1949)

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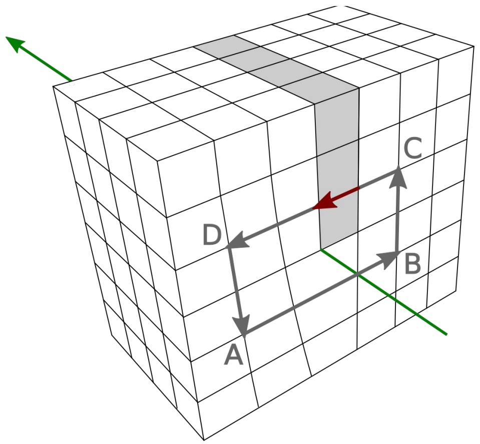
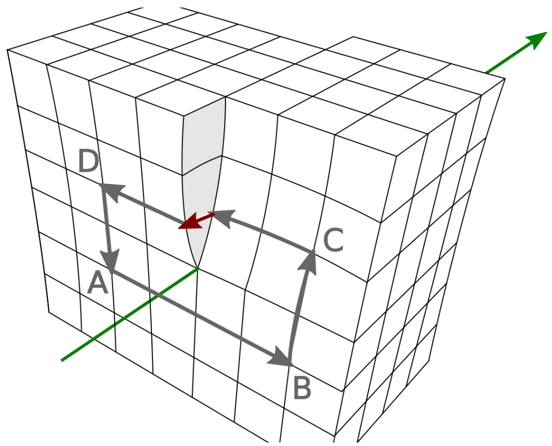


Symbol: ⊥

Screw

Results from a shear distortion, forming a helical ramp in the crystal lattice ($\boldsymbol{b} \parallel \boldsymbol{\xi}$).



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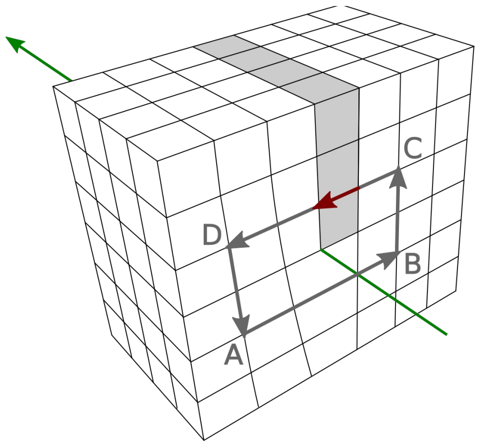

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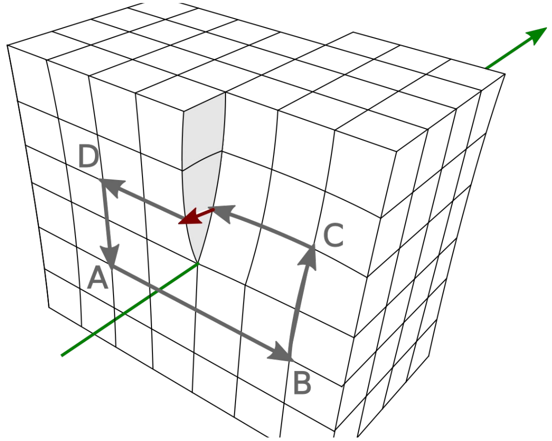
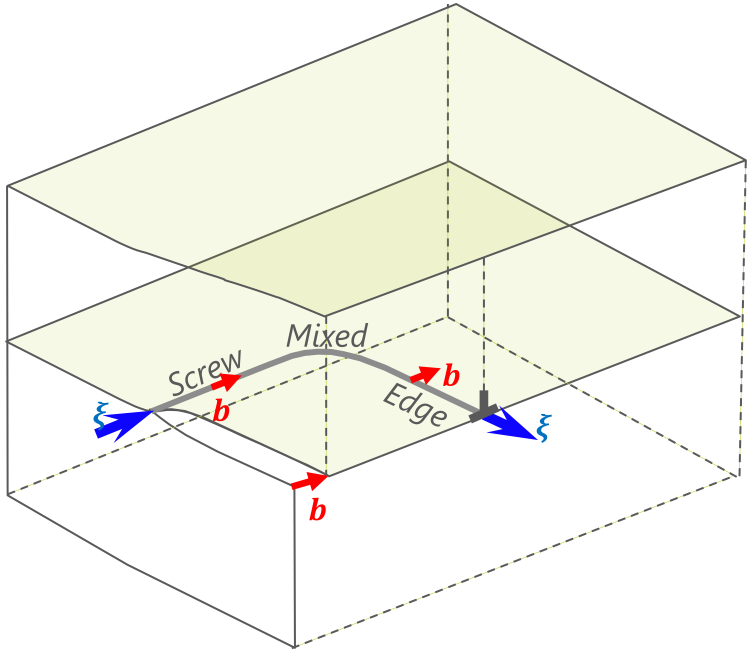


Mixed

A combination of edge and screw dislocations ($\boldsymbol{b} \angle \boldsymbol{\xi}$).



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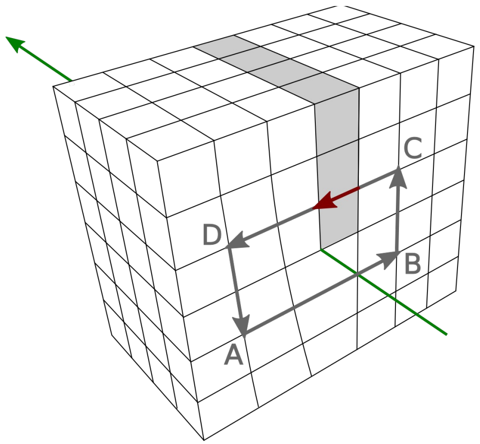

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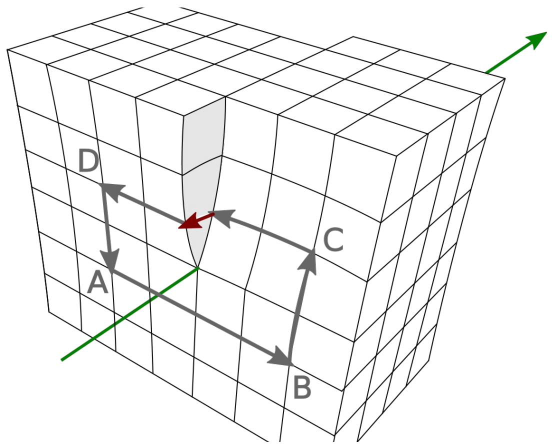

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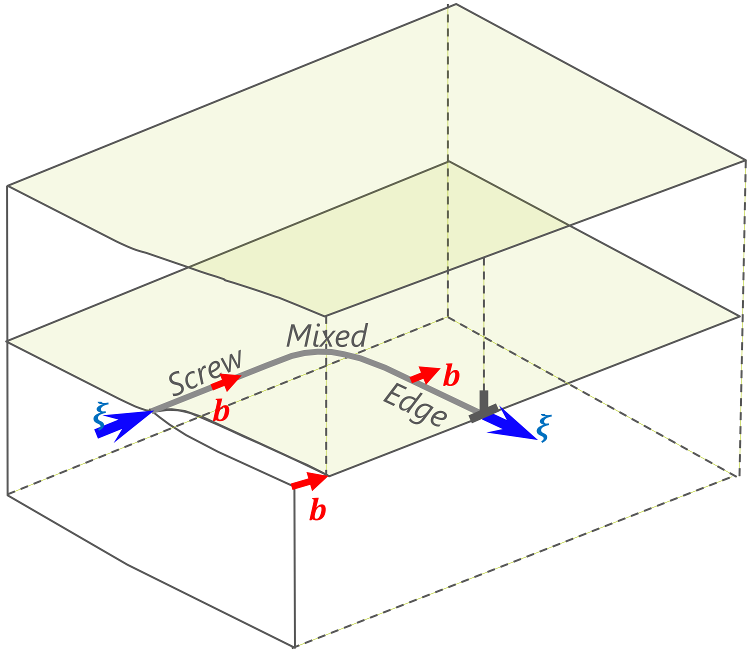

↳Dislocations are the carriers of plastic deformation in crystalline materials.

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Volterra (1907): elastic foundation, read retrospectively

- **Mathematical framework**
  - Isotropic continuum cylinder subjected to six cut-displace-reweld operations
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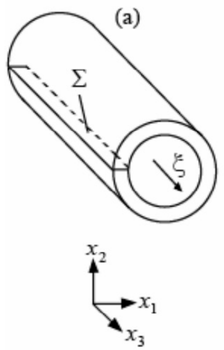

V. Volterra, *Ann. École. Norm. Super.*, 24, 400 (1907)

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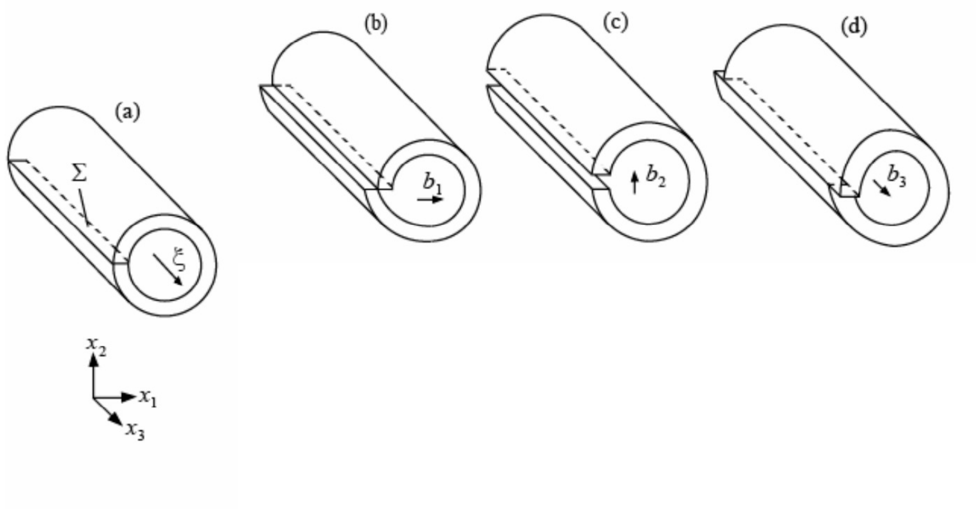

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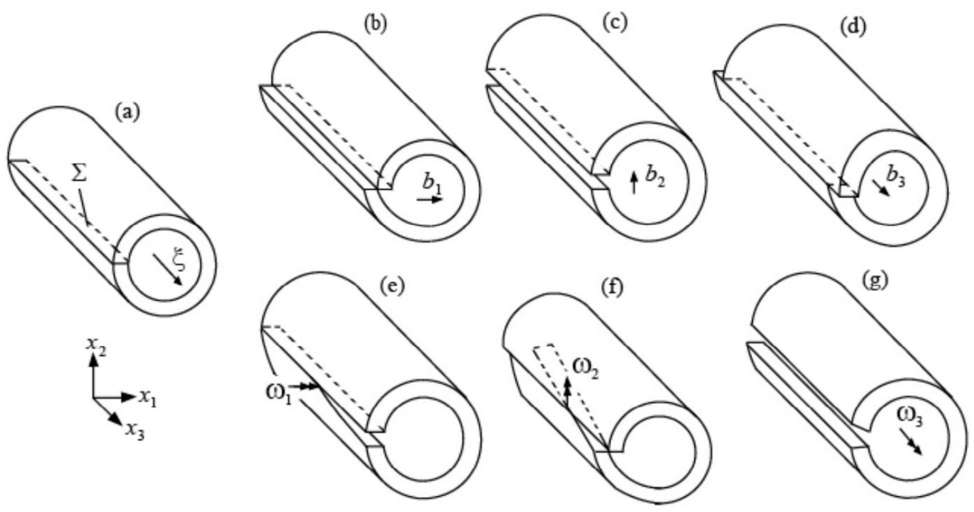

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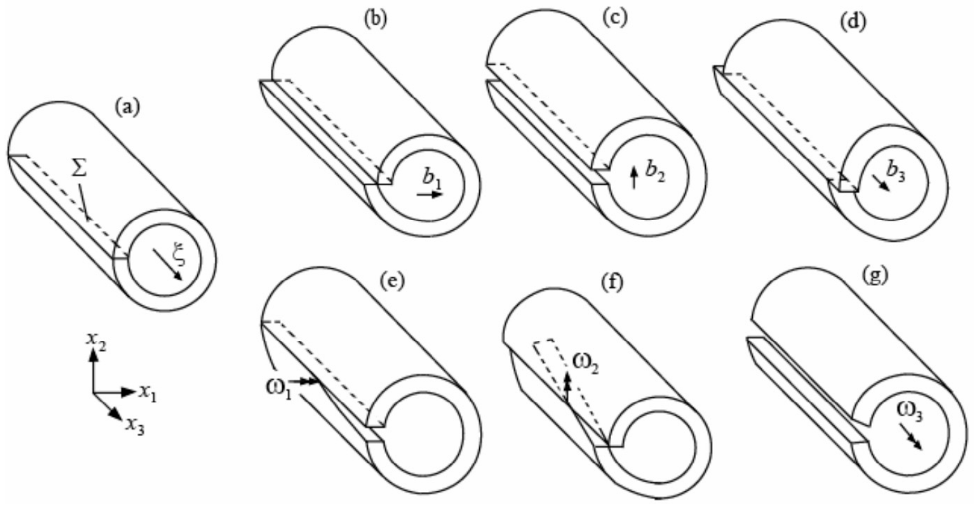

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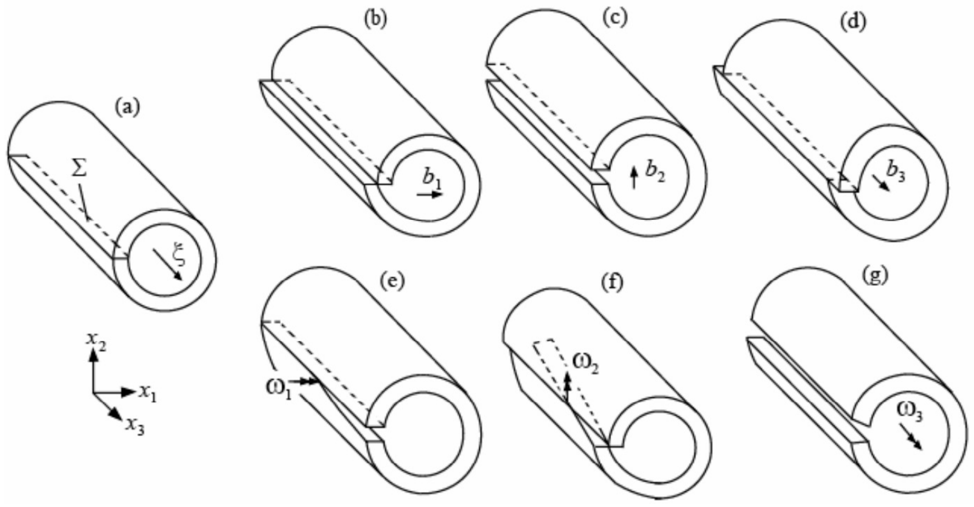
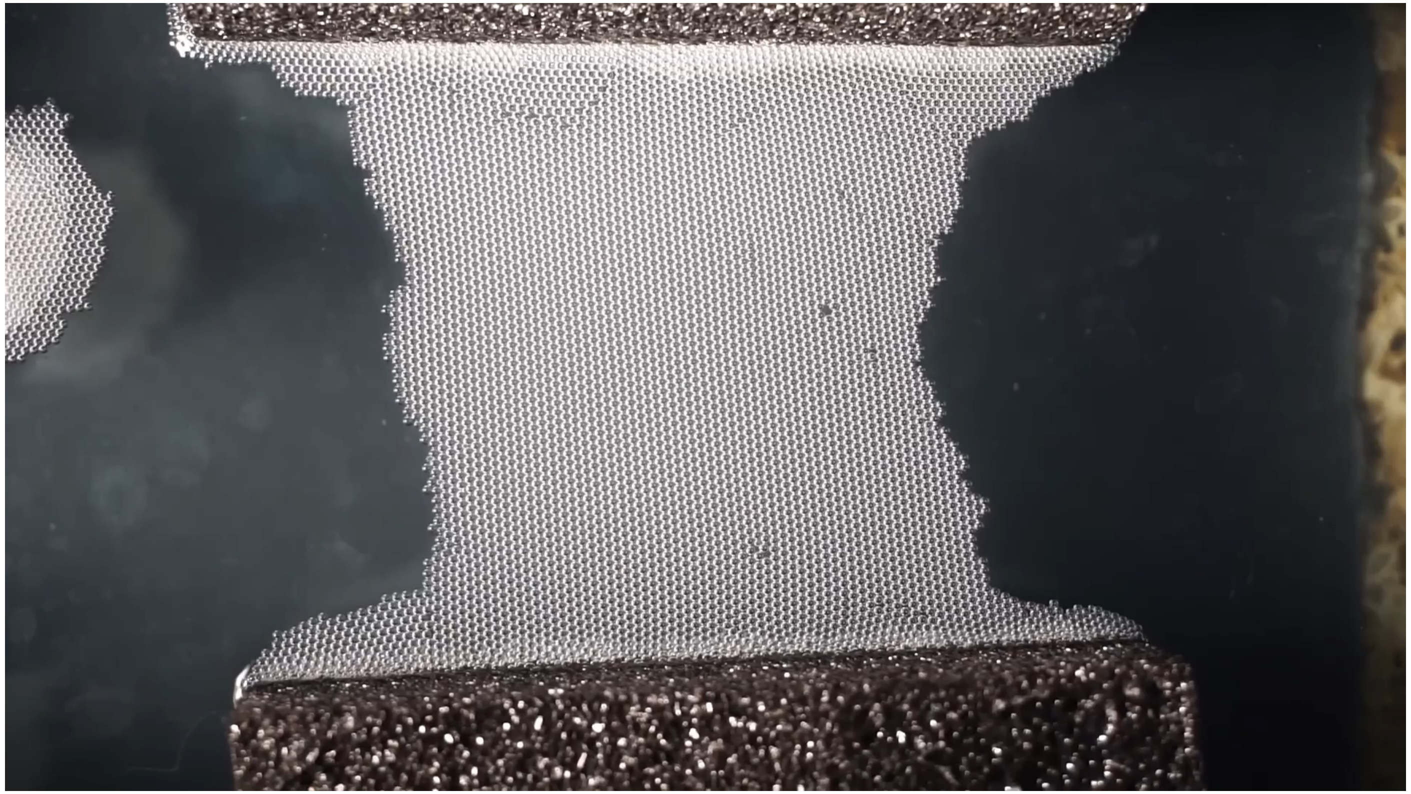
  - Retrospective connection to Volterra's work consolidated in the 1950s; term “Volterra dislocation” introduced then.

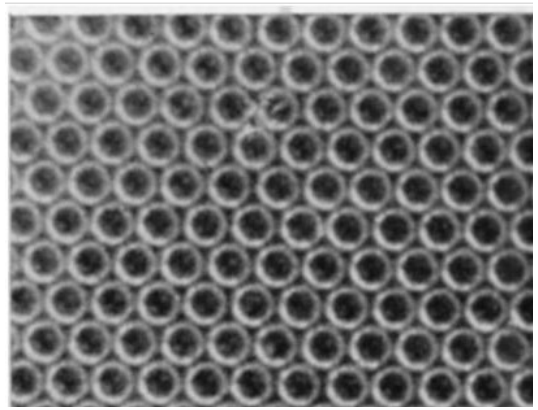


➱All six fundamental defect configurations had been mathematically predicted by 1907;
30 years before dislocations were postulated to explain plastic deformation in crystals!

