DISLOCATIONS

- ☐ Edge dislocation
- ☐ Screw dislocation
- ☐ Dislocations in crystals

Further reading

Introduction to Dislocations
D. Hull and D.J. Bacon
Pergamon Press, Oxford (1984)

Advanced reading (comprehensive)

Theory of Dislocations
J. P. Hirth and J. Lothe
McGraw-Hill, New York (1968)

- As seen before dislocations are 1D (line) defects.
- The role of dislocations goes *far beyond* just ‘plasticity by slip’.
- They play an important role in a variety of deformation processes like
  - creep, fatigue and fracture.
- They can play a ‘constructive role’ in crystal growth.
- They can provide short circuit paths for diffusion (pipe diffusion).
- Understanding the importance of dislocations in material behaviour cannot be overstated
  → hence it is very important to thoroughly understand the structure and behaviour of dislocations.

Caution Note: In any chapter, amongst the first few pages (say 5 pages) there will be some ‘big picture’ overview information. This may lead to ‘overloading’ and readers who find this ‘uncomfortable’ may skip particular slides in the first reading and come back to them later.

Dislocations

- ☐ The importance of understanding dislocations and their effect on material behaviour cannot be overstated.
- ☐ Though often the importance of dislocations in the context of plastic deformation* by slip** is highlighted; its role in materials science is far greater. (The next slide shows some of these roles).
- ☐ In this context it is important to note that even in crystalline materials there are alternate mechanisms of plastic deformation (as shown in an upcoming slide)
  → Twinning*** also being an important one.
- ☐ The important thing to be kept in mind is the role of dislocations in *weakening* crystals (taken up after the above mentioned slides).

* Plastic deformation
→ permanent deformation that remains when all external loading/constraints are removed

** Slip → is a technical term referring to plastic deformation caused by dislocations
◘ the 'first step' of the process is the small surface step which is created when a dislocation leaves a crystal

*** Twinning
→ process by which one part of the crystal gets related to another part, by a symmetry operator (usually a mirror); which is not a symmetry operator of the crystal.

Path to understanding the role of Dislocations in material behaviour

Consider a dislocation in an infinite crystal

Stress fields, strain fields, energy etc.

$E_d, \sigma_{xx}, \sigma_{yy}, \tau_{xy}, \varepsilon_{xx}, \varepsilon_{xy} \ldots$

Take into account finite crystal effects

Free surfaces, grain boundaries etc.

Consider interaction of dislocations with other defects

Interactions with other dislocations, interstitials, precipitates etc.

Collective behaviour and effects of external constrains

*Long range interactions & collective behaviour & external constraints***

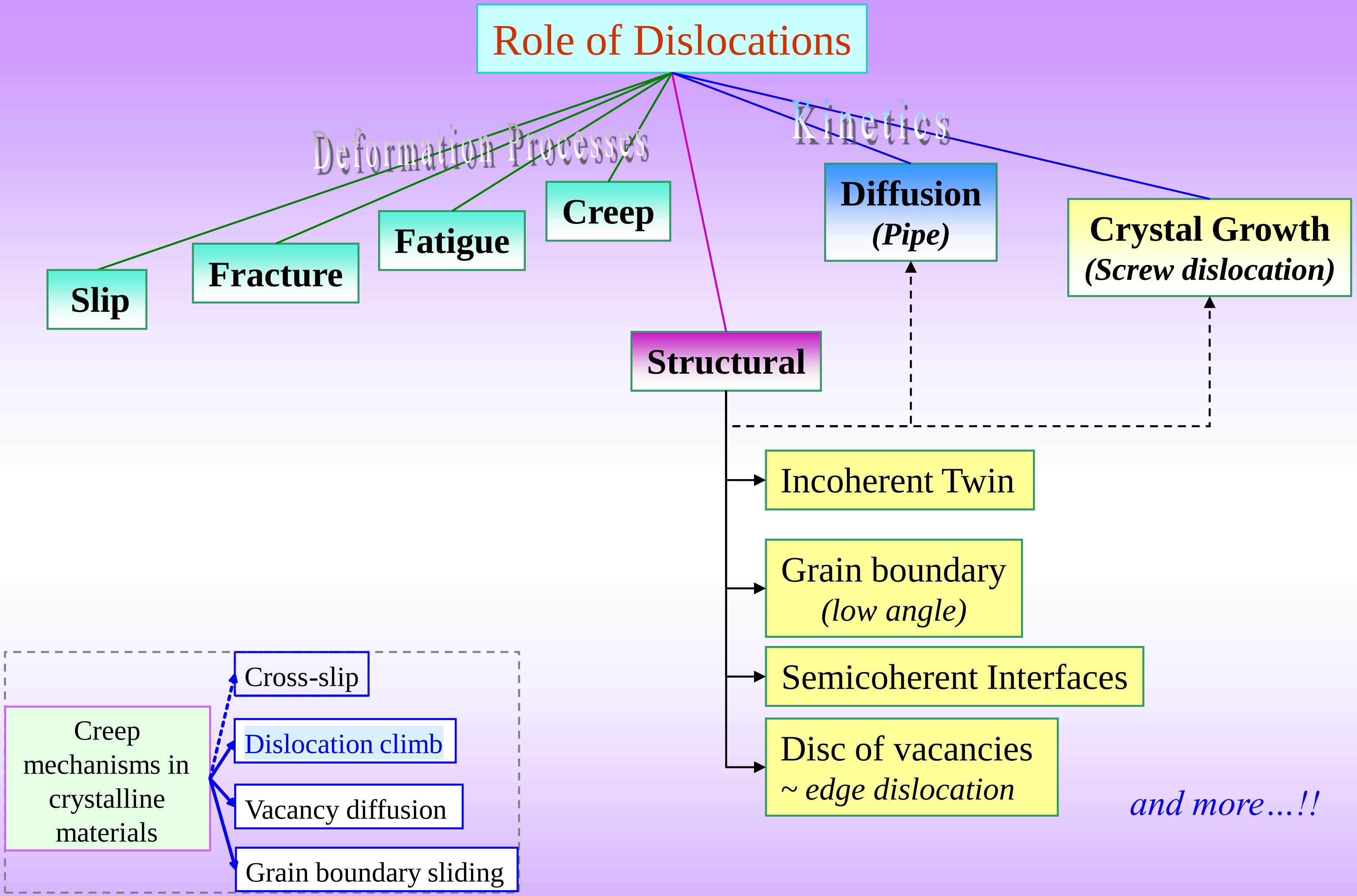
Though these points are written as a sequence many of these have to be considered in parallel

- Static and dynamic effects and interactions should be included*

* Dynamic effects include:

- *(Altered) Stress field of a moving dislocation*
- *Interactions evolving in time*

Note: the above step by step method may often not be the most practical one and there are techniques which take up collective behaviour directly



Role of Dislocations

Deformation Processes

Slip

Fracture

Fatigue

Creep

Kinetics

Diffusion
(Pipe)

Crystal Growth
(Screw dislocation)

Structural

Incoherent Twin

Grain boundary
(low angle)

Semicoherent Interfaces

Disc of vacancies
~ edge dislocation

and more…!!