V. Volterra, *Ann. École Norm. Super.*, 24, 400 (1907)

Dislocations are the carriers of plastic deformation





L. Bragg & J.F. Nye, *Proc. R. Soc. Lond.* (1947)

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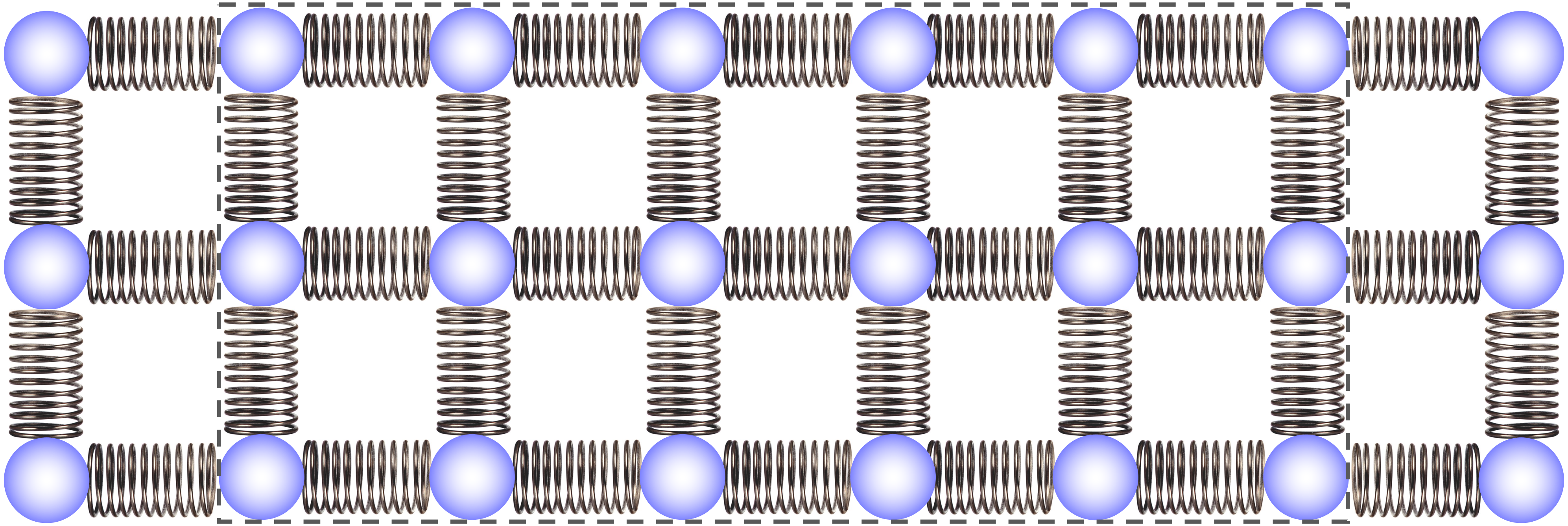
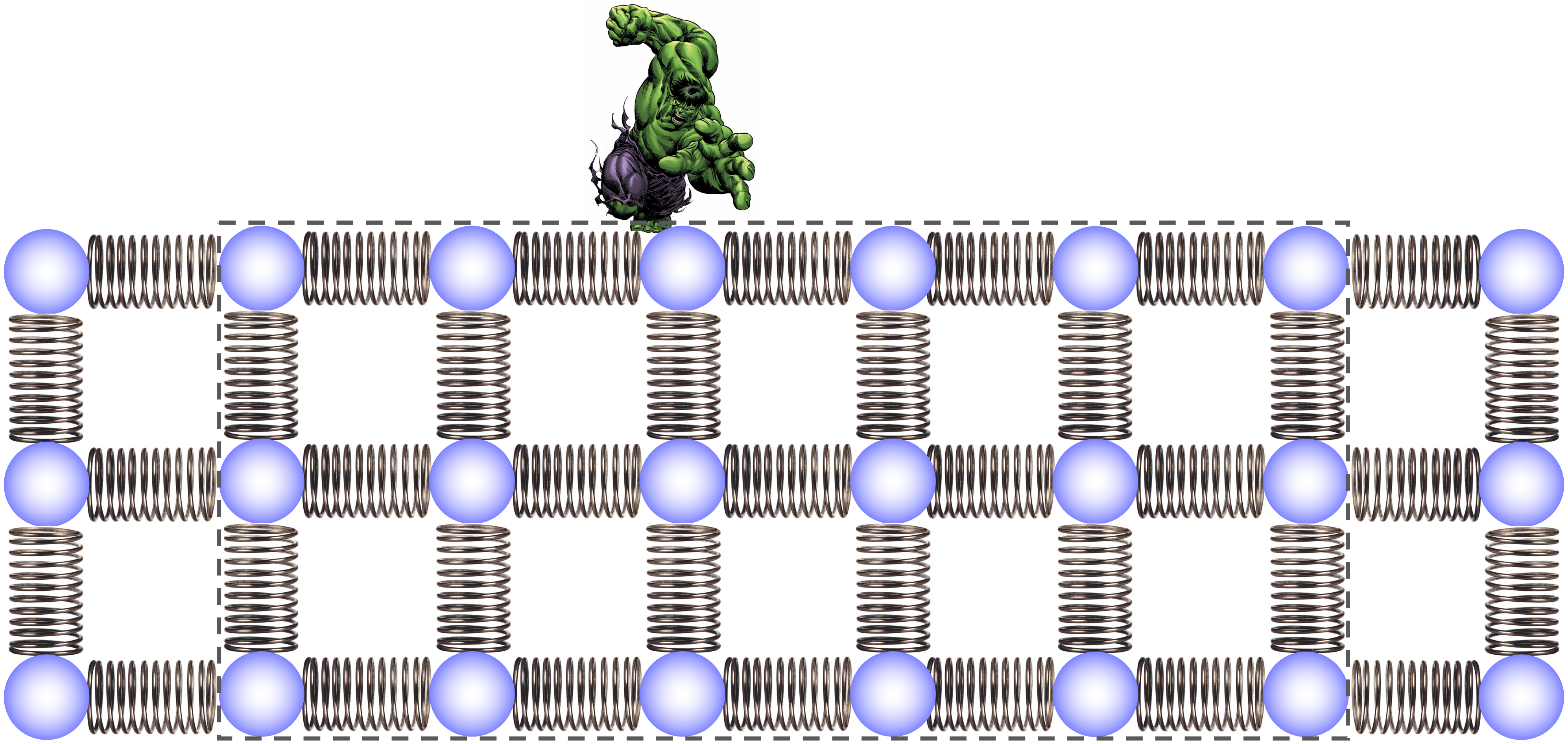
Initial size of the structure $L \times l \times h$



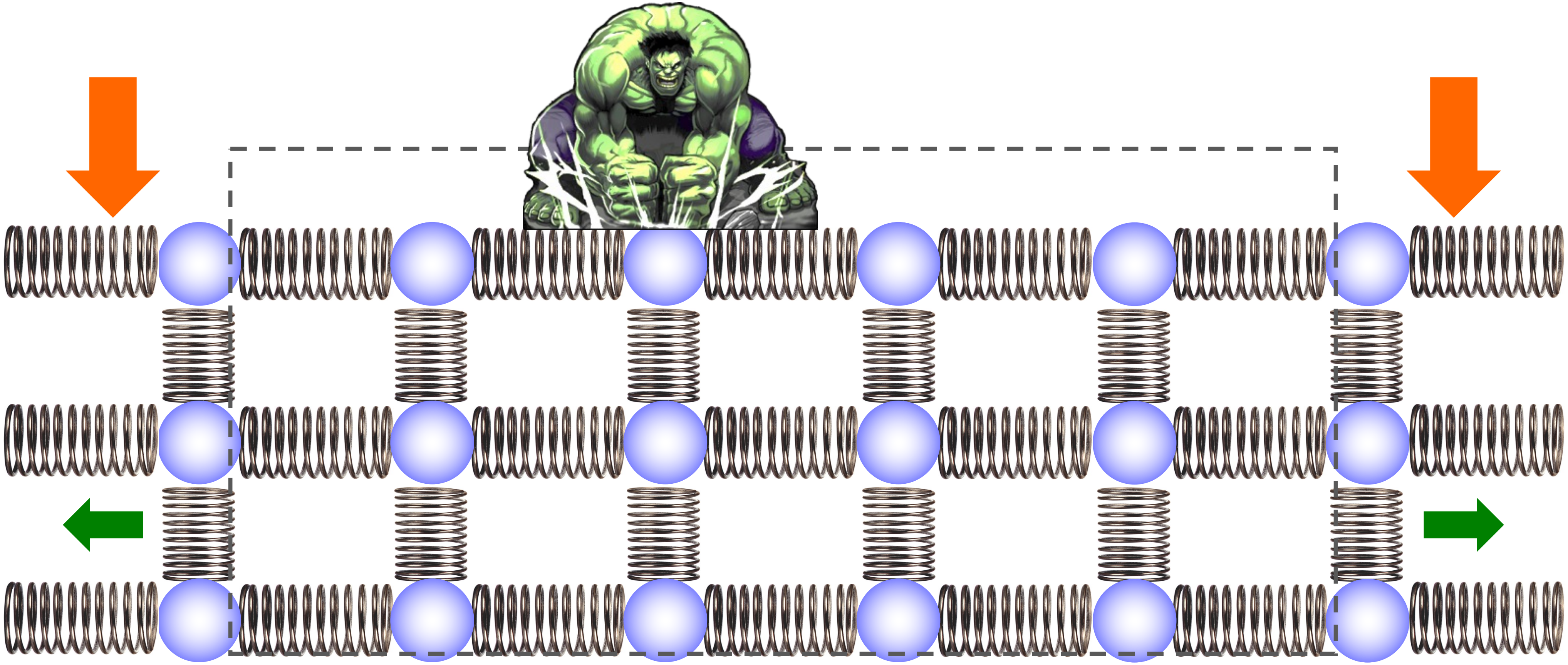
Dislocations are the carriers of plastic deformation

Application of a vertical load



Dislocations are the carriers of plastic deformation

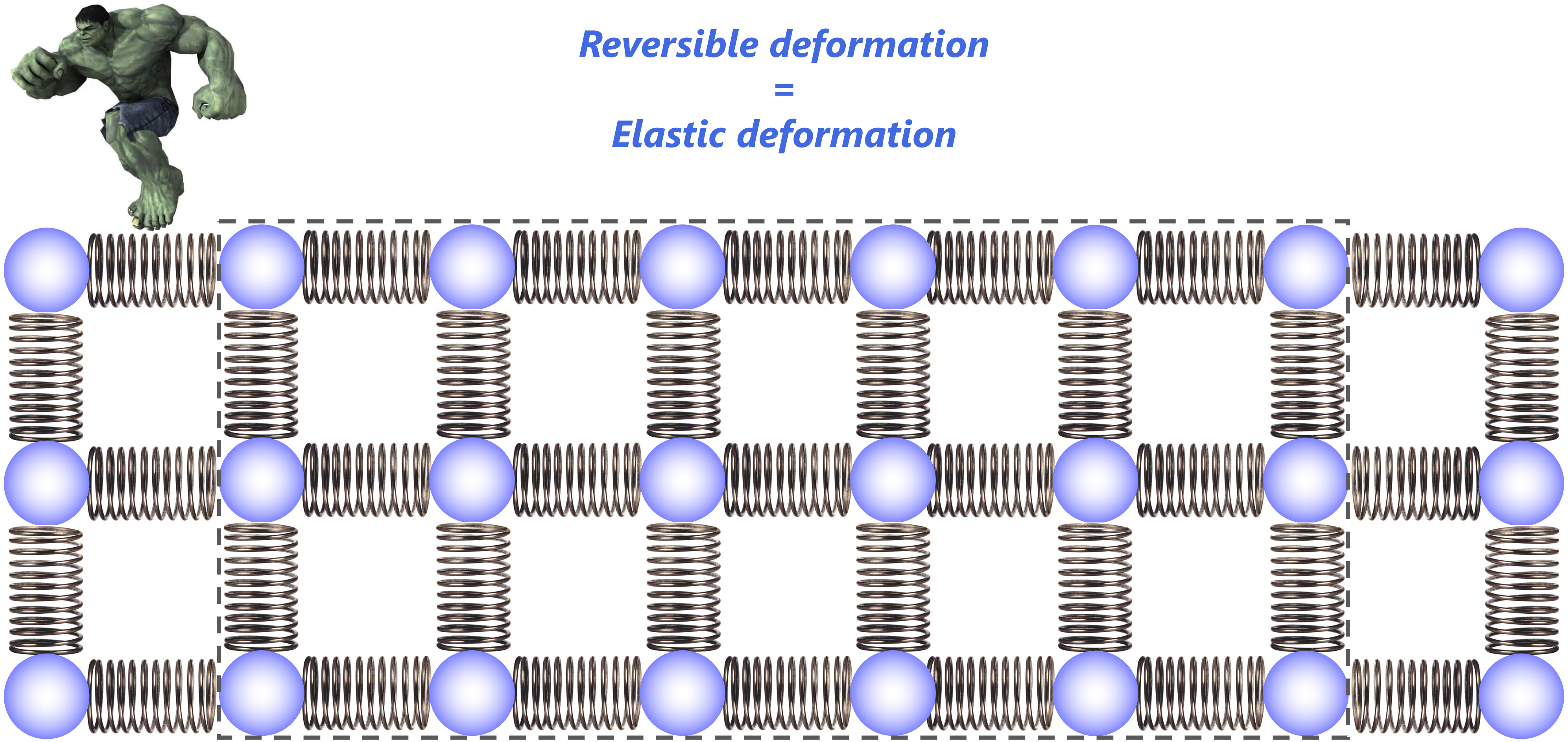
Under the load, the vertical springs are compressed and the horizontal ones are stretched.



Dislocations are the carriers of plastic deformation

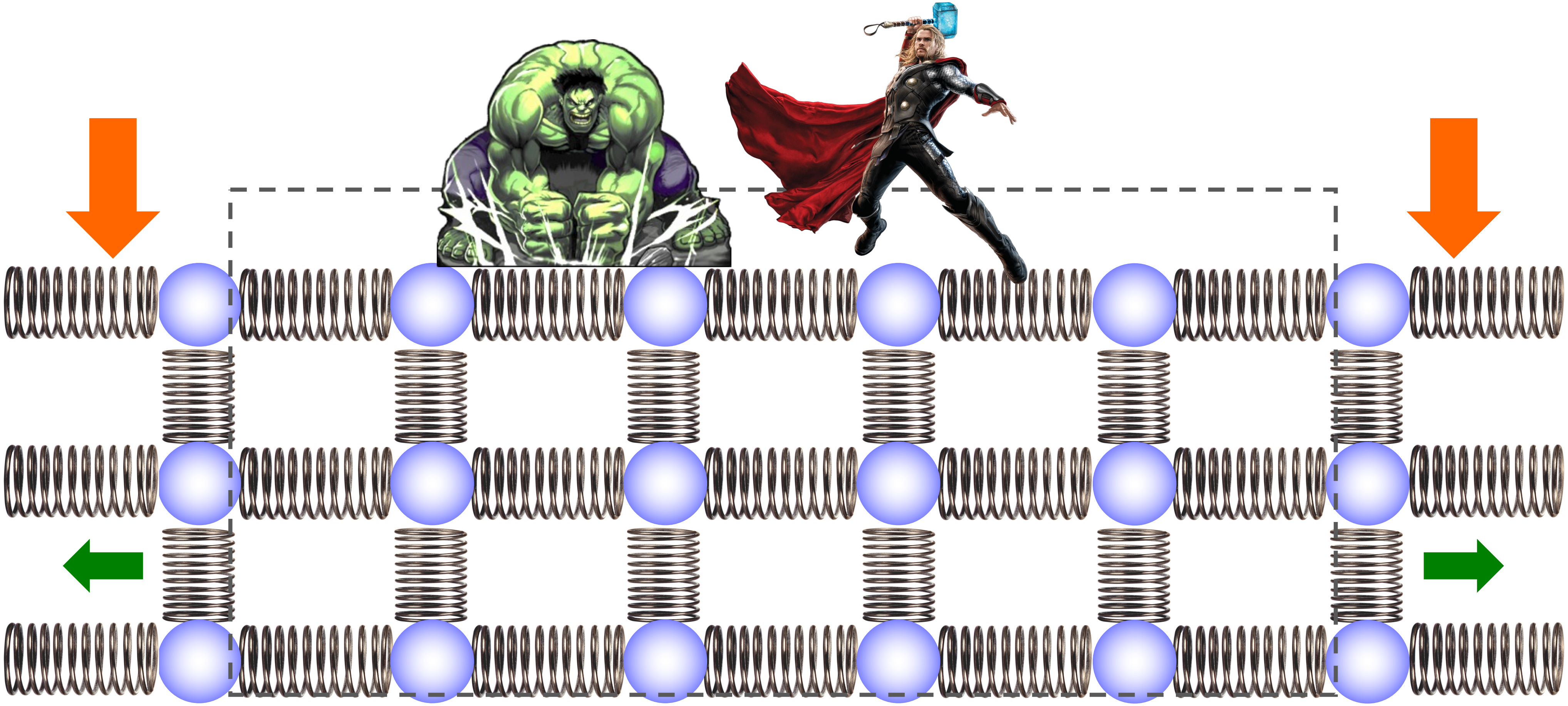
When the load is removed, the structure returns to its original dimensions.

Reversible deformation
=
Elastic deformation



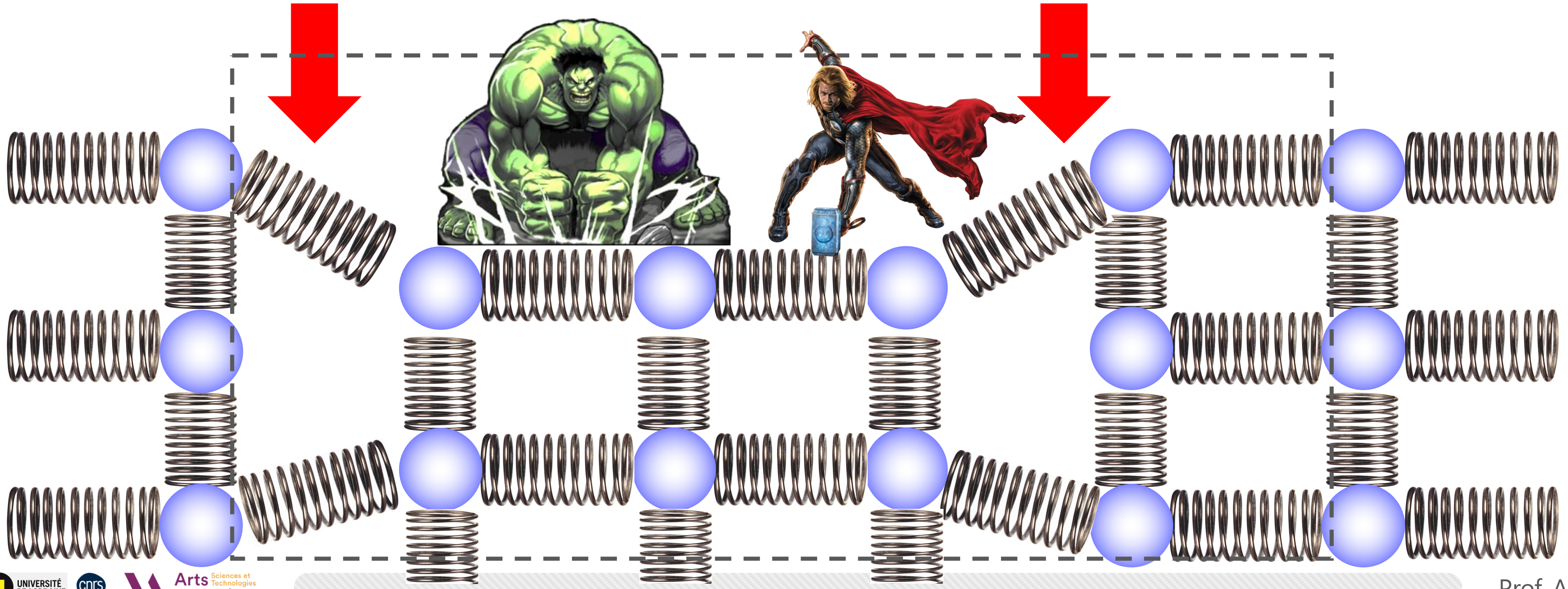
Dislocations are the carriers of plastic deformation

Under the load, the vertical springs are compressed and the horizontal ones are stretched.
A higher load is applied.



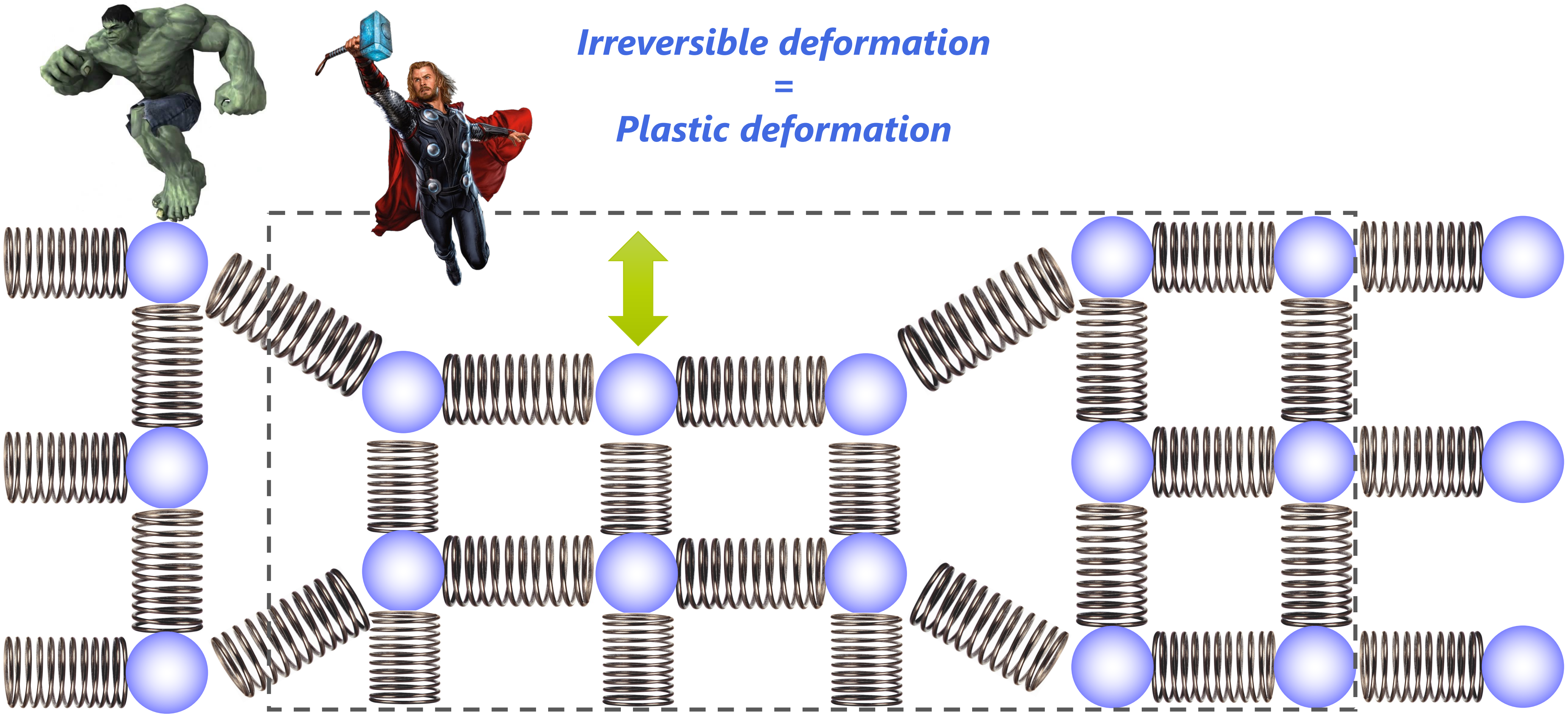
Dislocations are the carriers of plastic deformation

Under the load, the vertical springs are compressed and the horizontal ones are stretched.
Some springs are broken.



Dislocations are the carriers of plastic deformation

Since some springs are broken, the structure does not return to its original shape.



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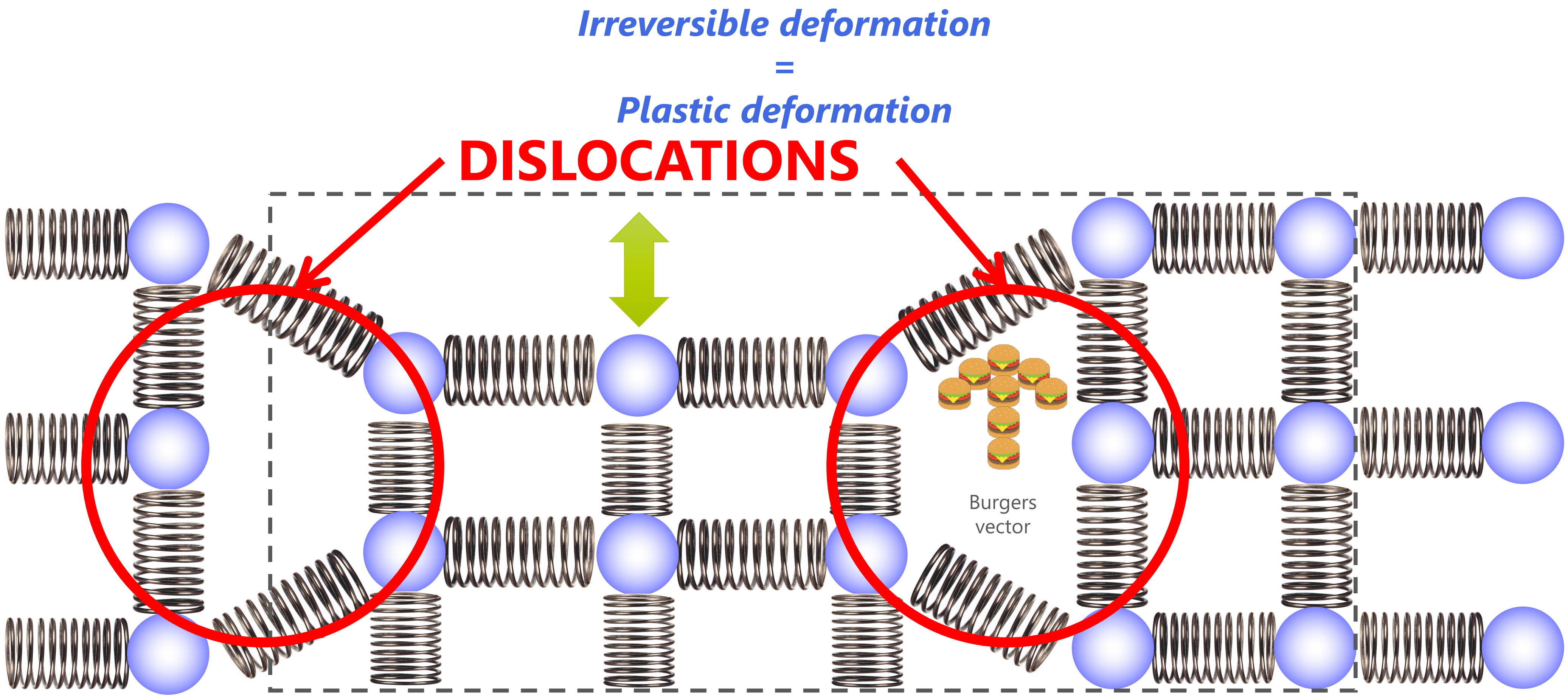


Key properties of dislocations

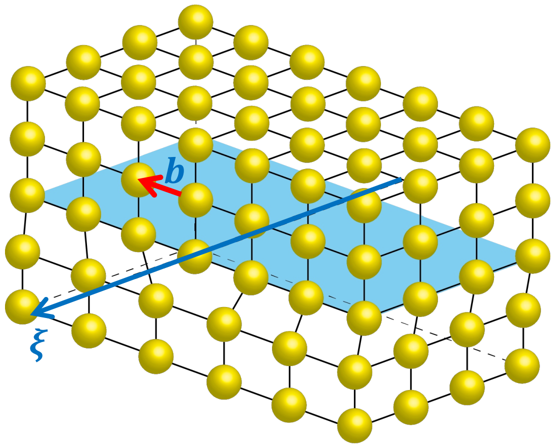
- ❖ The Burgers vector, $\boldsymbol{b}$, remains constant along the dislocation line.
- ❖ The direction of dislocation line, $\boldsymbol{\xi}$, can change along the dislocation line.

  $\Rightarrow$ The dislocation character $\widehat{(\boldsymbol{b},\boldsymbol{\xi})}$ can also.
- ❖ A dislocation cannot start and end inside a perfect crystal.

  $\Rightarrow$ Dislocations form loops.
- ❖ However, a dislocation can terminate at a grain boundary, a surface, or another dislocation.
- ❖ The plane defined by $(\boldsymbol{b},\boldsymbol{\xi})$ is the glide plane.

  $\Rightarrow$ No glide plane is defined for screw dislocations.
- ❖ The symbol of an edge dislocation: $\perp, \vdash, \dashv$.
- ❖ No standard symbol for screw or mixed dislocations.
- ❖ The sum of the Burgers vectors of the dislocations meeting at a node is zero.

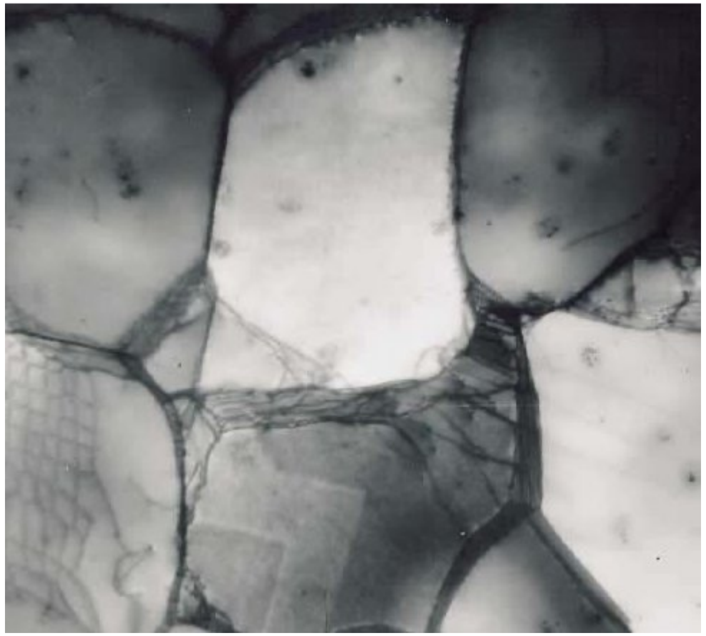
  $\Rightarrow \sum_i \boldsymbol{b_i} = 0.$



J.P. Hirth & J. Lothe, Theory of Dislocations, *Wiley* (1982)
. Hull & D.J. Bacon, Introduction to Dislocations, *Butterworth-Heinemann* (2011)

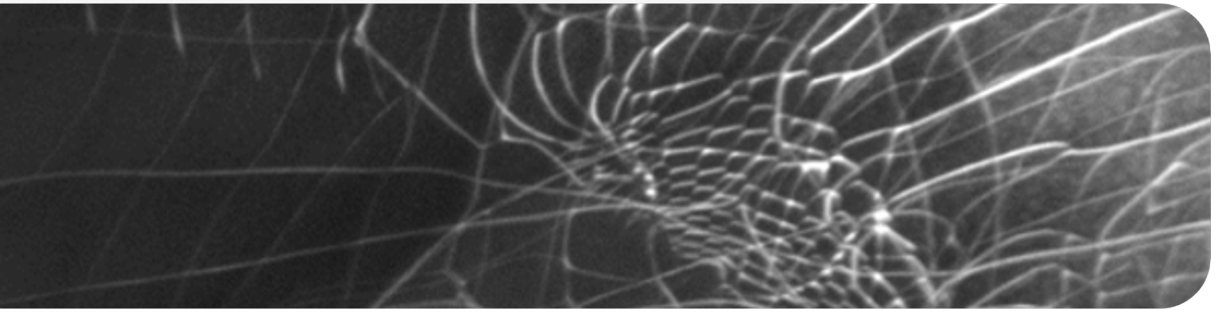
First observation of dislocations

- First direct TEM observation of dislocations in aluminum foils
- Specimens: high-purity Al, deformed and annealed, thinned to ~0.5 µm
- Dislocation substructures: subgrains (~1 µm), low-angle boundaries, networks, nodes
- Contrast mechanism due to strain fields & Bragg diffraction, no decoration needed



➪Preliminary but foundational: validated dislocation theory with direct imaging

P. B. Hirsch, R. W. Horne & M. J. Whelan, *Philos. Mag.*1; 677–684 (1956)

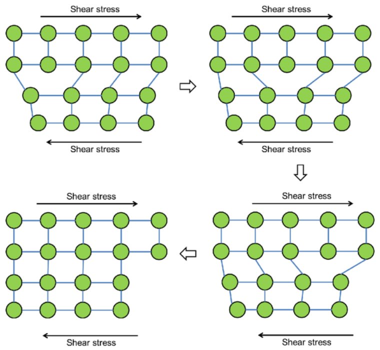


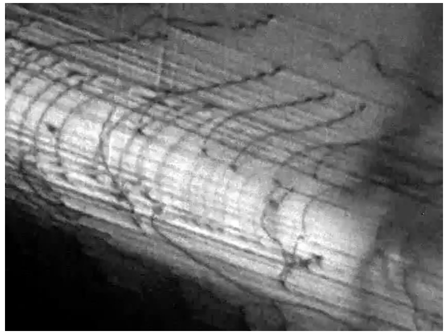
Dislocation mechanics, sources and microstructure

Dislocation movement

❖ Glide

- Glide
- Motion of a dislocation within its slip plane.
- Driven by the resolved shear stress (Schmid law).
- Conserves the number of atoms → no diffusion needed.
- Main mechanism of plastic deformation at low and moderate temperatures.
- Dislocations can move at speeds approaching a significant fraction of the speed of sound in the crystal under high stress





J. Kacher & I.M. Robertson, Acta Materialia 60; 6657–6672 (2012)

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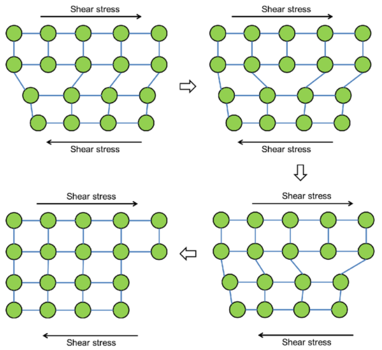
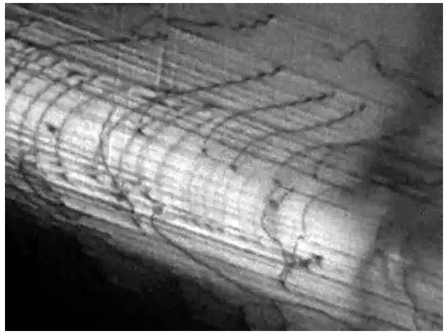
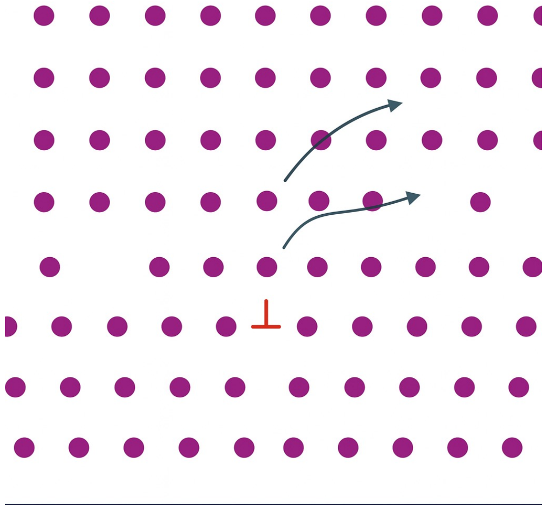




❖ Climb

- Motion out of the slip plane.
- Controlled by diffusion of vacancies/atoms.
- Requires point defect exchange.
- Lets dislocations bypass obstacles.
- Important at high temperatures (diffusion-driven).
- Much slower than glide.



J. Kacher & I.M. Robertson, Acta Materialia 60; 6657–6672 (2012)

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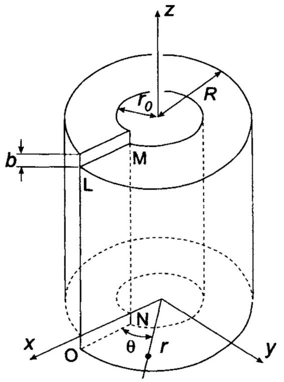

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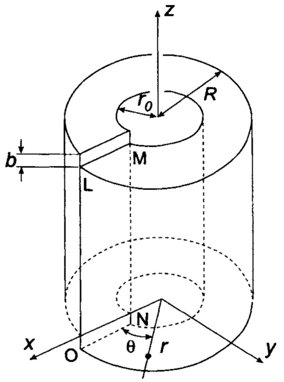

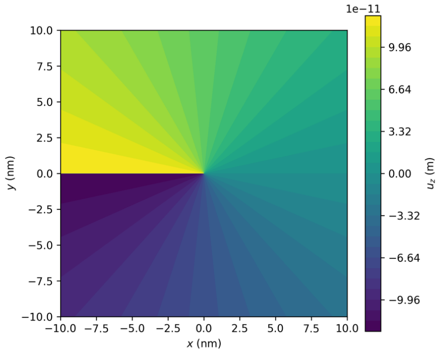

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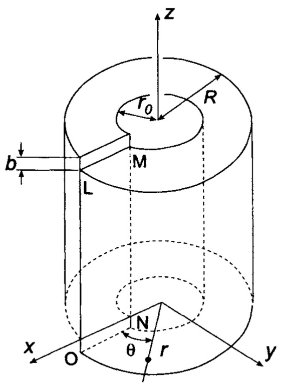

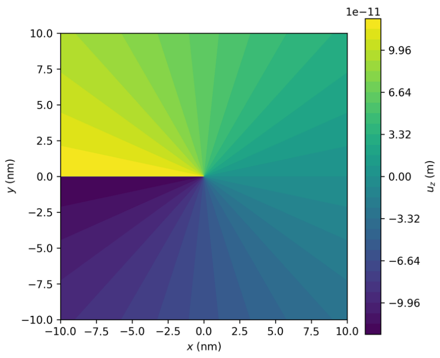

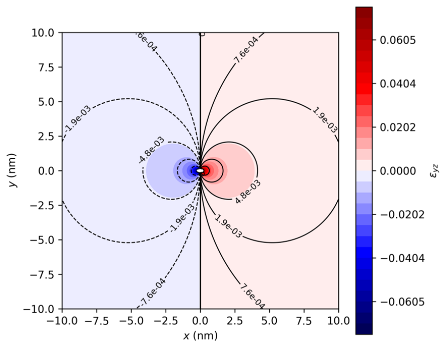

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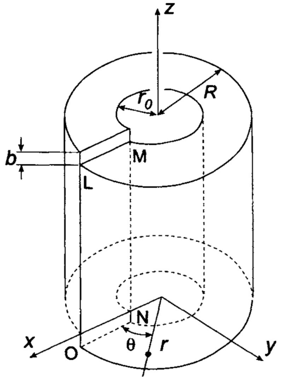