Creep mechanisms in crystalline materials

Cross-slip

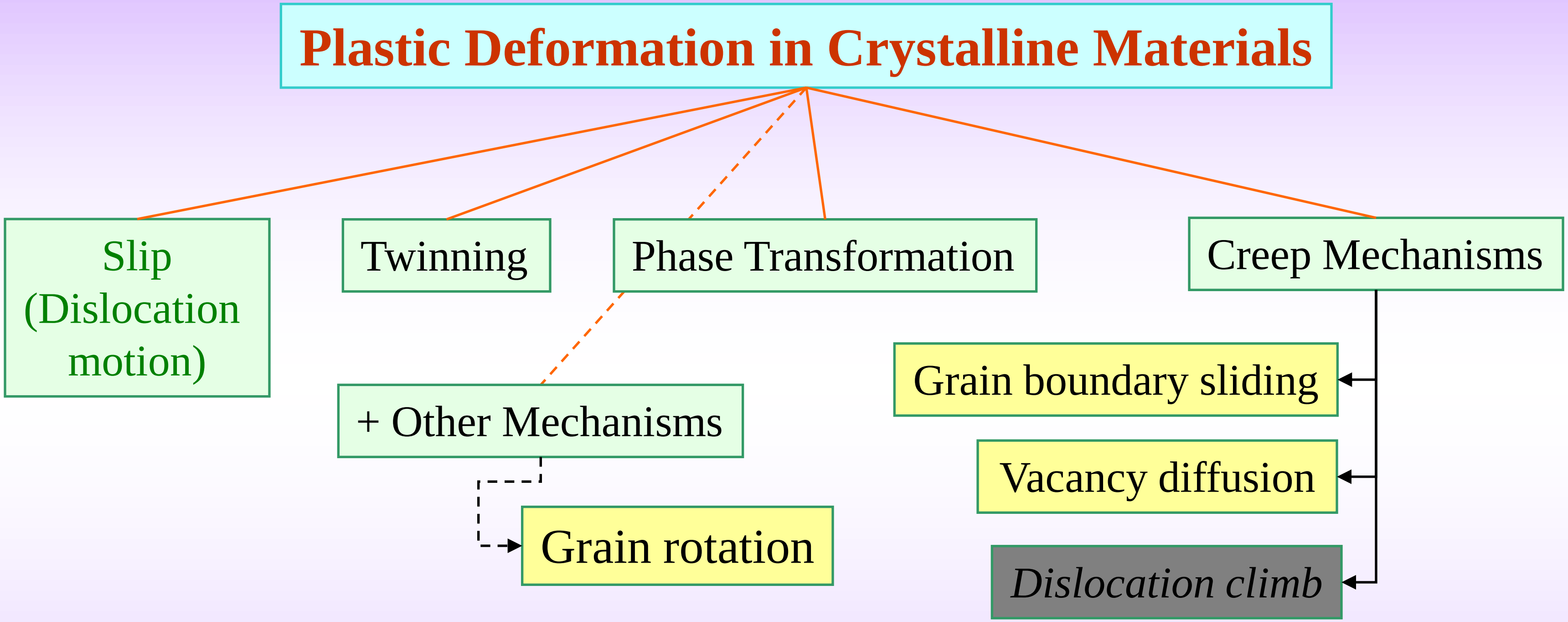
Dislocation climb

Vacancy diffusion

Grain boundary sliding

Note: Structural dislocations can also play a role in deformation and kinetic processes

Though plasticity by slip is the most important mechanism of plastic deformation, there are other mechanisms as well *(plastic deformation here means permanent deformation in the absence of external constraints)*:



Plastic Deformation in Crystalline Materials

Slip (Dislocation motion)

Twinning

Phase Transformation

Creep Mechanisms

+ Other Mechanisms

Grain rotation

Grain boundary sliding

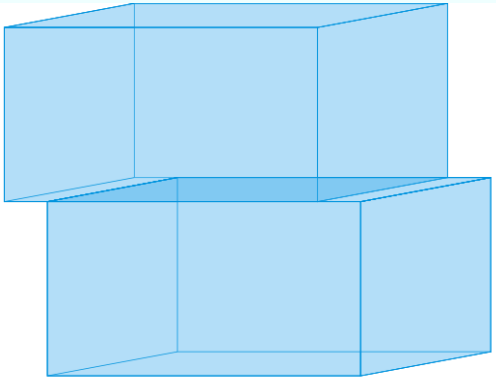
Vacancy diffusion

Dislocation climb

Note: Plastic deformation in amorphous materials occur by other mechanisms including flow (~viscous fluid) and shear banding

Weakening of a crystal by the presence of dislocations

- To cause plastic deformation by shear (*all of plastic deformation by slip require shear stresses at the microscopic scale**) one can visualize a plane of atoms sliding past another (fig below**)
- This requires stresses of the order of GPa (calculation in the next slide)
- But typically crystals yield at stresses ~MPa
- ⇒ This implies that 'something' must be weakening them drastically
- It was postulated in 1930s[#] and confirmed by TEM observations in 1950s, that the agent responsible for this weakening are dislocations



Shearing of a whole part of a crystal with respect to another

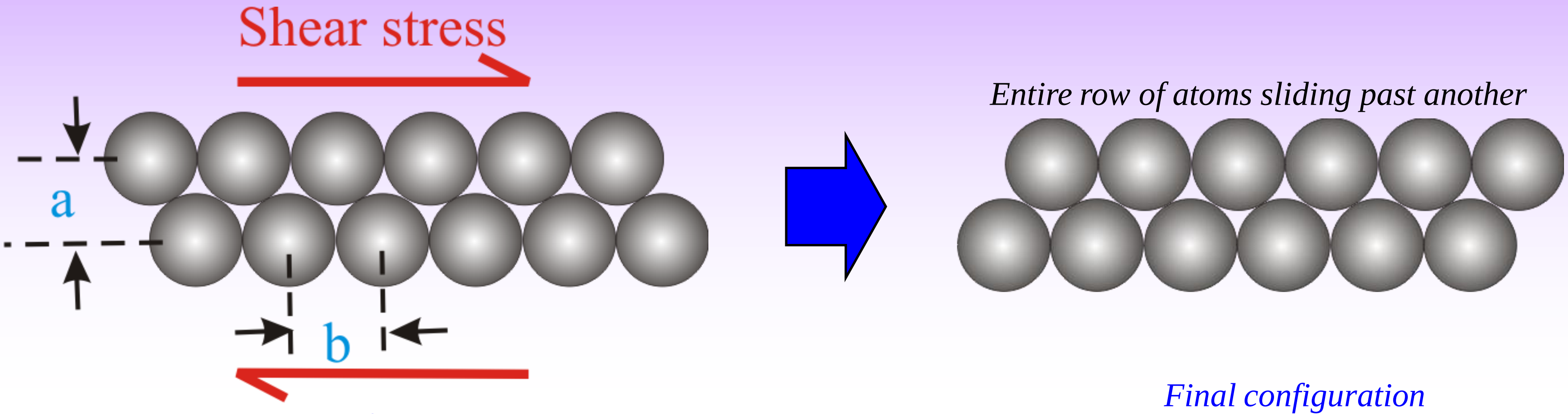
* Even if one does a pure uniaxial tension test with the tension axis along the z- axis, except for the horizontal and the vertical planes all other planes 'feel' shear stresses on them