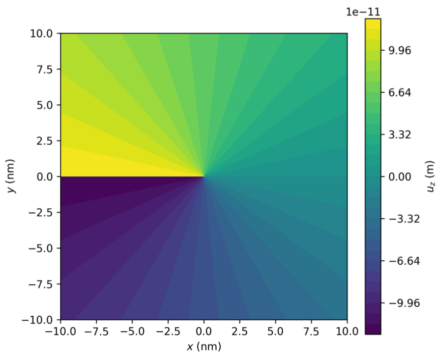

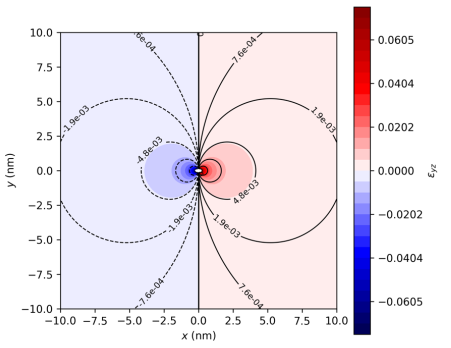

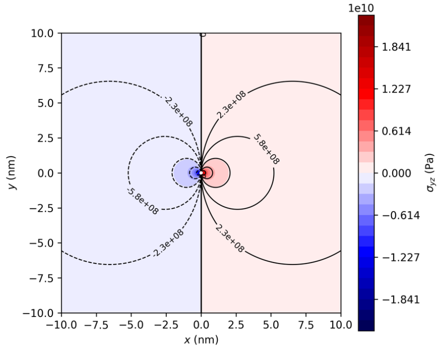

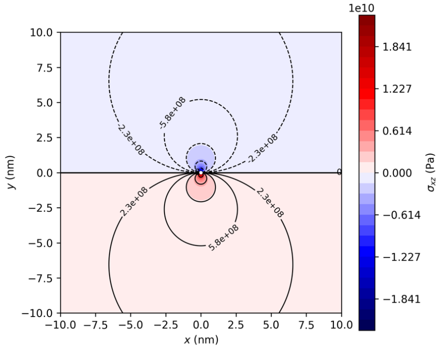

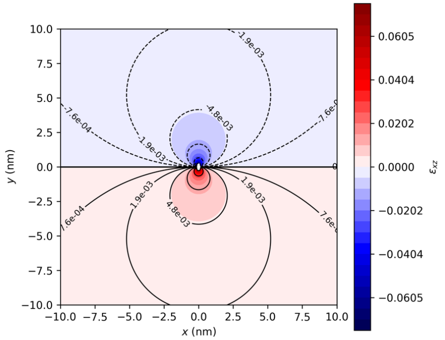

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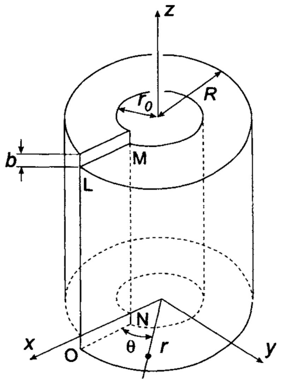

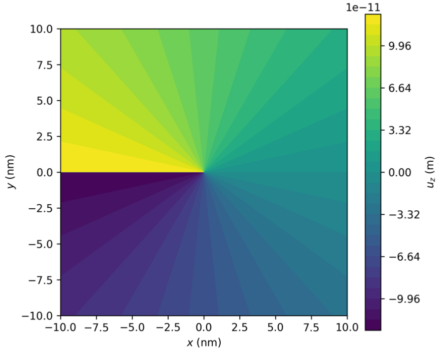

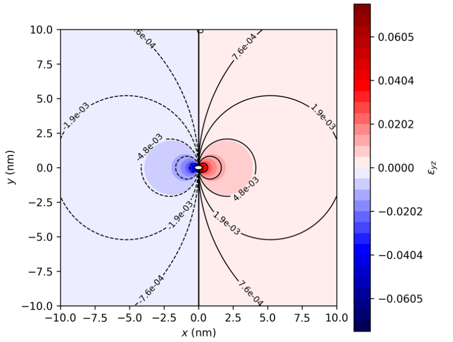

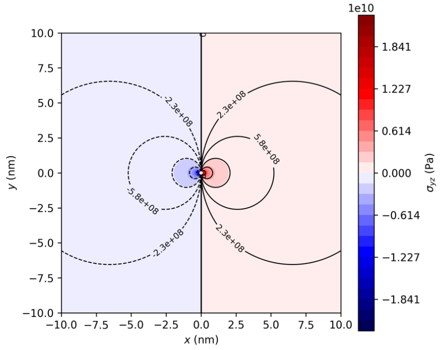

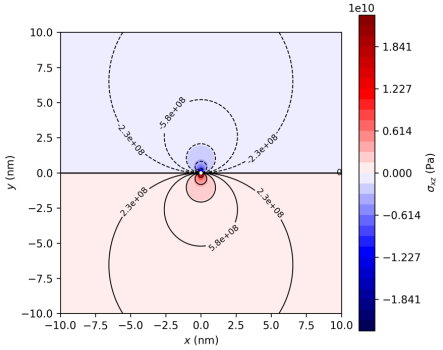

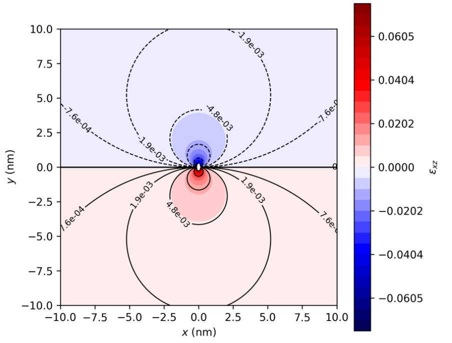

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$$D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{xx} = -Dy\frac{(3x^2+y^2)}{(x^2+y^2)^2};\ \sigma_{yy} = Dy\frac{(x^2-y^2)}{(x^2+y^2)^2}$$

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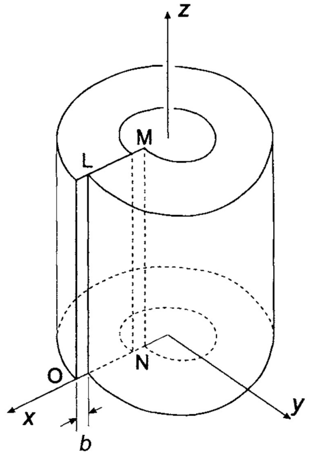

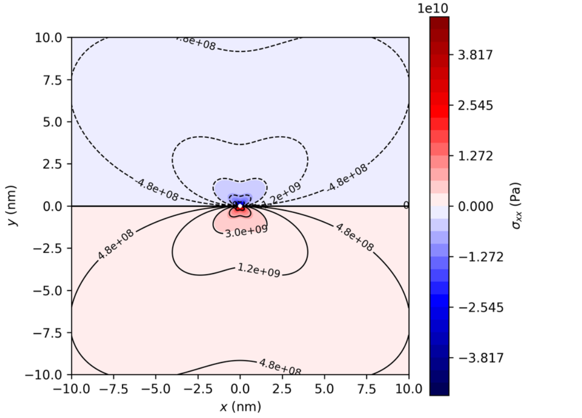

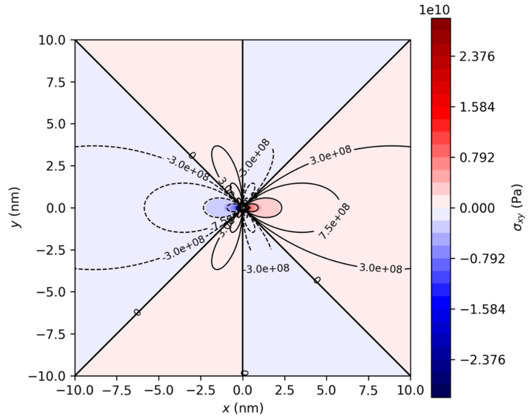

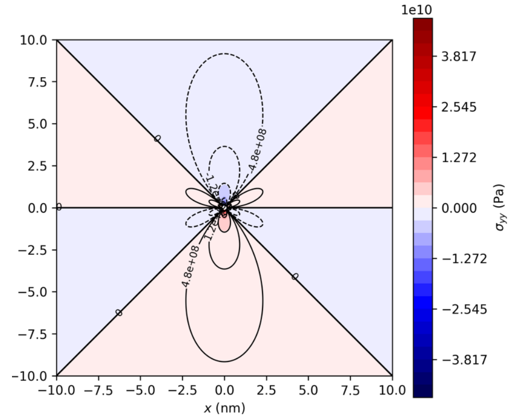

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↳Dislocation energy $\propto Gb^2\ln\frac{R}{r_0}$ → diverges in infinite crystal, cut off by the core.

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Glide force

- Driving force for dislocation motion in the slip plane.

- Origin: resolved shear stress acting on the Burgers vector.

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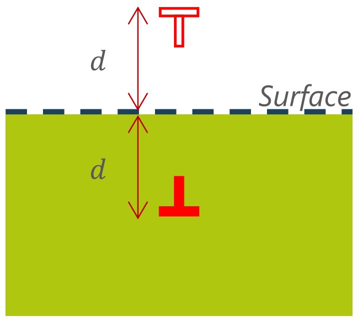
Effect of free surfaces on dislocations



❖ **Surface presence alters the elastic field of a dislocation loop.**

⇒ An image force appears to satisfy the zero-traction boundary condition at the surface.

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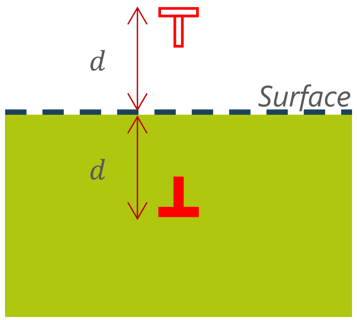

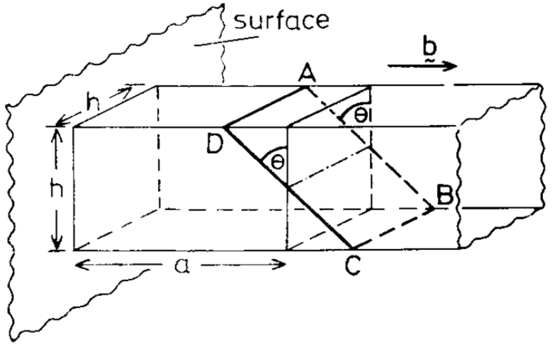

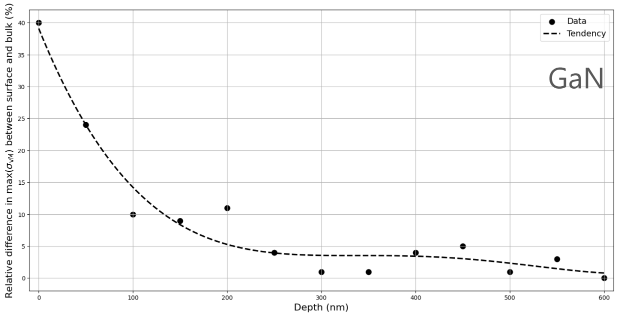

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- **Surface effects are short-ranged:**
  - Significant influence when depth $a \leq 2h - 3h$

    a: distance from loop center to surface; h: loop size (length of one side of rectangular loop)
  - For $a > 3h$, the dislocation behaves as in an infinite medium.

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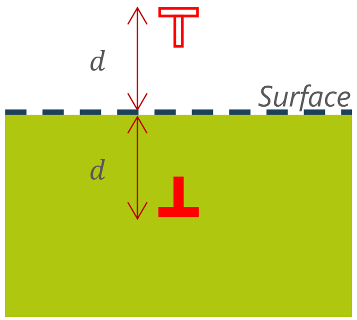
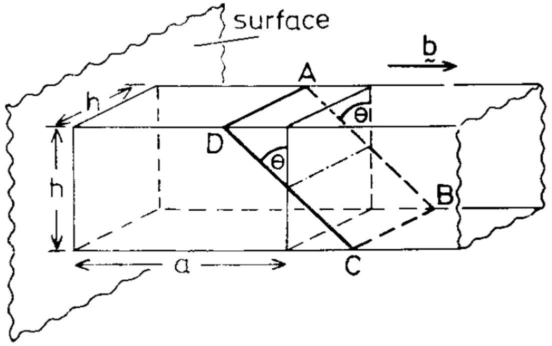
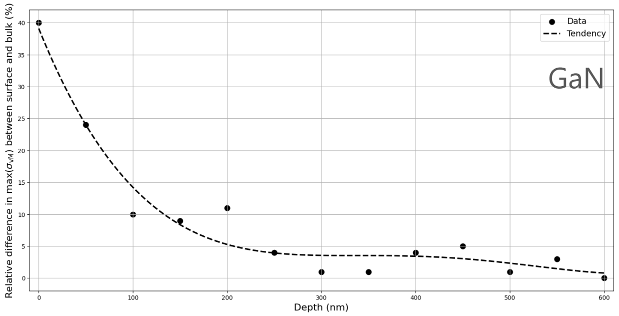






- ❖ **Surface presence alters the elastic field of a dislocation loop.**

  ⇒ An image force appears to satisfy the zero-traction boundary condition at the surface.

  ⇒ Physically, it corresponds to the attraction between the real dislocation and a virtual dislocation of opposite Burgers vector ($-\boldsymbol{b}$) placed symmetrically on the other side of the surface.

- ❖ **Surface effects are short-ranged:**
  - Significant influence when depth
    $$a \leq 2h - 3h$$
    a: distance from loop center to surface; h: loop size (length of one side of rectangular loop)
  - For $a > 3h$, the dislocation behaves as in an infinite medium.

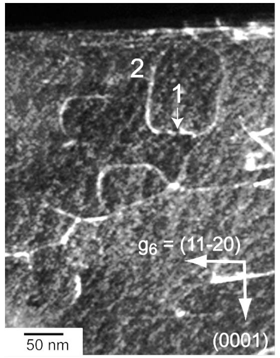
↳The behavior of dislocations is influenced by the presence of free surfaces

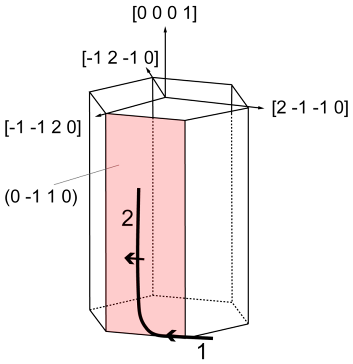
P.P. Groves et al., *Philos. Mag.* (1970)
F. El Ajjouri et al., *Philos. Mag.* (2026)

Some dislocation configurations

Cross-slip

- Mechanism: a screw dislocation can move from its original slip plane to a cross-slip plane.
- **Effect:** essential for work hardening





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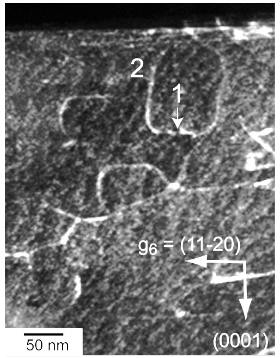
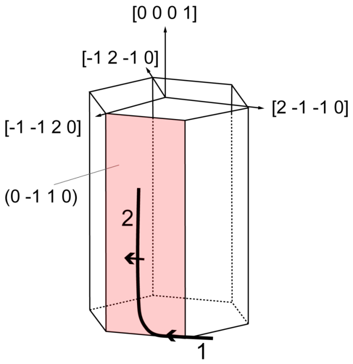


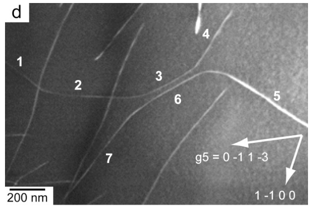


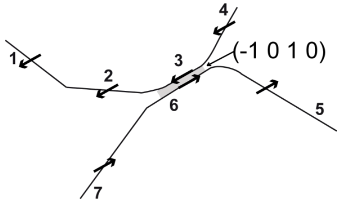
Dipole/pair

- Two dislocations on parallel slip planes.
  - Opposite signs → form a dipole
    - At small separation, they attract and create a stable locked pair.
    - Effect: dipoles act as strong obstacles to further glide

    ⇒ **Contribute to strain hardening.**

  - Same sign → form a pair.
    - They repel each other but can move together as a bound configuration.
    - Effect: can act as mobile sources of stress fields and enhance forest interactions.





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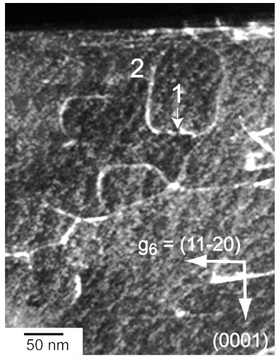

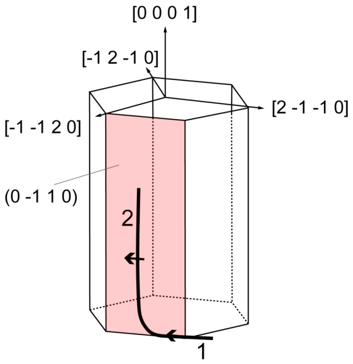

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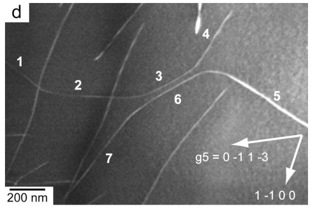
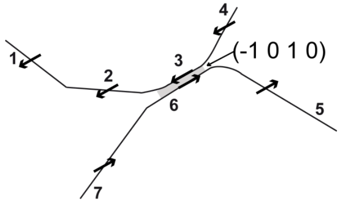




Reaction

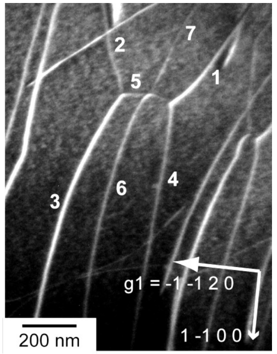
- When two dislocations on different slip systems interact, they can react:

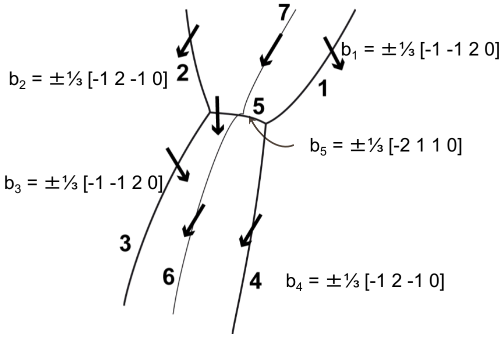
$$\boldsymbol{b_1} + \boldsymbol{b_2} \rightarrow \boldsymbol{b_3}$$

- Effect: formation of sessile dislocations

  ⇒ Strong barriers to motion

  ⇒ Strain hardening.





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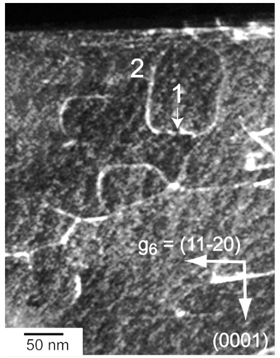

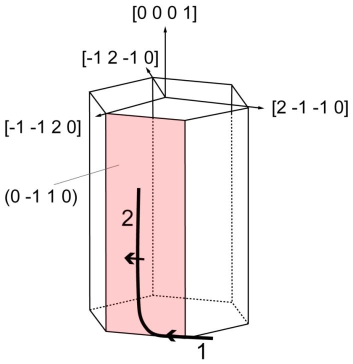

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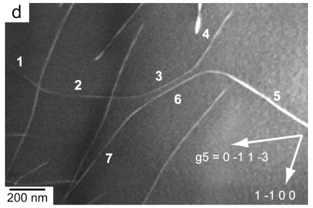

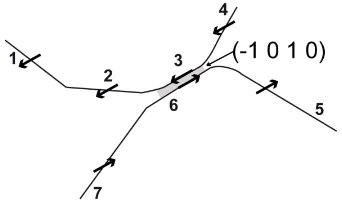

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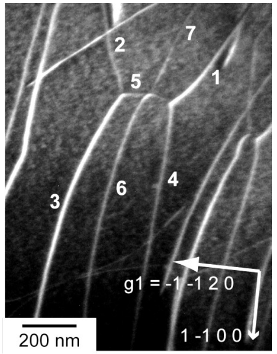

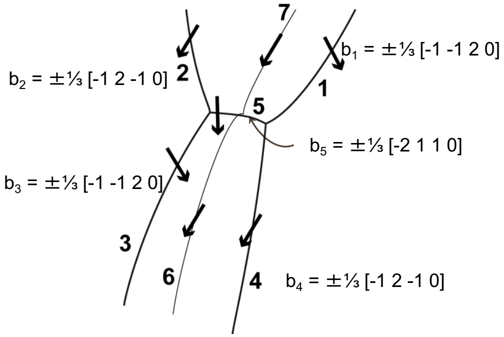

Dislocation configurations are key to understanding how dislocation interactions lead to strain/work hardening.