** As to how this atomic slip is connected to macroscopic permanent shape changes will be considered later

[#] By Taylor, Orowan and Polyani

Plastic deformation of a crystal by shear

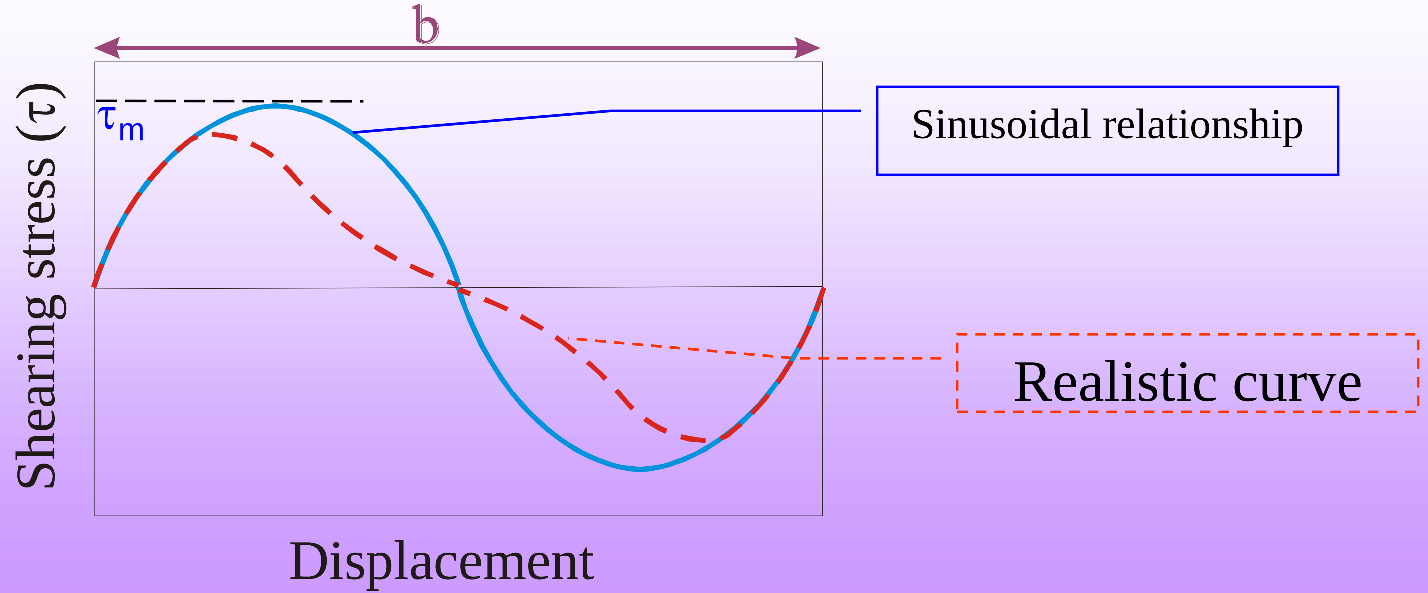
Let us consider the shearing of an entire plane of atoms over one another
→ causing plastic deformation by shear



Starting configuration

Final configuration

The shear stress displacement curve looks as shown in the diagram on the right



As a first approximation the stress-displacement curve can be written as

$$\tau = \tau_m Sin\left(\frac{2\pi x}{b}\right)$$

At small values of displacement Hooke's law should apply

$$\tau = G\gamma = G\frac{x}{a}$$

$\Rightarrow$ For small values of x/b

$$\tau = \tau_m\left(\frac{2\pi x}{b}\right)$$

$$G\frac{x}{a} = \tau_m\left(\frac{2\pi x}{b}\right)$$

Hence the maximum shear stress at which slip should occur

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

If b ~ a

$$\tau_m \sim \frac{G}{2\pi}$$

$$\boxed{\tau_m \sim \frac{G}{2\pi}}$$

- The theoretical shear stress will be in the range 3 – 30 **GPa**

- The shear modulus of metals is in the range 20 – 150 GPa

$$\tau_m \sim \frac{G}{2\pi}$$

- The theoretical shear stress will be in the range 3 – 30 **G**Pa

- Actual shear stress is 0.5 – 10 **M**Pa *(experimentally determined)*
- I.e. (Shear stress)$_{\text{theoretical}}$ > 100 × (Shear stress)$_{\text{experimental}}$!!!!

DISLOCATIONS

Dislocations severely weaken the crystal

Whiskers of metals *(single crystal free of dislocations, Radius ~ 10^{-6}m) can approach theoretical shear strengths*

Whiskers of Sn can have a yield strength in shear ~10^{-2} G *(10^3 times bulk Sn)*

- ❑ As we have seen before dislocations can play diverse kinds of role in materials structure and its behaviour
- ❑ Perhaps the most important of these is the weakening of the crystal in the presence of dislocations
- ❑ From a slide before we know the path to understanding the role of dislocations in materials involves their interactions with other dislocations and defects present in the material (and the evolution of the system with time/deformation)
  → *This path will include the 'hardening' of the crystal, i.e strengthening of the weakened crystal*
  → *In this context it will be noted that many dislocations will interact with each other and there will be a strengthening effect*

Dislocations: path breaking ideas

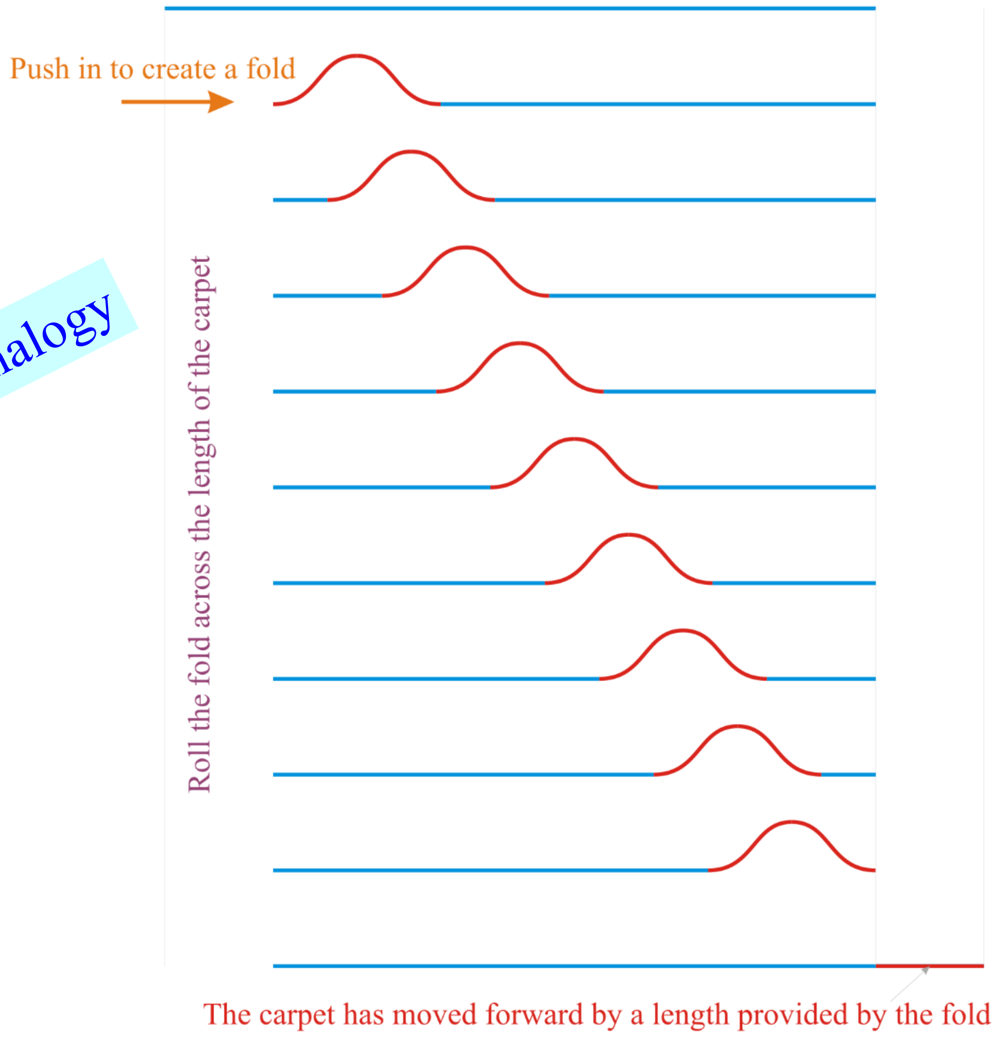
- ▪ As late as 1930 the reason behind this weakening of the crystal was not clear *(to imagine that this was the post Relativity, post Quantum Mechanics era, wherein deep questions regarding the larger scale of the universe and the sub-atomic realms were being conquered → but why a rod of copper can be bent easily was not known!)*
- ▪ Taylor, Orowan and Polanyi (independently) postulated the presence of dislocations as a mechanism leading to the weakening of the crystal
- ▪ The continuum construction of a dislocation (and other defects) was proposed by Volterra in 1905.
- ▪ The presence of dislocations was Electron microscopically confirmed in the 1950s

- o ◘ 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.
- o Vito Volterra, 1905.