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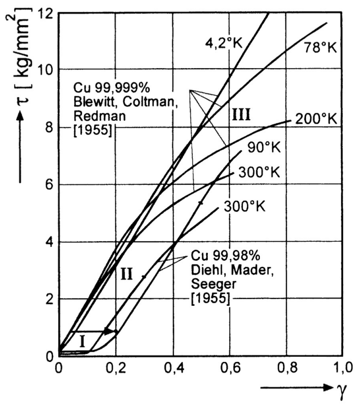

Fig. 2. Shear stress versus shear strain curves of single crystals [orientation near (100)] of 99.999% copper at various low temperatures [53] and for a single-slip orientation [51].

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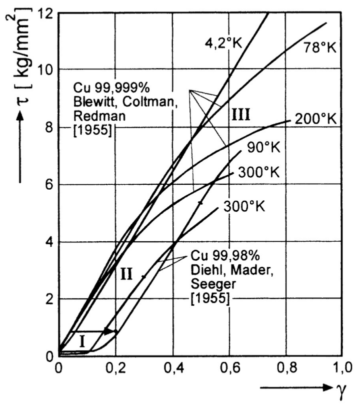
($\alpha \approx 0.3 - 0.5$; dimensionless constant reflecting dislocation interaction strength)



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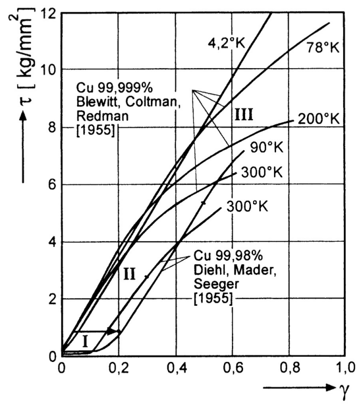
First term: storage (mean free path $\Lambda \sim 1/\sqrt{\rho}$; Second term: dynamic recovery (thermally activated annihilation)



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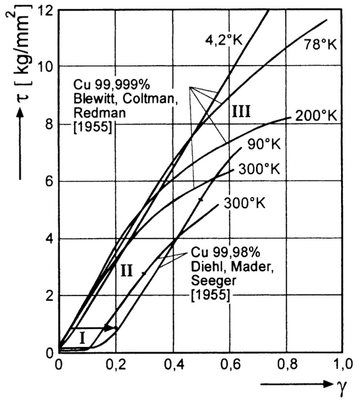
- Consequence on hardening rate $\theta = \mathrm{d}\tau/\mathrm{d}\gamma$:

$$\theta = \theta_0 - \theta_{recovery}(T, \dot{\gamma})$$

$\Rightarrow$ θ decreases with increasing temperature and decreasing strain rate.



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✓ Schematic $\tau\theta - \tau$ plot.
✓ Storage dominates at low stress.
✓ Dynamic recovery increases with τ.

$\Rightarrow$ **Dynamic recovery accelerates hardening rate θ decreases until plastic flow saturates.**

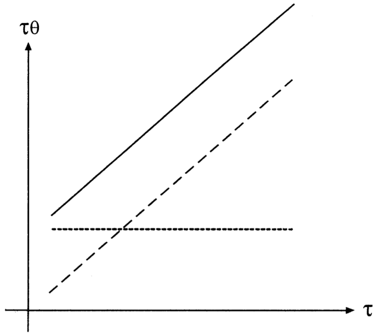


Fig. 14. Dislocation storage rate when the mean free path is constant (dots); when it is proportional to the dislocation spacing (dashes); and when both superpose (solid).

↳Work hardening is the macroscopic signature of dislocation storage controlled by the configurations generated during plastic flow.

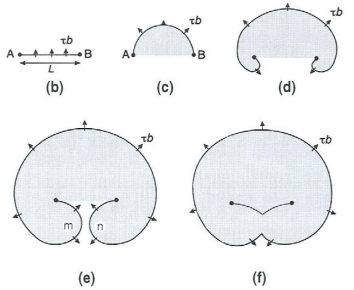
U.F. Kocks & H. Mecking, Prog. Mater. Sci. 48, 171 (2003)

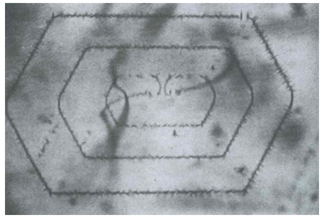
Dislocation sources

Frank-Read

- Pinned dislocation segment bows out under shear stress.
- At $\sim 180°$ curvature, reconnection occurs
  $\Rightarrow$ dislocation loop emitted.
- The process repeats → dislocation multiplication.
- Critical activation stress:

$$\tau_{max} = \frac{\alpha G b}{L};\ \alpha = 0.5 - 1$$





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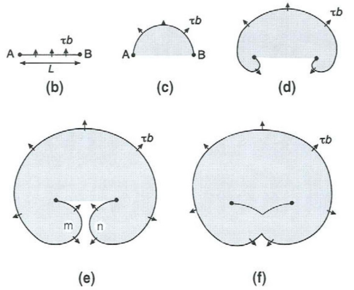
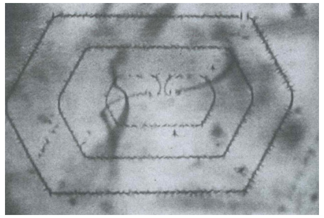
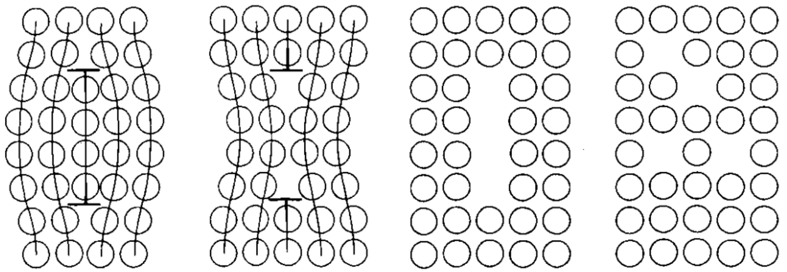




Vacancy collapse

- Cluster of vacancies coalesces into a void-like defect.
- Collapse produces a prismatic dislocation loop.
- Important in irradiated and quenched materials.



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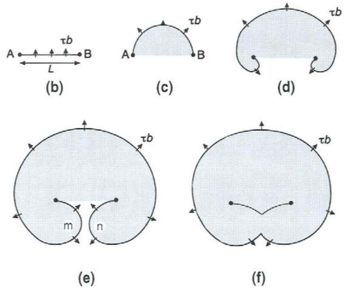

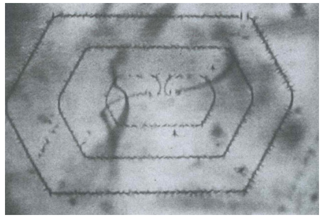

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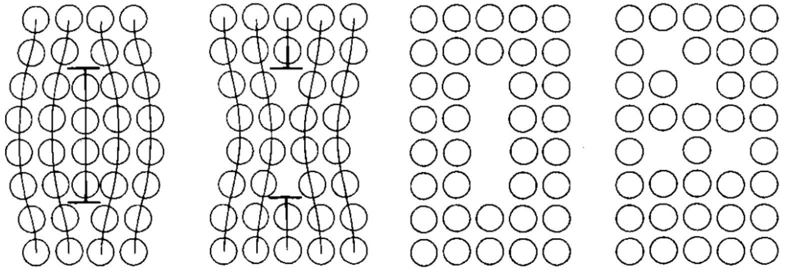

Other

- Single-arm sources (pinned at one end).
- Cross-slip of screw dislocations.
- Dislocation reactions/junctions.
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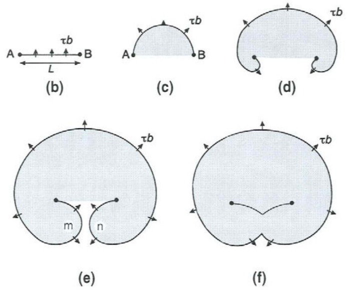

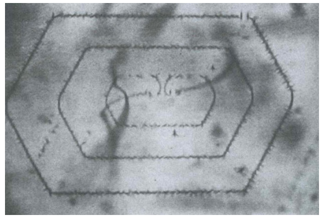

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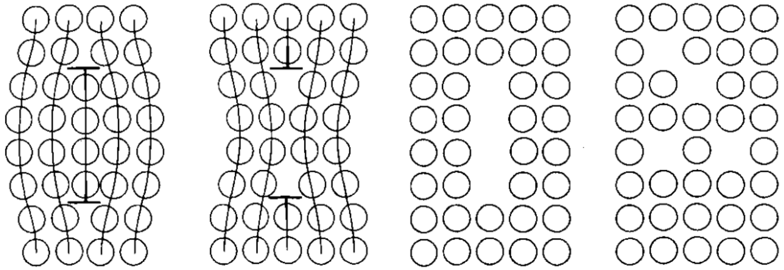

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Dislocation sources sustain the dislocation population required for plastic deformation..

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Different types of dislocation densities

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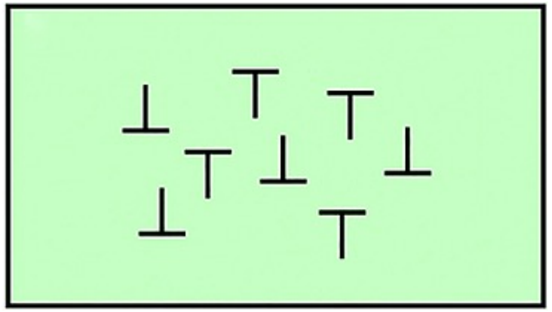

⇒ No lattice curvature at long range

J.F. Nye, *Acta Metal.* (1953)

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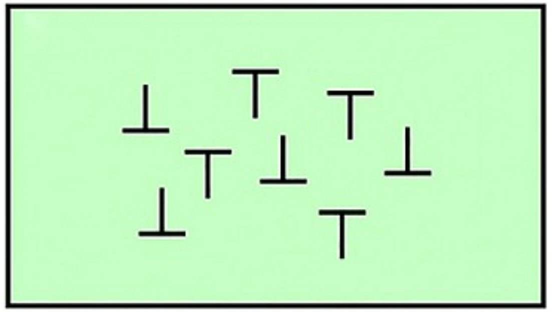

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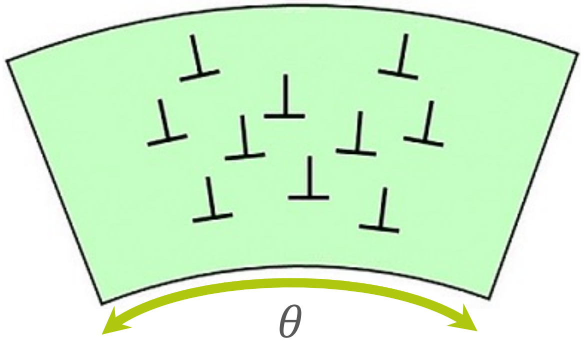

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$$\rho_{GND} \propto \frac{\theta}{||\boldsymbol{b}||\delta x}$$

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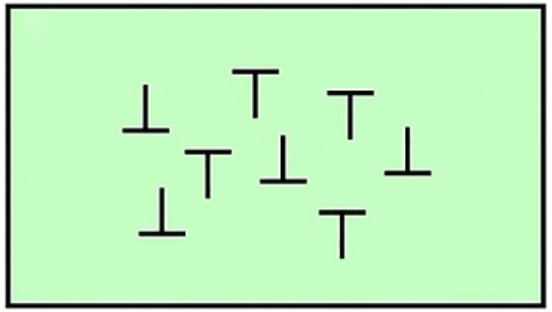

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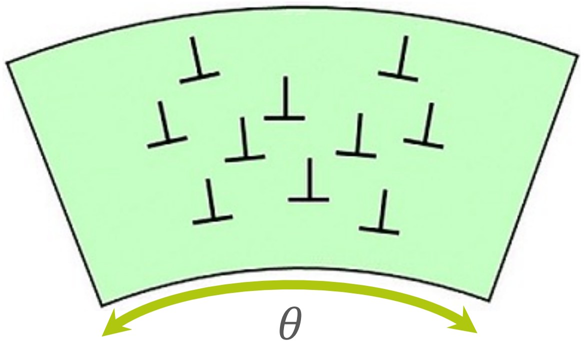


⇒ Lattice curvature at long range

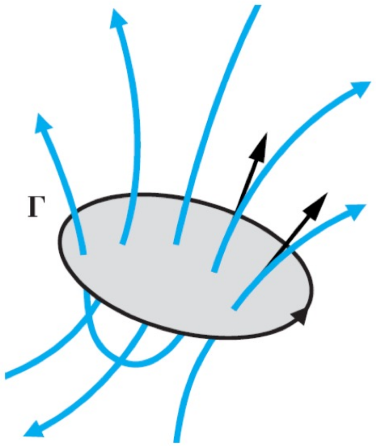
$$\rho_{\text{GND}} \approx \frac{1}{\|\boldsymbol{b}\|}\|\boldsymbol{\alpha}\|; \|\boldsymbol{\alpha}\| = \sqrt{\alpha_{ij}.\alpha_{ij}}$$

$$\boldsymbol{\alpha} = curl\ \boldsymbol{\varepsilon} + \text{tr}(\boldsymbol{\kappa_e}) \cdot \mathbb{I} - \boldsymbol{\kappa}_{\boldsymbol{e}}^T$$

$$\kappa_{ij} \cong \frac{\Delta\omega_i}{\Delta x_j};\ \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

J.F. Nye, *Acta Metal.* (1953)

The Nye tensor



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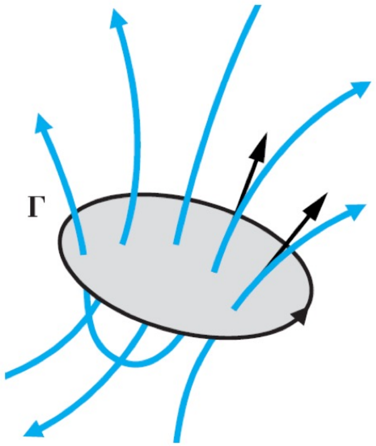

- The net Burgers vector on the closed circuit Γ limiting the surface S

$$\boldsymbol{B} = \left(\oint_{\Gamma} \boldsymbol{u}(\boldsymbol{x})\boldsymbol{n}\mathrm{d}S \right) \boldsymbol{b} = \oint_{\Gamma} \tilde{\boldsymbol{\alpha}}\boldsymbol{n}\mathrm{d}S$$

Where

$$\tilde{\boldsymbol{\alpha}} = \boldsymbol{b} \otimes \boldsymbol{u}(\boldsymbol{x})$$

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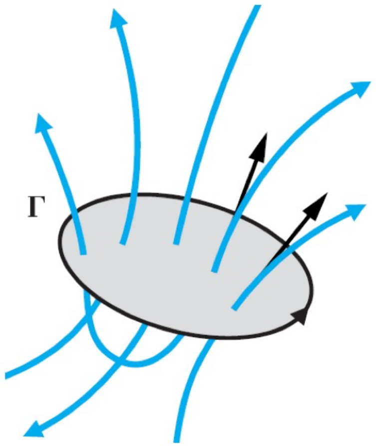

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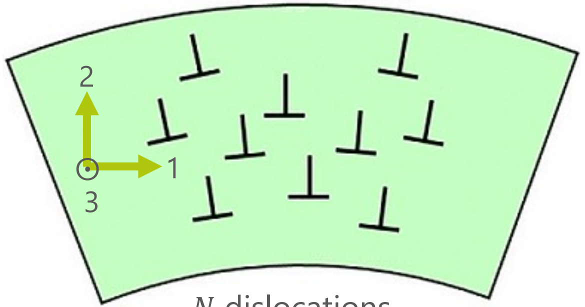
Edge dislocations (1 of 2 types)

$$\boldsymbol{B}_{edge} = Nb\boldsymbol{e_1} = \tilde{\boldsymbol{\alpha}}\boldsymbol{e_3}S$$

$$\tilde{\boldsymbol{\alpha}} = \frac{N}{S}\boldsymbol{b}\otimes\boldsymbol{u}(\boldsymbol{x}) = \frac{N}{S}b\boldsymbol{e_1}\otimes\boldsymbol{e_3} = \rho_{GND}\boldsymbol{e_1}\otimes\boldsymbol{e_3}$$



N dislocations

Screw dislocations

$$\boldsymbol{B}_{screw} = Nb\boldsymbol{e_3} = \tilde{\boldsymbol{\alpha}}\boldsymbol{e_3}S$$

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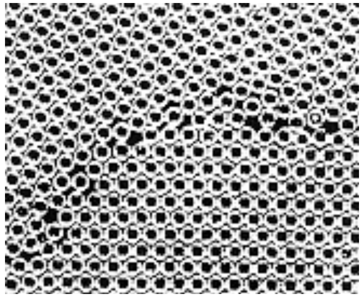
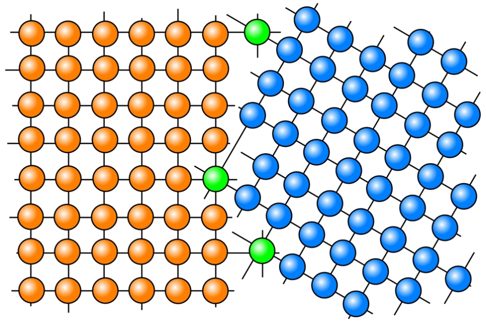
J.F. Nye, *Acta Metal.* (1953)

Grain boundaries

L. Bragg & J.F. Nye, *Proc. R. Soc. Lond.* (1947)





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L. Priester, *Springer Science & Business Media.* (2012)
F. Habiyaremye et al. MSEA, 817, 141364 (2021)

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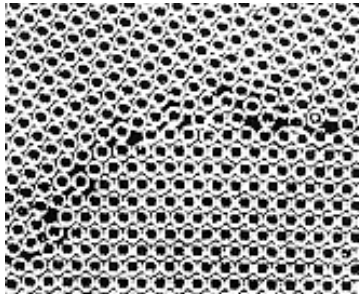
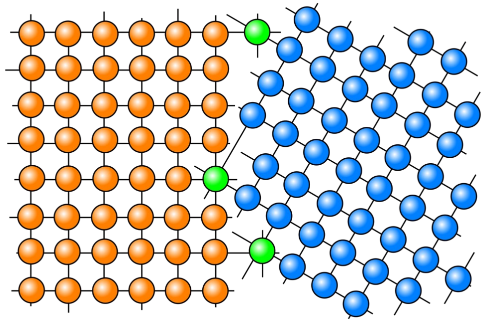
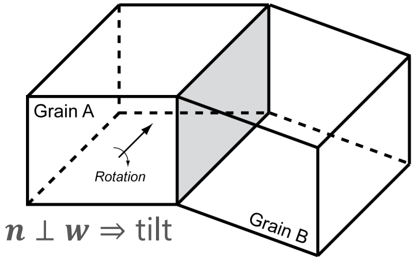
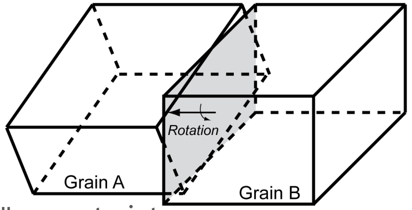