- The analogy usually given to understand the role of dislocations in weakening a crystal is the one of ‘pulling a carpet’.
- If one tries to pull an entire carpet (a long and wide one), by sliding it against the floor, the effort required is large.
- However, if a ‘bump’ is made in the carpet (as in the figure in the following slide) and this bump is moved across the length of the carpet, then the carpet moves forward by a small distance (as provided by the bump).

- The force required to move the bump will be considerably small as compared to the force required to pull the entire carpet.
- By creating and moving a series of bumps successively the carpet can be moved forward ‘bit by bit’. *(Graphic on next slide).*

The ‘carpet-pulling’ analogy



The Volterra Dislocation

Continuum description of a dislocation

- The continuum* concept of a dislocation (and other defects) was proposed by Vito Volterra in 1905.
- His ideas and calculations based on his ideas predate their application to crystals. However, continuum calculations based on Volterra's idea are used even today to understand the behaviour of dislocations in crystals.
- Continuum calculations of stress fields, displacement fields etc. related to dislocations are found to be valid to within a few atomic spacing (i.e. the continuum description fails only within about 5 atomic diameters/Burgers vector).
- In this chapter the stress fields of dislocations shown are based on elastic continuum theories.**

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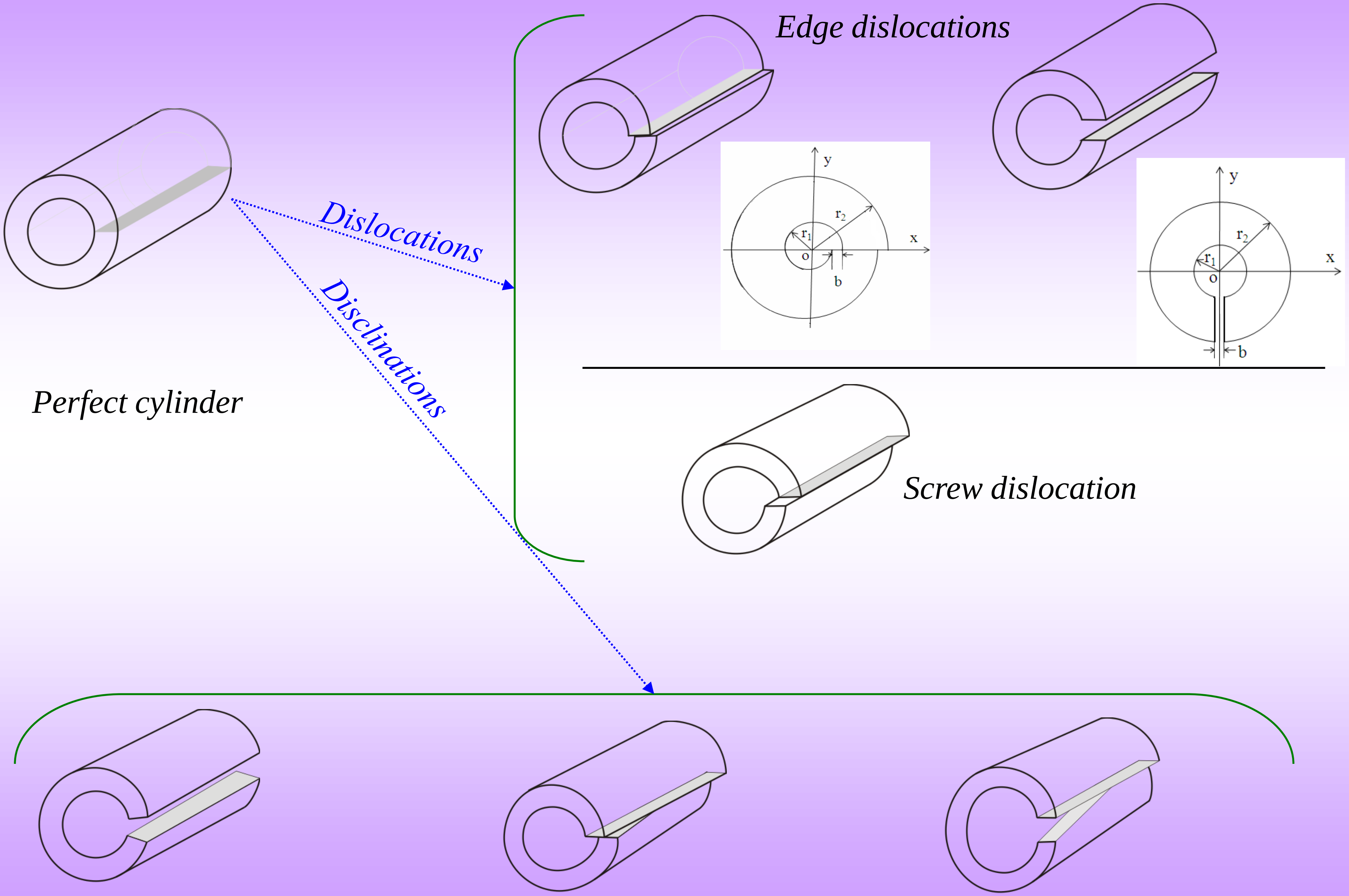
* Continuum implies that we are not 'worried' about atoms! *(Antonym → Discretum).*

** This is a 'strange' aspect: we have used elasticity theory to calculate the stress fields of the very (most important) agent responsible for plastic deformation

Deformations of a hollow cylinder showing the formation of various defects (Volterra constructions)