$\boldsymbol{n} \perp \boldsymbol{w} \Rightarrow$ tilt



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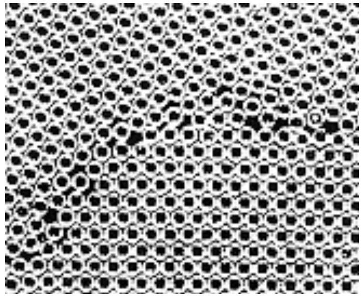

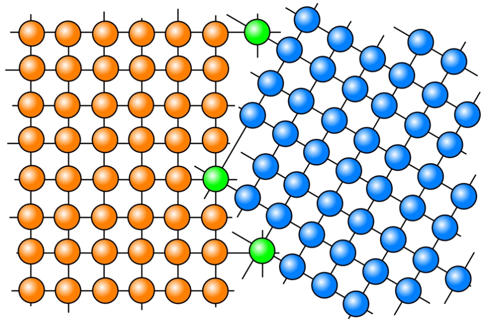

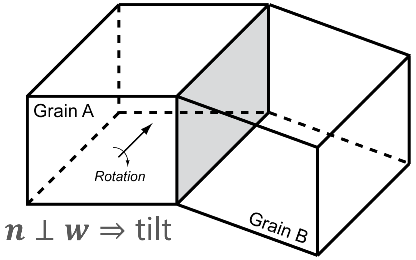

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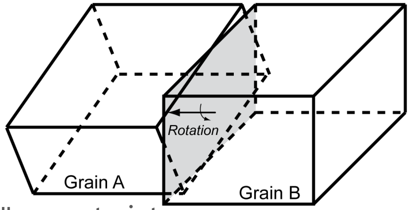

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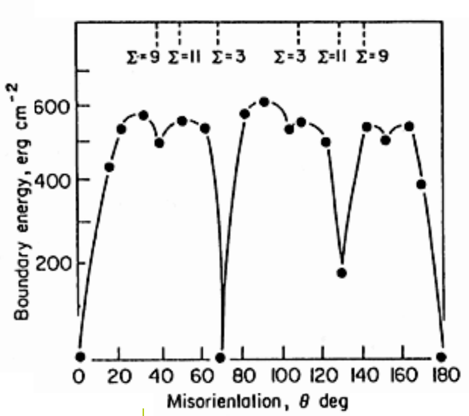
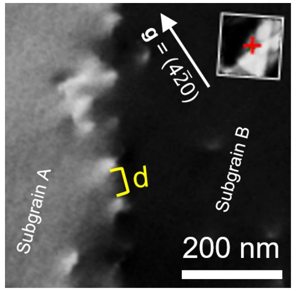
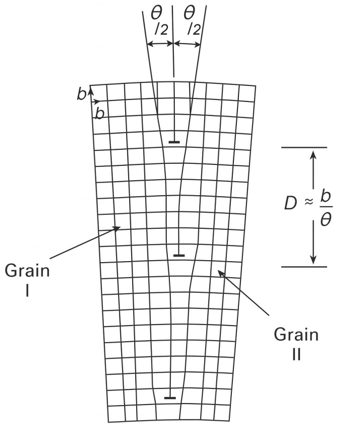




- $D = 60 \pm 5.52$ nm
- $\boldsymbol{b} = \frac{a}{2}\langle 110 \rangle$

$\Rightarrow \theta = 0.24 \pm 0.02°$



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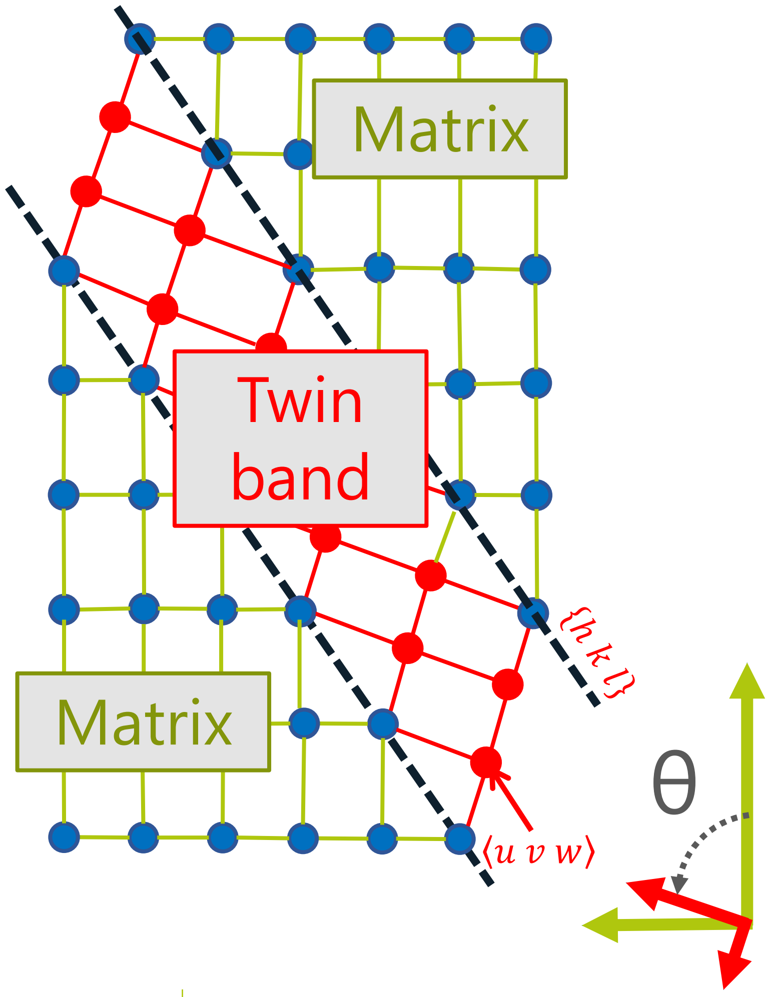
- Low-Angle GB (LAGB): $\theta \lessapprox 15°$

$$\theta = 2\sin^{-1}\left(\frac{|\boldsymbol{b}|}{2D}\right)$$

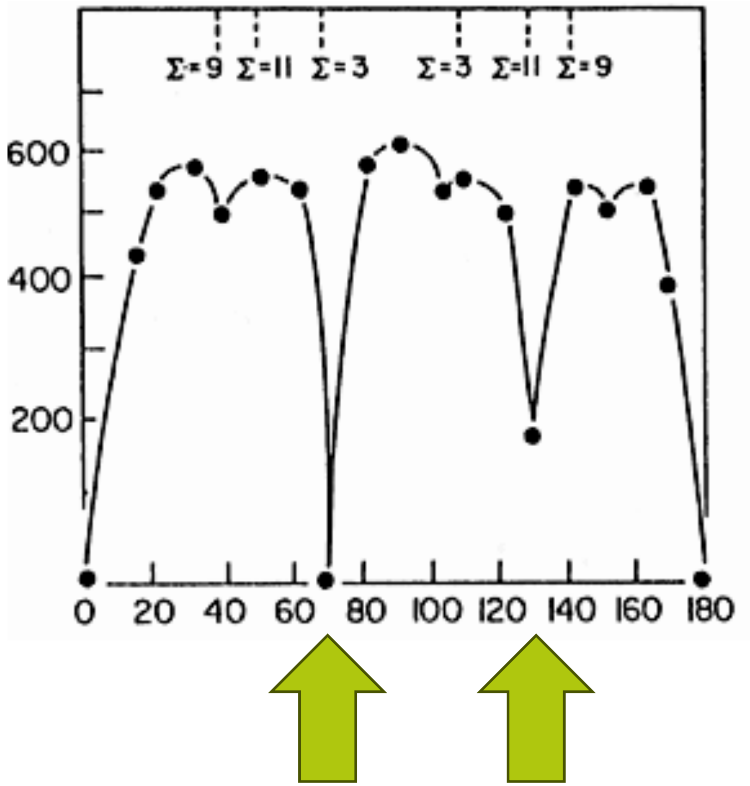
- High-Angle GB (HAGB): $\theta \gtrapprox 15°$

L. Priester, *Springer Science & Business Media.* (2012)
F. Habiyaremye et al. MSEA, 817, 141364 (2021)

Focus on the twinning



- Identical crystalline structure
- Mirror reflection
- System: $\langle u\ v\ w\rangle\{h\ k\ l\}$
- Low-energy HAGB ($\sum 3$ in FCC)
- Tilted by a specific angle (θ)

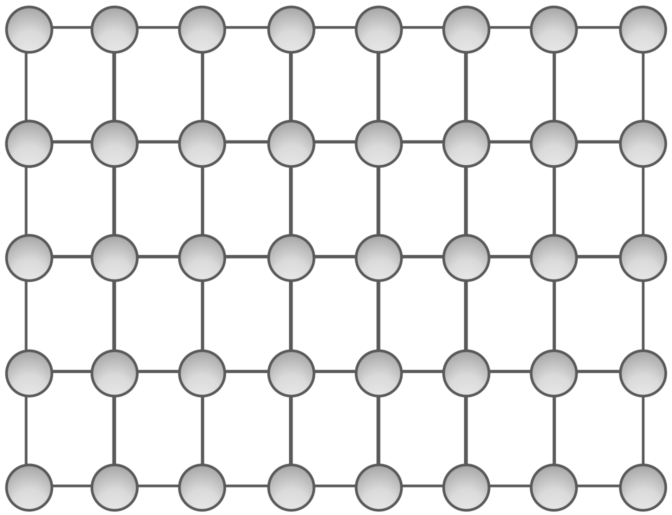


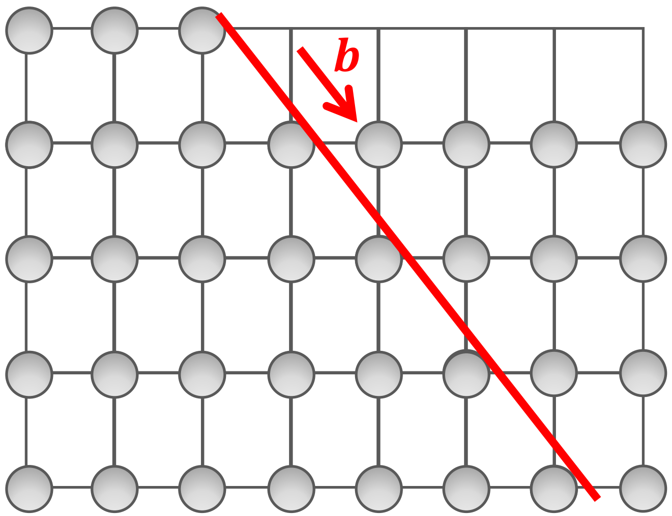
L. Priester, *Springer Science & Business Media.* (2012)
R. Genin, *PhD Defense* (2025)

Partial dislocations and stacking fault

- If $\boldsymbol{b}$ is a vector of the lattice

  $\Rightarrow$ **Perfect dislocation**





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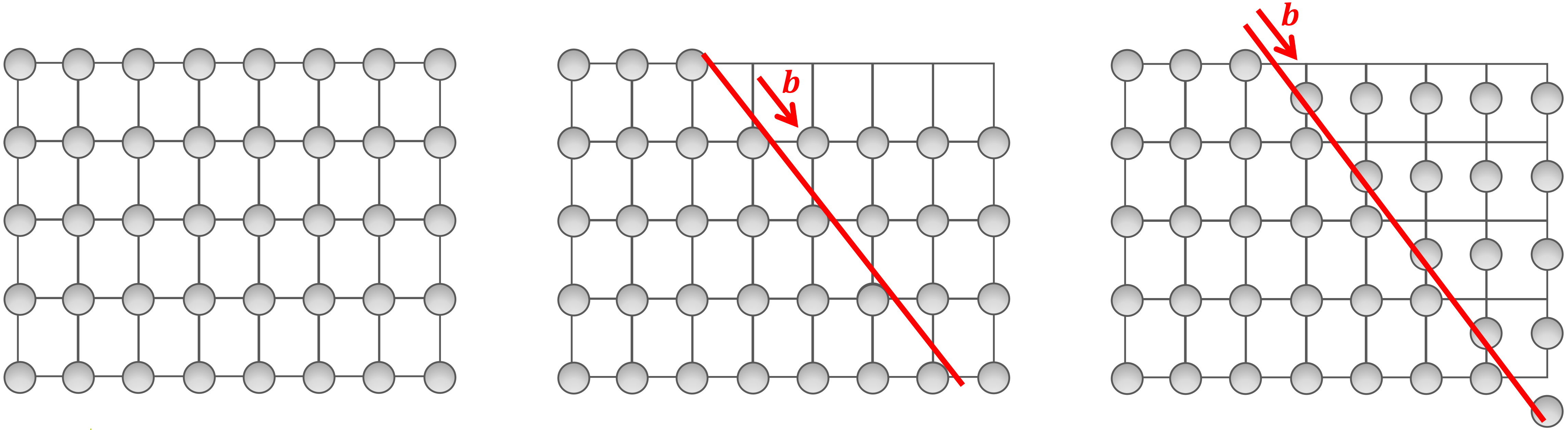

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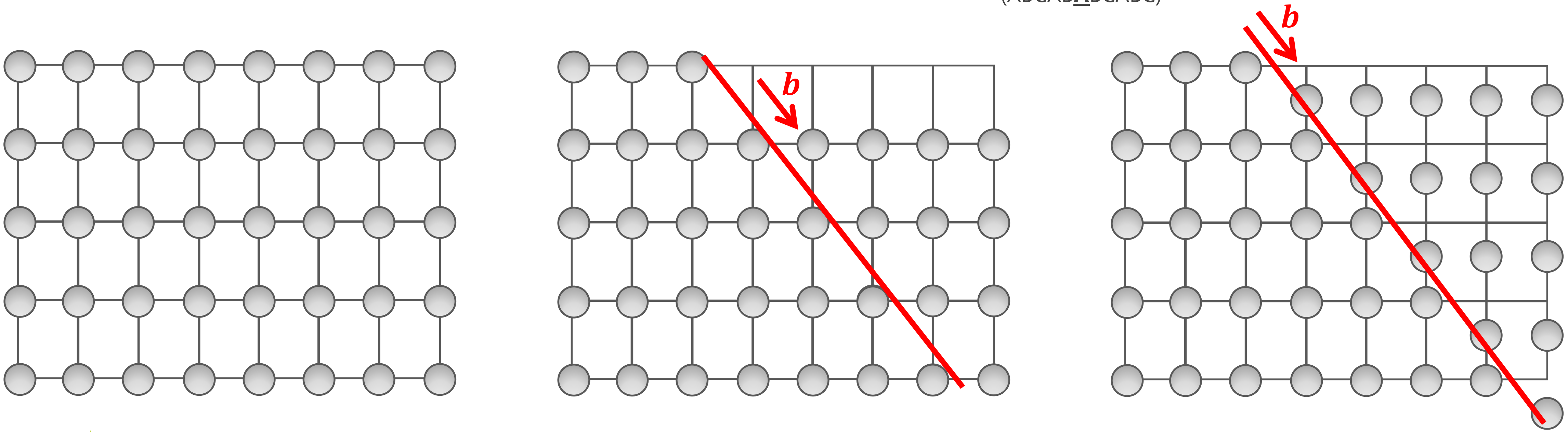
- If $\boldsymbol{b}$ is smaller than a vector of the lattice

  $\Rightarrow$ **Partial dislocation and stacking fault**

- Stacking faults
  - Planar defect where the normal stacking sequence of close-packed planes is interrupted.
  - Types:
    - Intrinsic stacking fault → missing plane in the sequence (ABCAB_ABC)
    - Extrinsic stacking fault → extra plane inserted. (ABCAB**A**BCABC)



Peierls stress and γ-surface

❖ Peierls stress

- **Definition:** minimum shear stress to move a dislocation across the periodic lattice potential.
- **Origin:** the dislocation core experiences the periodic γ-surface energy

$$\tau_P \approx CG\exp\left\{-\frac{2\pi w}{b}\right\}$$

(C: dimensionless constant; w: dislocation core width)

R. Peierls, Proc. Phys. Soc. 52, 34 (1940); .R.N. Nabarro, Proc. Phys. Soc. 59, 256 (1947)
K. Gouriet et al. *Philos Mag.*, (2015)

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❖ Effect on dissociation

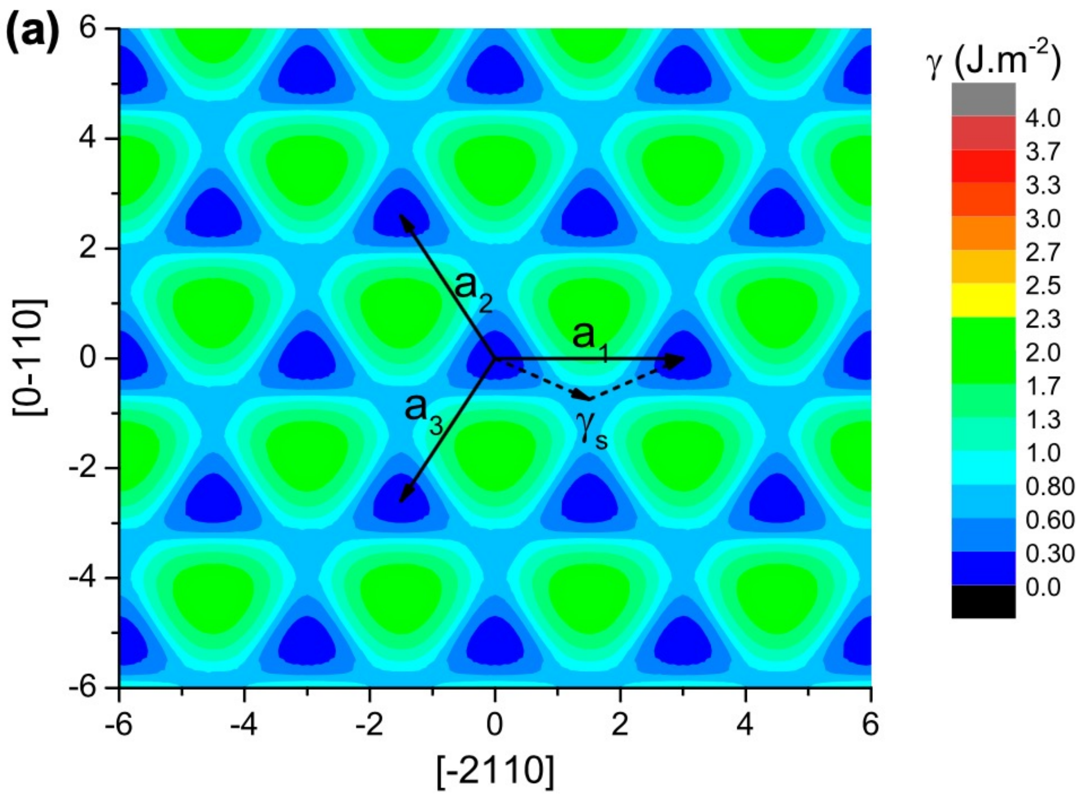
- Perfect dislocation splits into two partials.

$$\boldsymbol{b} \rightarrow \boldsymbol{p_1} + \boldsymbol{p_2} + SF$$

- A stacking fault forms between the partials (SF).
- Separation distance between partials:

$$d \approx \frac{Gb^2}{8\pi\gamma(1-\nu)}$$

- Effect of the stacking fault energy (γ) on τ_P:
  - ➢ Low γ → large separation, very low τ_P
  - ➢ High γ → small separation, higher τ_P