Perfect cylinder

Dislocations

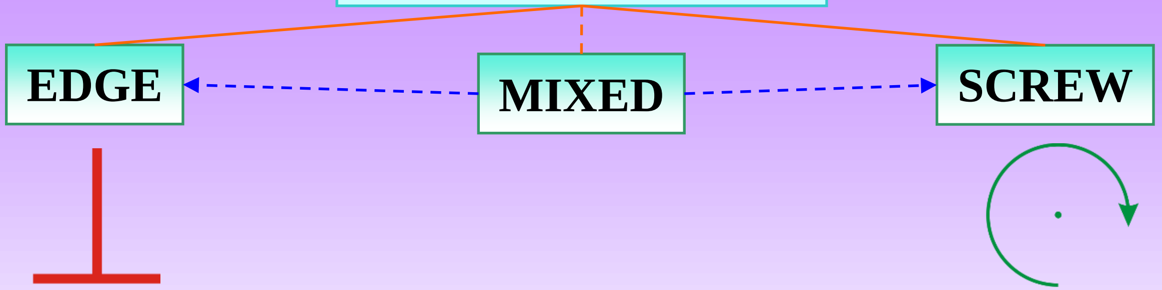
Disclinations

Edge dislocations

Screw dislocation

Disclinations

DISLOCATIONS

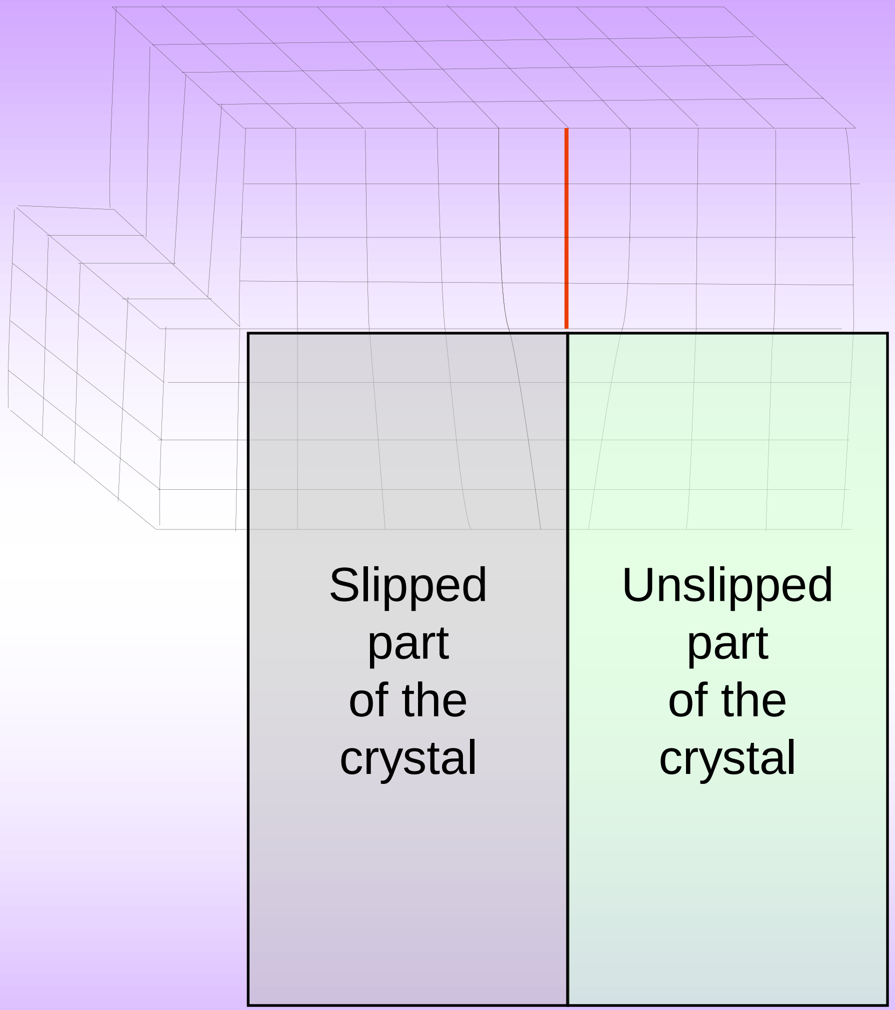


- If one looks at a sample of Aluminum under a TEM, one usually finds curved dislocation lines ⇒ Usually dislocations have a mixed character and *Edge* and *Screw* dislocations are the *ideal extremes*.
- Not only this, the character of the dislocation (i.e the percentage of screw and percentage of edge character) will change from position to position along the dislocation line.
- However, under special circumstances Pure Edge, Pure Screw or a Mixed Dislocation with a fixed percentage of edge character can form.

  (e.g. in GeSi epitaxial films on Si substrate 60° misfit dislocations form- i.e. the dislocation lines are straight with the angle between ***b*** *and* ***t*** *being 60°)*

  → more about these aspects will be considered later
- The edge dislocation is easier to visualize and hence many of the concepts regarding dislocations will be illustrated using the example of the pure edge dislocation.

TEM micrograph showing dislocation lines



Slipped part of the crystal

Unslipped part of the crystal

Dislocation can be considered as a boundary between the slipped and the unslipped parts of the crystal lying over a slip plane*

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* *this is just a way of visualization and often the slipped and unslipped regions may not be distinguished*

A dislocation has associated with it two vectors:

$\vec{t} \rightarrow$ *A unit tangent vector along the dislocation line*

$\vec{b} \rightarrow$ *The Burgers vector*

- The Burgers vector is like the *'SOUL of a dislocation'*. It 'can be defined' even if there is no dislocation in the crystal (it is the shortest lattice translation vector for a full/perfect dislocation), it defines every aspect of the dislocation (its stress fields, energy, etc.) and expresses itself even in the 'death' of the dislocation (i.e. when the dislocation leaves the crystal and creates a step of height 'b').
- Burgers vector of a perfect dislocation is the shortest translation vector (for a full/perfect dislocation) and can be determined by the Burgers circuit (coming up).
- Hence, Burgers vector is an invariant for a crystal, while the line vector is not. If one looks at a transmission electron micrograph showing a dislocation line in Aluminium, it will not be straight– i.e. the line vector is not fixed (usually*).

TEM micrograph showing dislocation lines

Dislocation lines

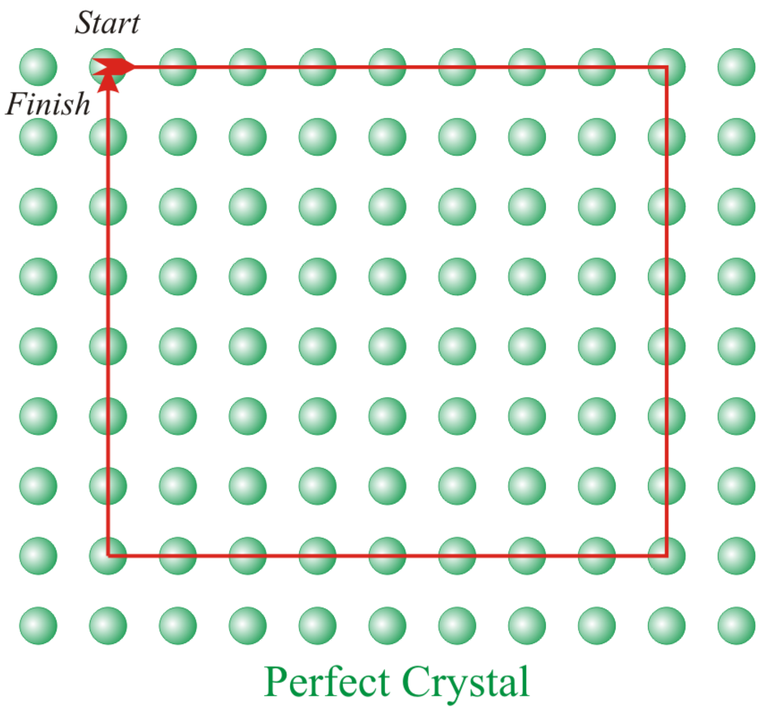
** In special cases we might have straight dislocation lines.*

Burgers Vector

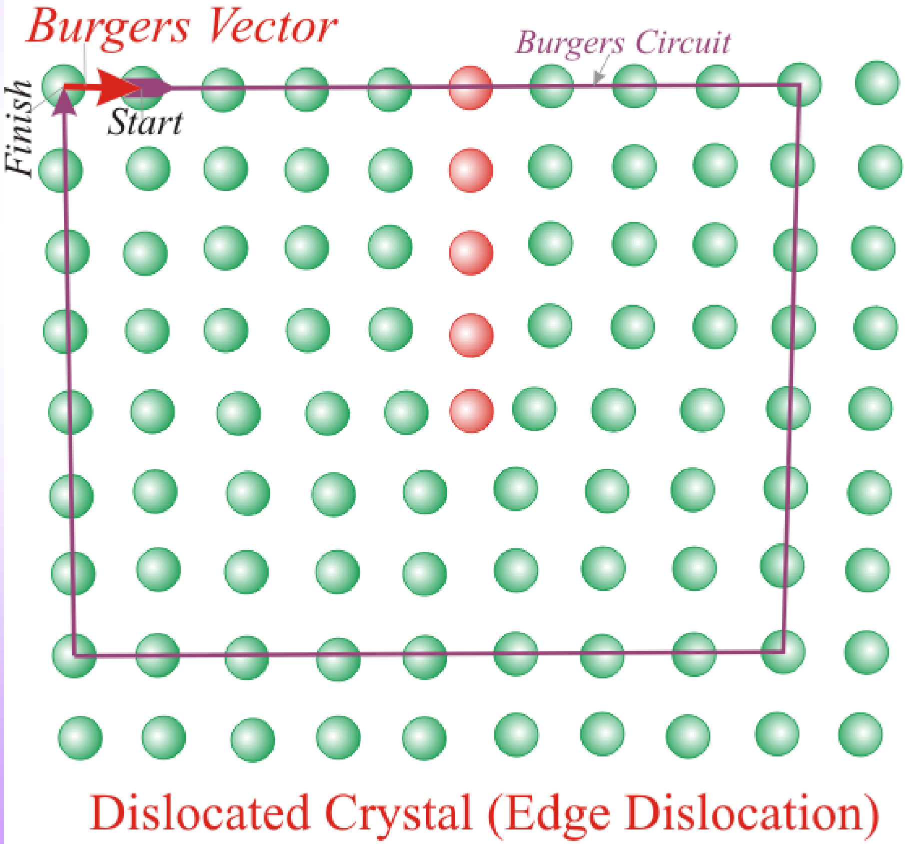
Edge dislocation

Determination of Burgers vector in a dislocated crystal using Right Hand Finish to Start Rule (RHFS)

- In a perfect crystal make a circuit (e.g. as in the figure shown: 8 atomic steps to right, 7 down, 8 left & 7 up). The circuit is *Right Handed*.
- Follow the same steps in the dislocated crystal. The 'missing link' (using some convention like RHFS) is the Burgers vector.
- 'Burgers circuit' and RHFS convention can be applied to both edge and screw dislocations.



Perfect Crystal



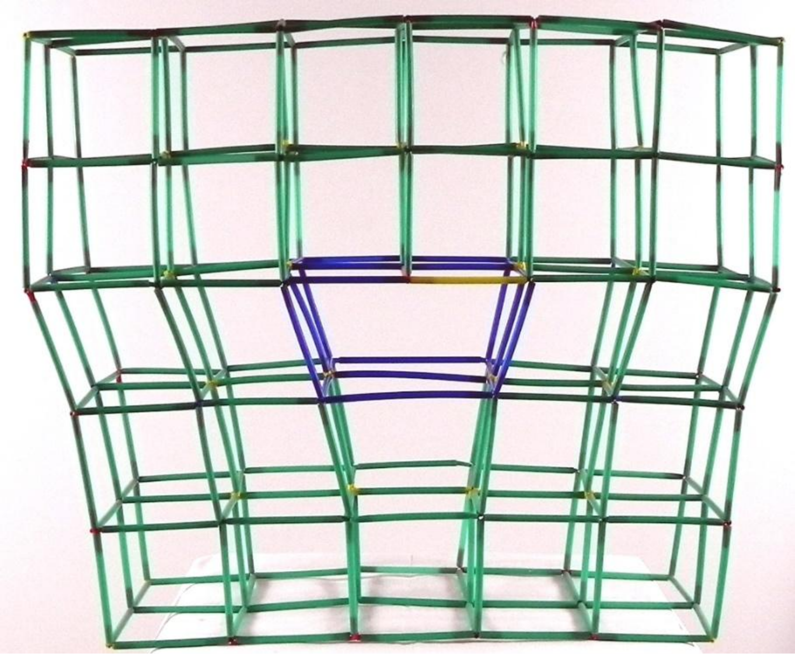
Dislocated Crystal (Edge Dislocation)

RHFS:
Right Hand Finish to Start convention

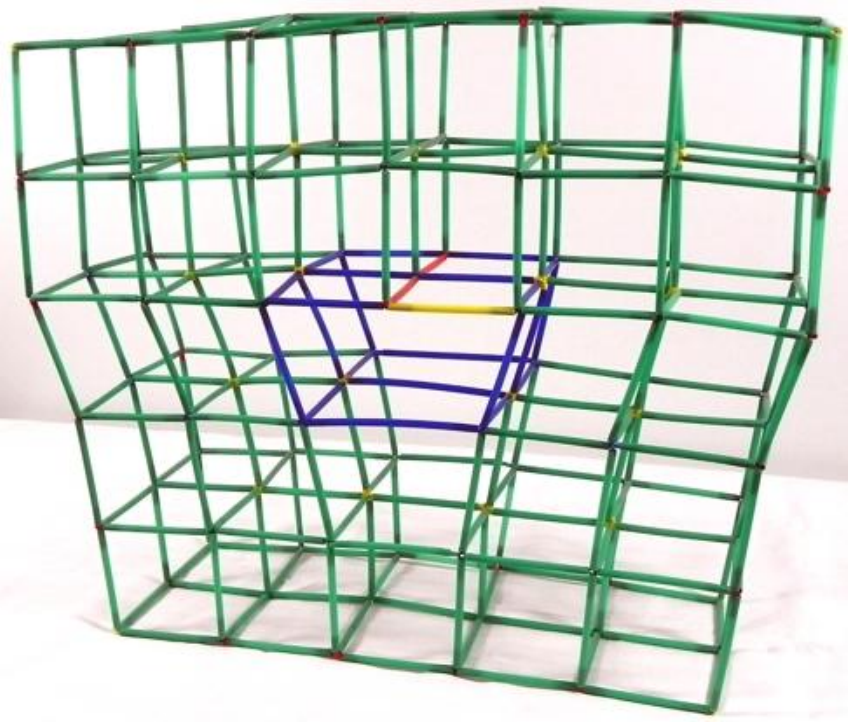
Note: the circuit has to be drawn 'far' away from the dislocation line

Some models of Edge Dislocation

Video: Edge Dislocation

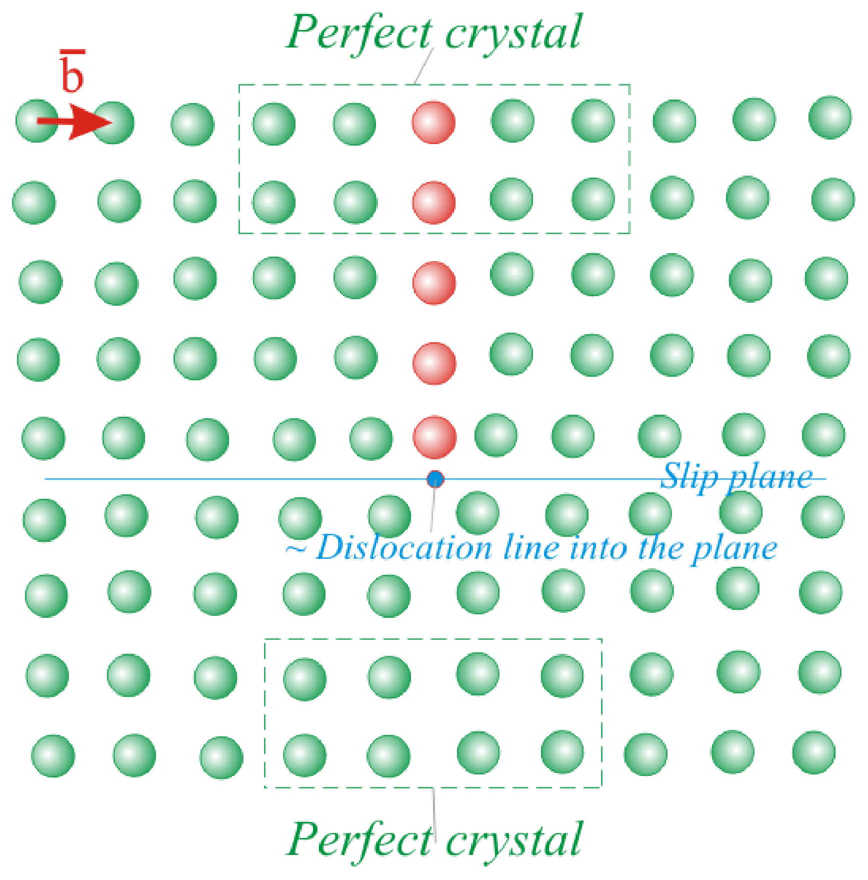


Model using magnetic balls
(not that accurate!)



Understanding the Edge dislocation

- ☐ The edge dislocation is NOT the ‘extra half-plane’, it is *neither* the ‘missing half-plane’ → it is the line between the ‘extra’ and the ‘missing’ half-planes.
- ☐ The regions far away from the dislocation line are perfect → all the ‘deformation’ is concentrated around the dislocation line.
- ☐ However, the stress field of the dislocation has a ‘long range’.