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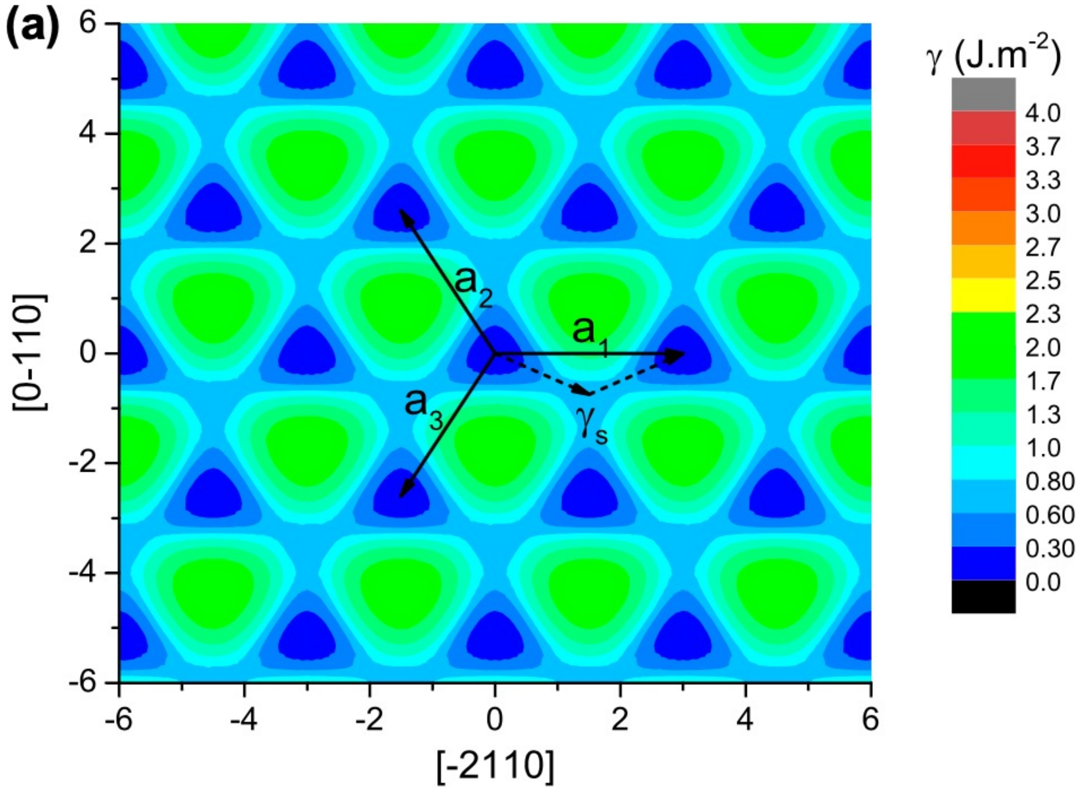
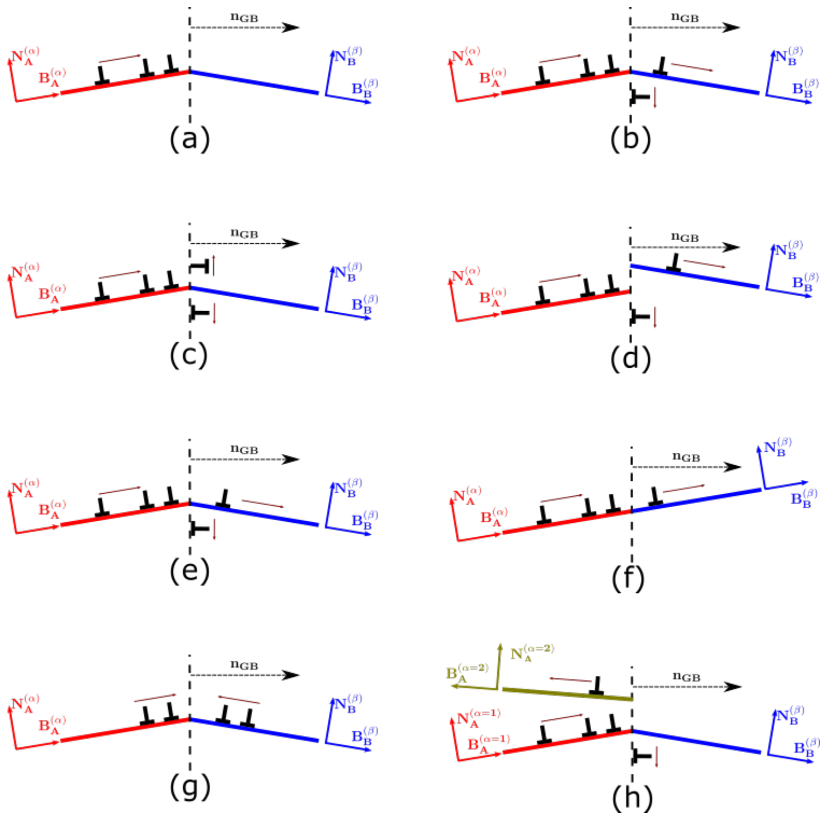


Dissociation into partials lowers the Peierls stress by effectively broadening the dislocation core.

K. Gouriet et al. *Philos Mag.*, (2015)

Dislocation/ grain boundary interactions



- **Blocking (pile-up)**
  - Dislocations accumulate at the GB.
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A. Guitton, *HDR, Université de Lorraine*, (2022)
.O. Hall, Proc. Phys. Soc. B 64, 747 (1951); .J. Petch, J. Iron Steel Inst. 174, 25 (1953)E. Bayersche et al. *J. Mater. Sci.* 51:2243–2258 (2016)

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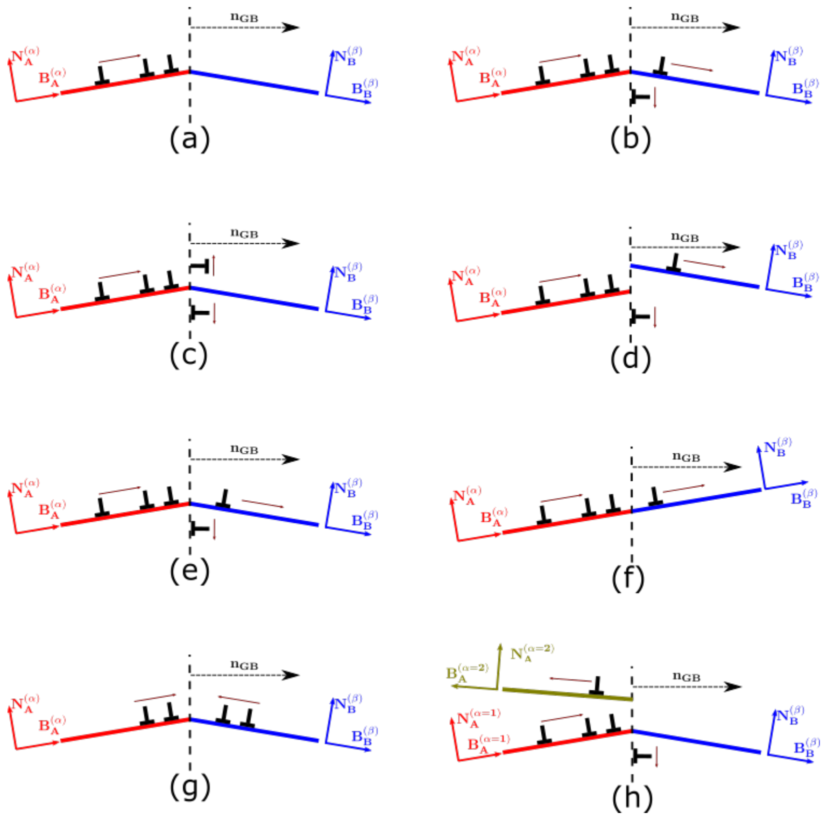

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  - Dislocations accumulate at the GB.
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- **Transmission across the GB**
  - Dislocation passes into the adjacent grain.
  - Governed by criteria:
    - Geometrical criterion:

$$LC_{\alpha\beta} = \left(N_\alpha^A \cdot N_\beta^B\right) \cdot \left(B_\alpha^A \cdot B_\beta^B\right) + \left(N_\alpha^A \cdot B_\beta^B\right) \cdot \left(N_\beta^B \cdot B_\alpha^A\right)$$

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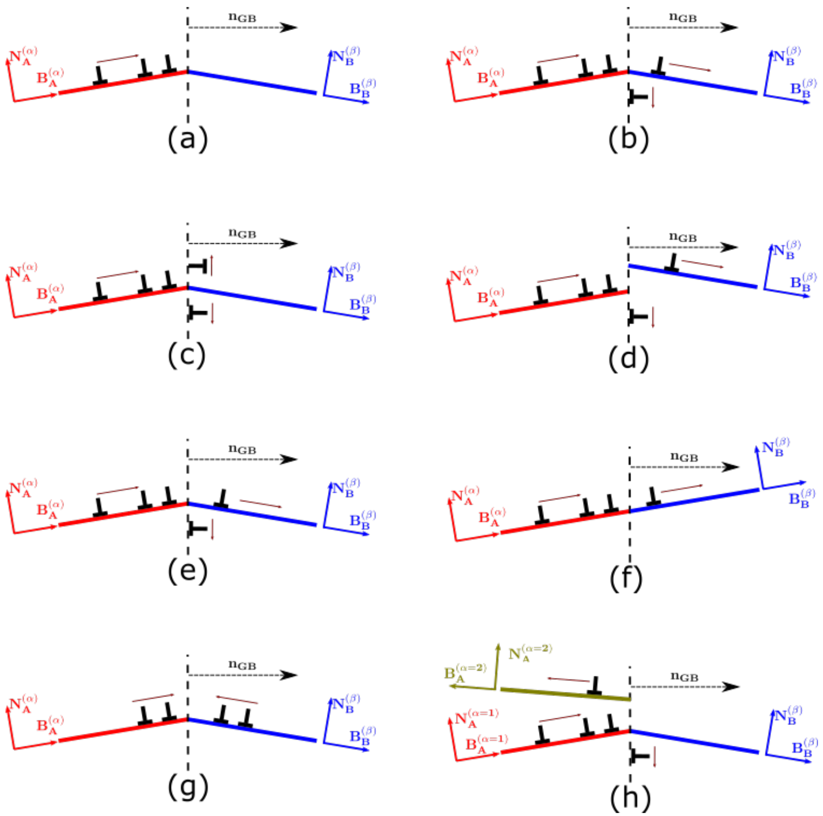

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  - Dislocation incorporated into the GB structure.
  - Alters GB energy and mobility.

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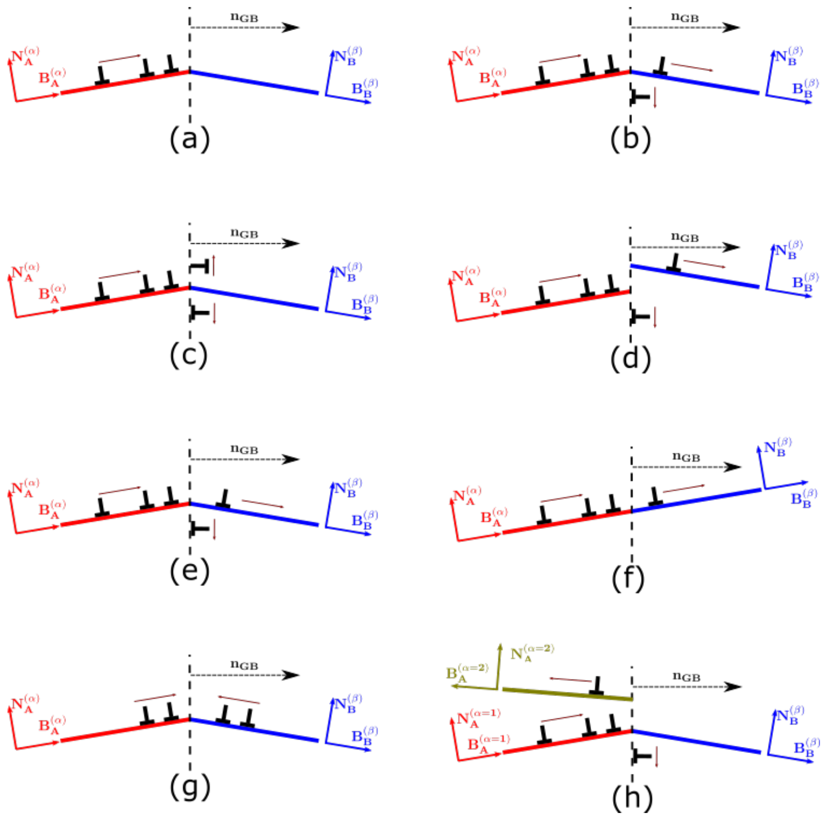

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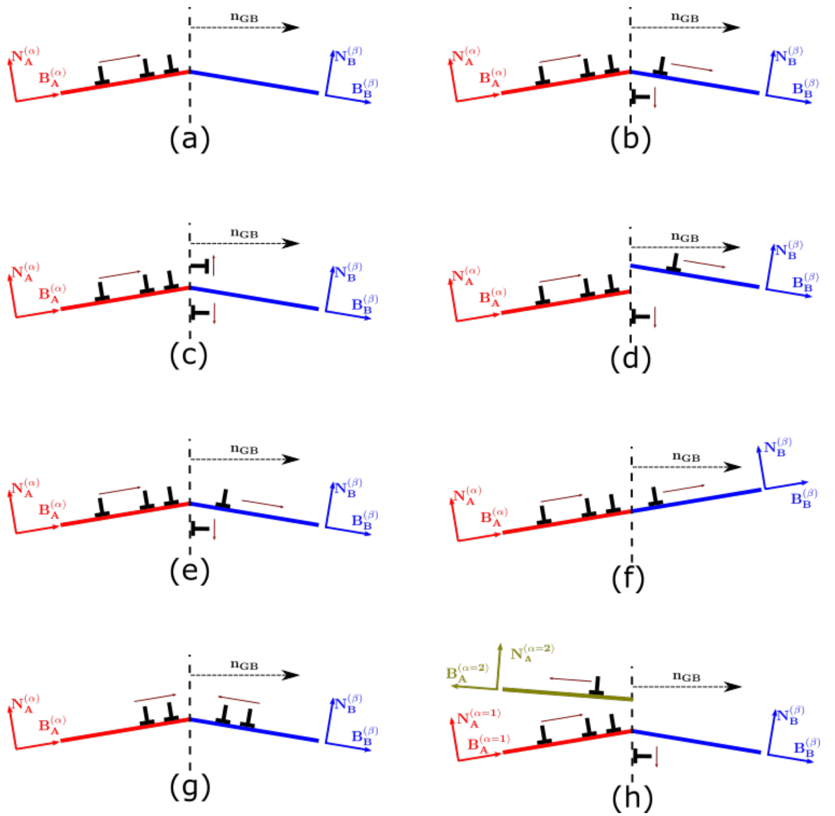

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  - Alters GB energy and mobility.
- **Emission / nucleation**
  - GB can act as a source of new dislocations in the neighboring grain.
- **Mechanical barrier effect**
  - Grain size controls strength → Hall–Petch relation:

$$\sigma_e = \sigma_0 + K d^{-\frac{1}{2}}$$

GBs are not passive walls; they block, transmit, absorb, and emit dislocations, ultimately shaping the strength of polycrystals.

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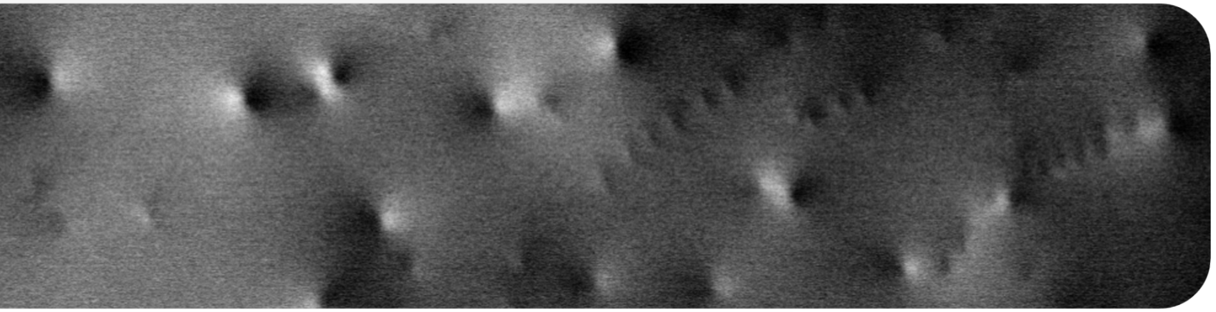
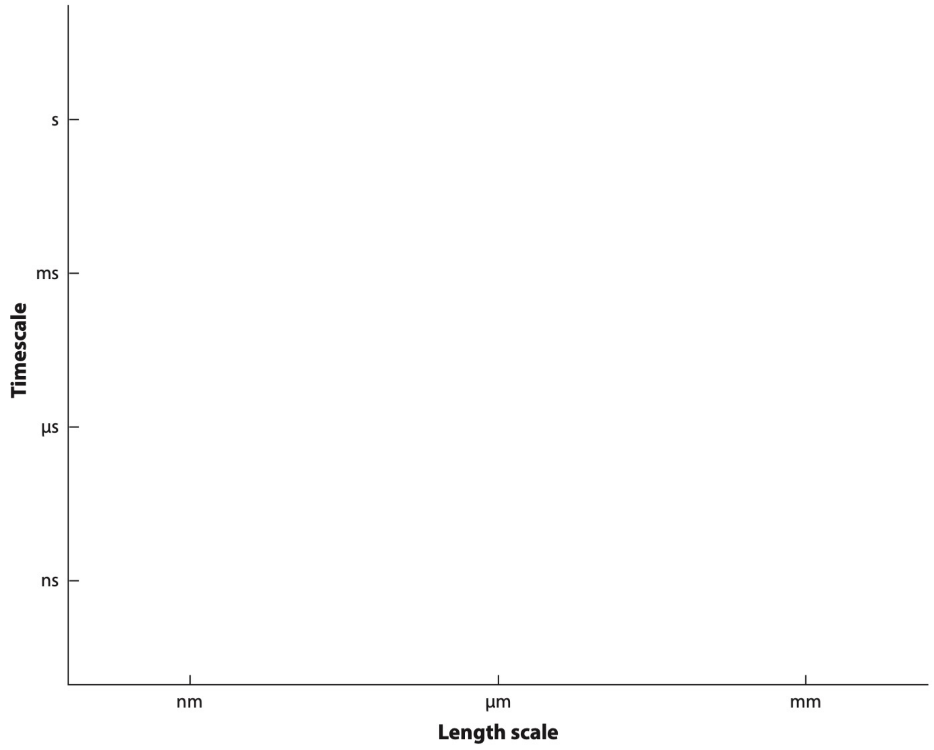


Modeling and simulation

Multiscale modeling of crystal plasticity

- Dislocation physics spans ~9 orders of magnitude in length (nm → mm) and ~12 orders of magnitude in time (ns → s).



N. Bertin, R.B. Sills, W. Cai, *Annu. Rev. Mater. Sci.* (2020)

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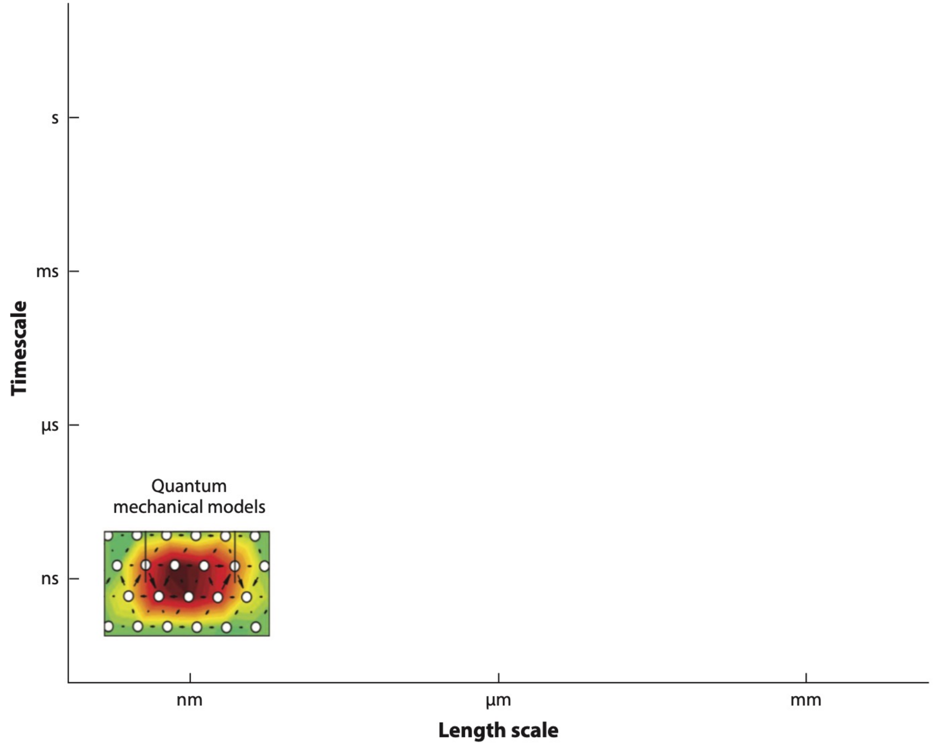

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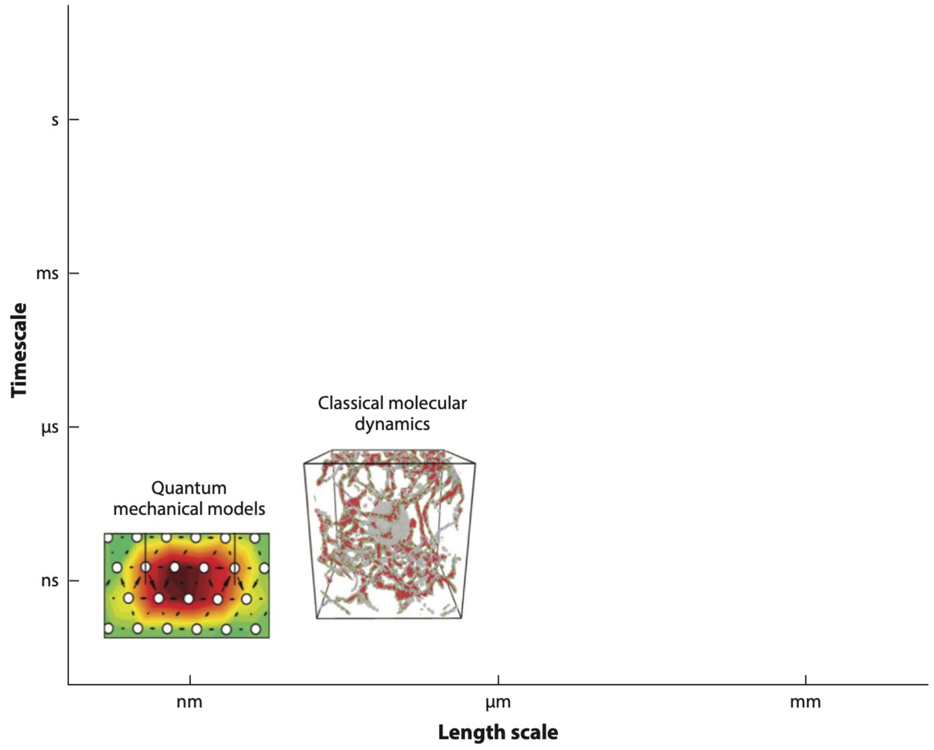

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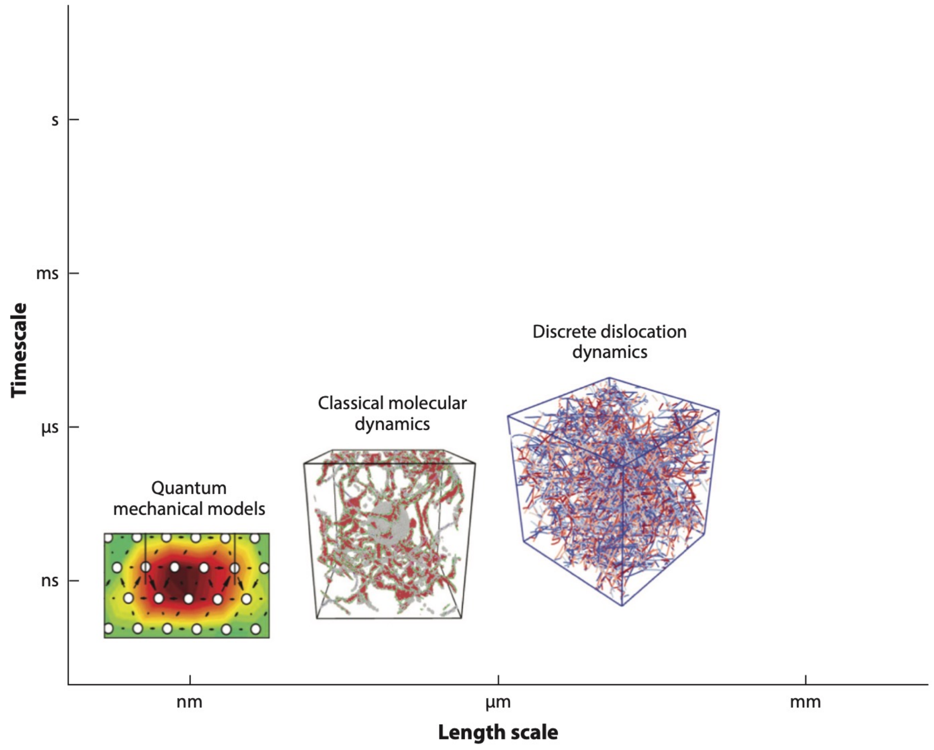
    - Discrete dislocation dynamics (DDD): forest hardening, pile-ups, Frank-Read sources (~µm, ~µs)



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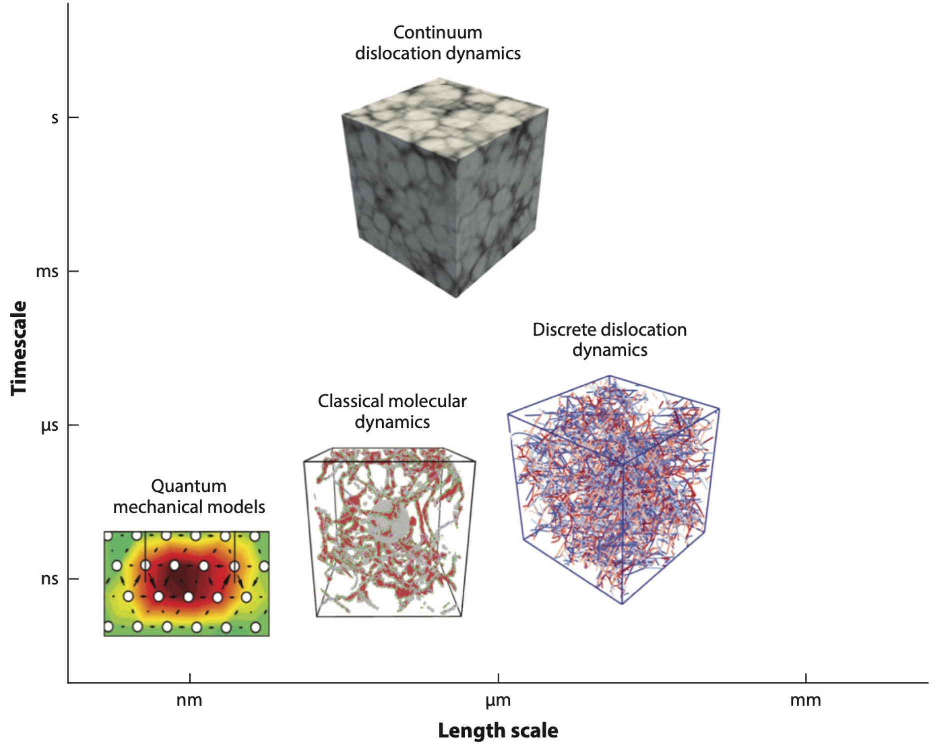

N. Bertin, R.B. Sills, W. Cai, *Annu. Rev. Mater. Sci*. (2020)

Multiscale modeling of crystal plasticity

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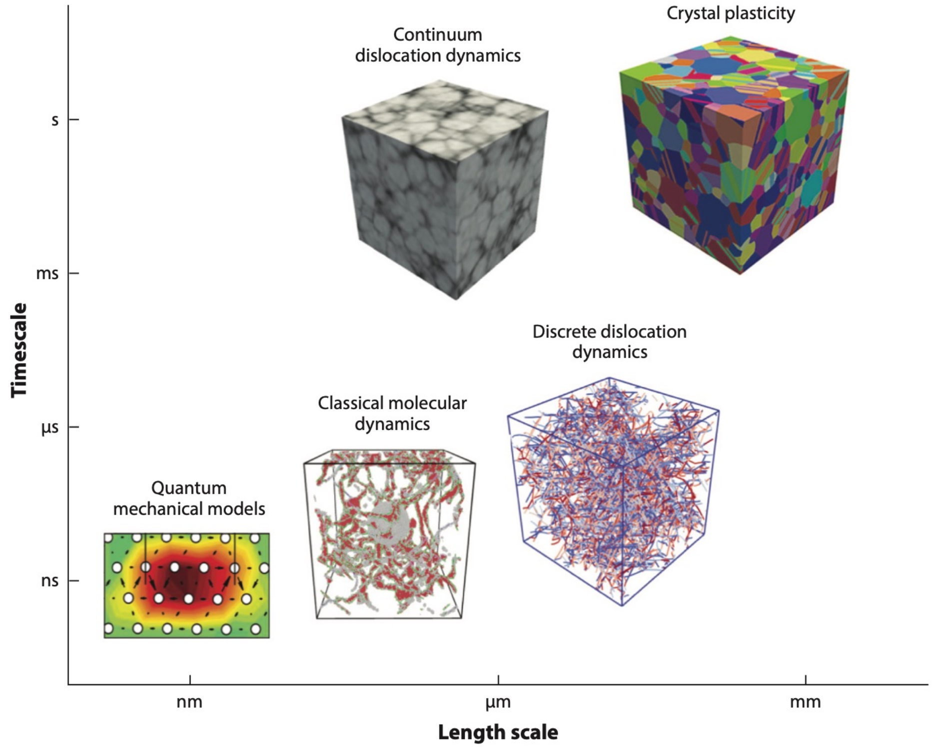

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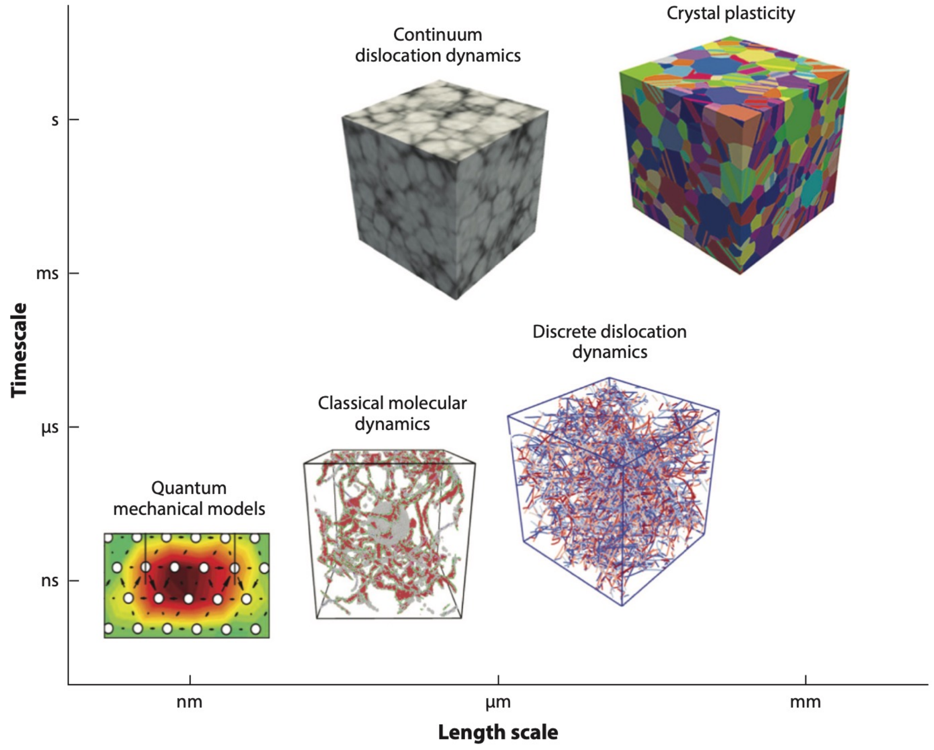

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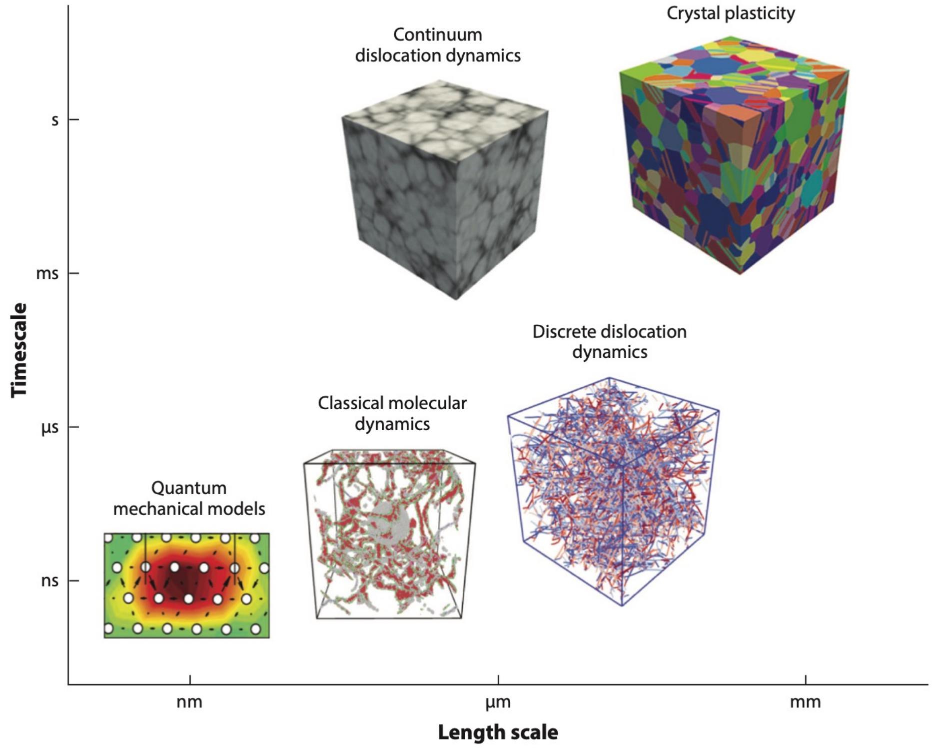

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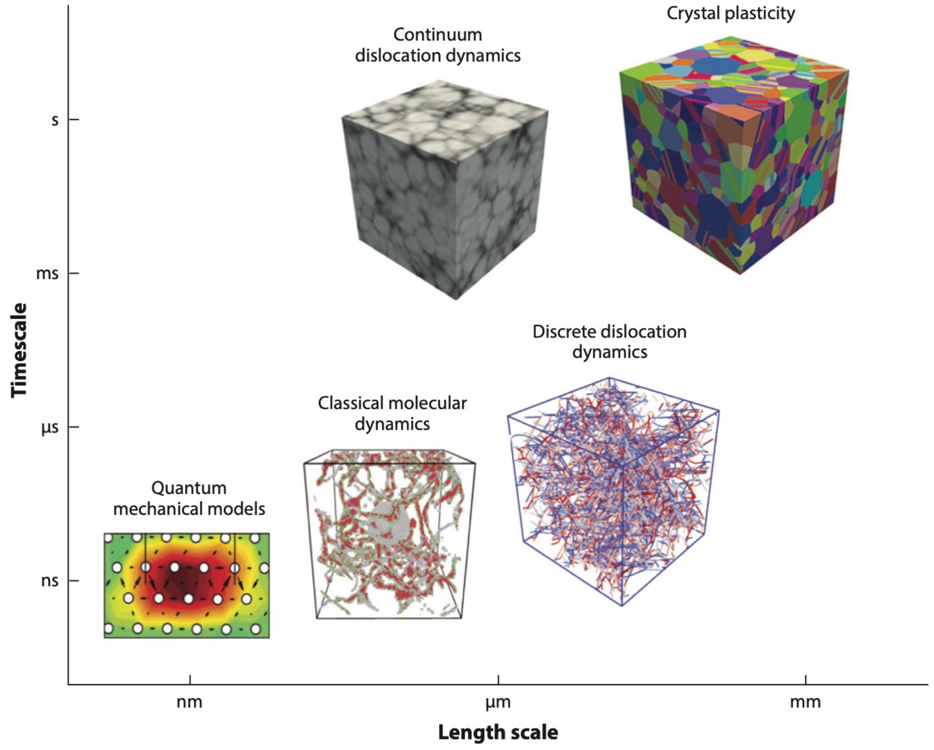

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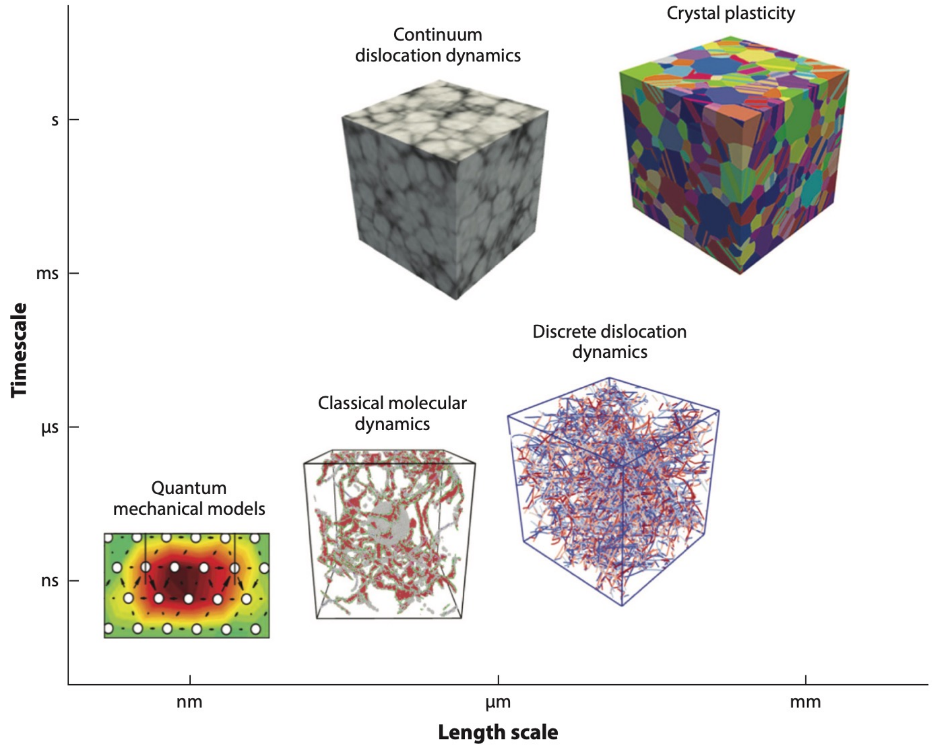

↳ Bridging these scales remains the central challenge of computational crystal plasticity.

N. Bertin, R.B. Sills, W. Cai, *Annu. Rev. Mater. Sci.* (2020)

Thanks for your listening!

If you need further information:

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LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX

UNIVERSITÉ DE LORRAINE

École Nationale d'Ingénieurs de Metz