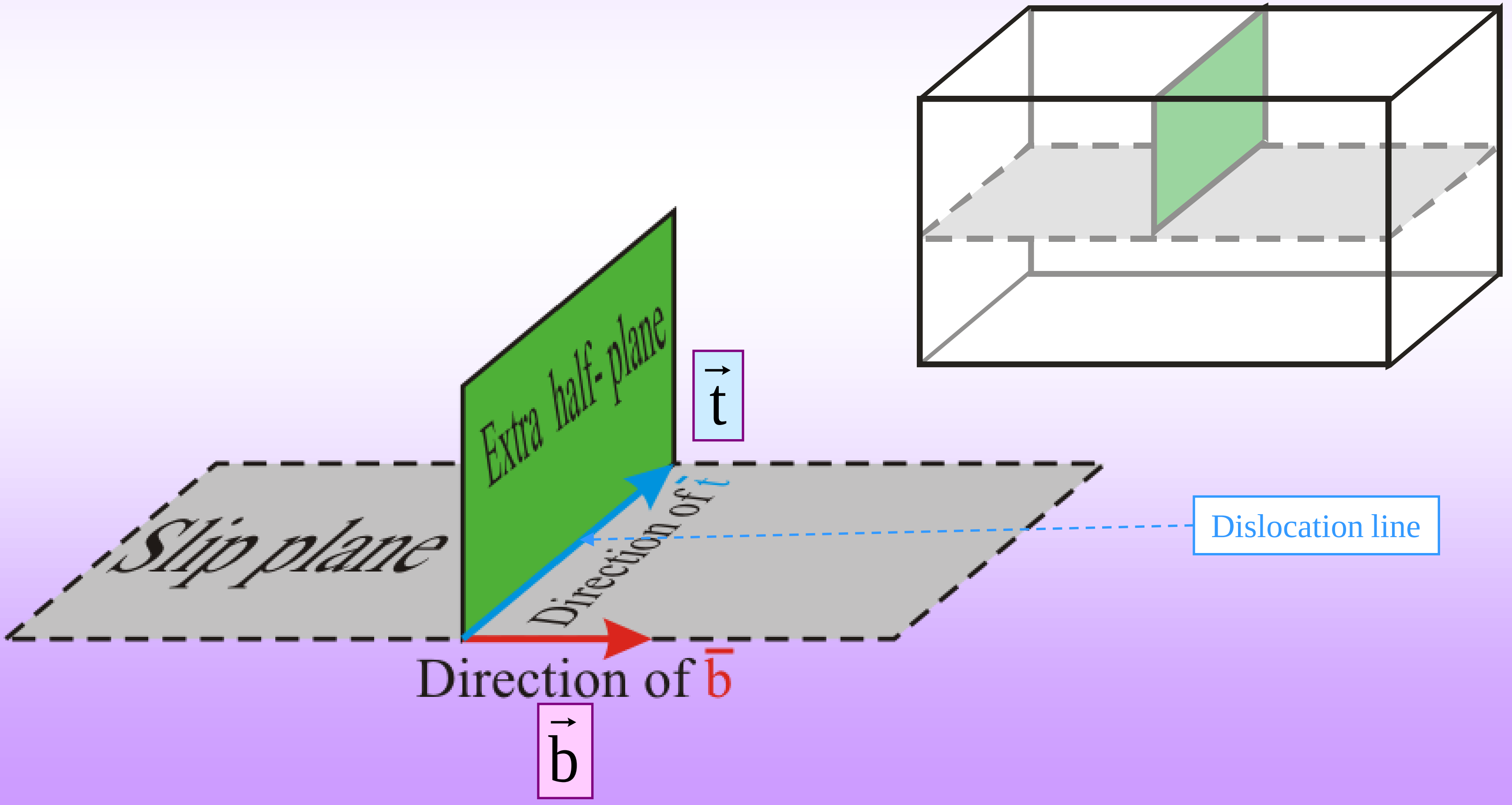


Note:

- The Burgers vector has to be drawn *‘far away’* form the dislocation line (sometimes it may be drawn close to dislocation line for convenience).
- The edge dislocation line is between the ‘missing’ and ‘extra’ half-planes.

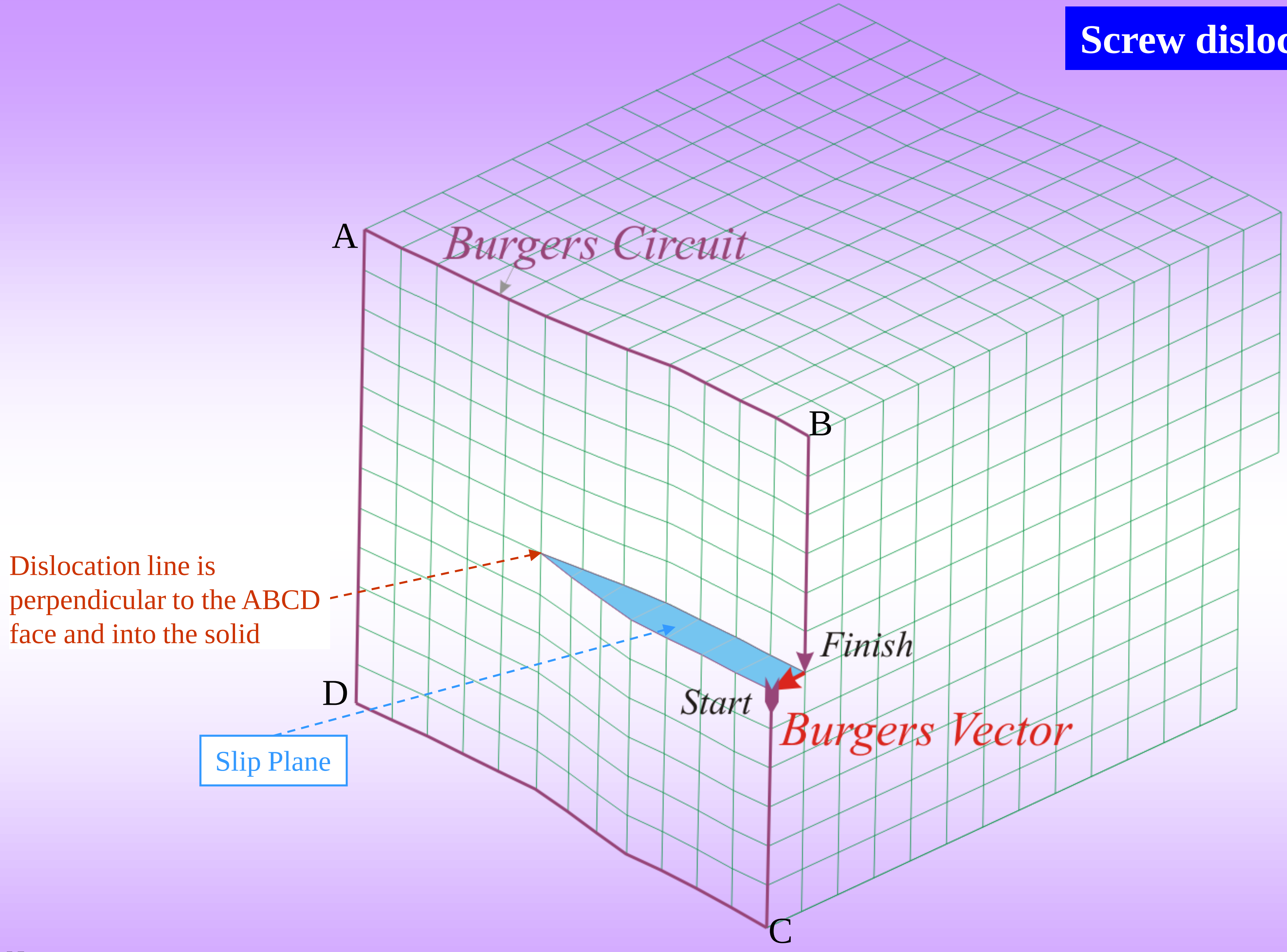
Edge dislocation

- Often to visualize the edge dislocation, only the extra ‘half’-plane and slip plane are shown. The remaining crystal is hidden away.
- The intersection of the extra half-plane and slip plane can be visualized as the dislocation line (one of the two possible directions is represents the line vector- shown in blue colour).



- Dislocation can be considered as the boundary between the slipped and the unslipped parts of the crystal lying over a slip plane.
- For an edge dislocation, the intersection of the extra half-plane of atoms with the slip plane defines the dislocation line.
- Direction and magnitude of slip is characterized by the Burgers vector of the dislocation
  (A dislocation is born with a Burgers vector and expresses it even in its death!).
- The Burgers vector can be determined by the Burgers Circuit.
- Right hand screw (finish to start) convention is usually used for determining the direction of the Burgers vector.
- As the periodic force field of a crystal requires that atoms must move from one equilibrium position to another ⇒ **b** must connect one lattice position to another *(for a full dislocation).*
- Dislocations tend to have as small a Burgers vector as possible.
- Dislocations are non-equilibrium defects and would leave the crystal if given an opportunity. *(The presence of dislocations increases the configurational entropy and hence the* $-T\Delta S$ *term would be negative. However, the 'T' at which they are stabilized is beyond the melting point of all crystals).*

Screw dislocation



Notes:

The figure shows a Right Handed Screw (RHS) dislocation (RHS is structurally distinct from LHS).

As for the edge dislocation the Burgers circuit has to be drawn far away from the dislocation line.

Geometric properties of dislocations

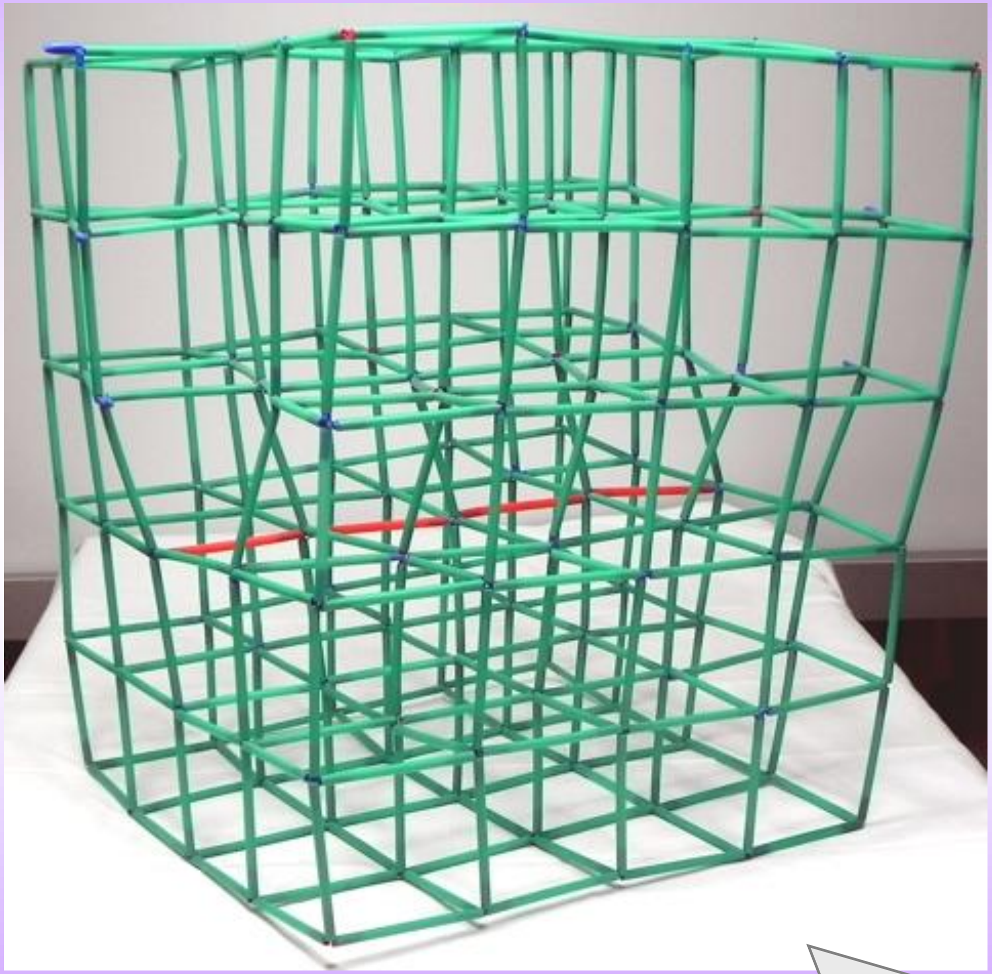
- In a edge dislocation : **b** is perpendicular to **t**.
- In a screw dislocation : **b** is parallel to **t.**
- Other properties are as in the table below.

Dislocation Property	**Type of dislocation**	
	Edge	**Screw**
Relation between dislocation line (**t**) and **b**	⊥	||
Slip direction** (& the 'direction' of step created when dislocation leaves the crystal)	|| to **b**	|| to **b**
Direction of dislocation line movement relative to **b**	||	⊥
Process by which dislocation may leave slip plane*	climb	Cross-slip

* *Note: edge dislocations cannot cross slip & screw dislocations cannot climb.*

** Slip is the end result when dislocation leaves the crystal to create a step. Slip is hence always parallel to **b**. Motion of a dislocation line is… well… "motion of a dislocation line".

Model of Screw Dislocation



Though it is difficult to understand anything from the photo of the model!

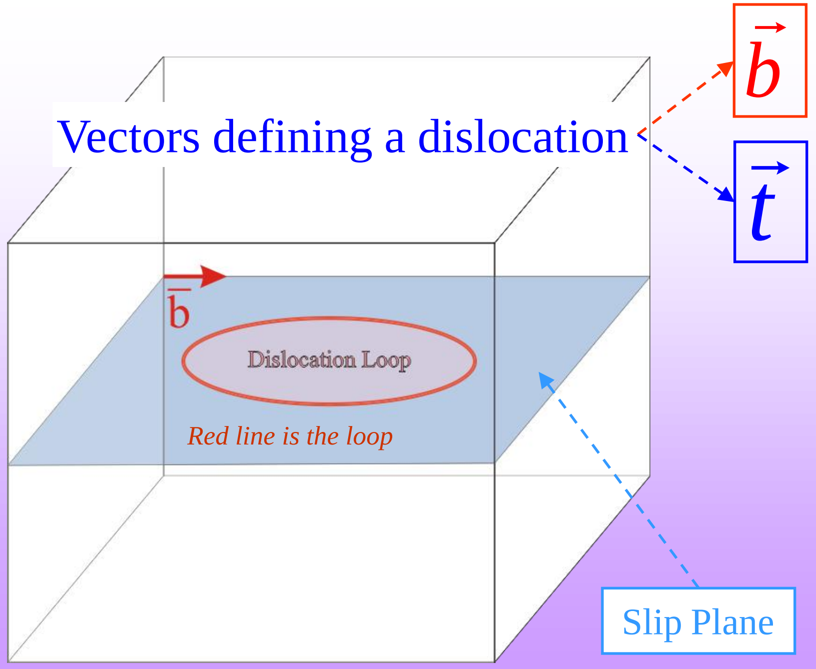
Mixed dislocations

Dislocations with mixed edge and screw character

- As we had noted, except in special circumstances, dislocations have mixed edge and screw character.
- In a curved dislocation the edge and screw character change from point to point.
- Typically in a dislocation loop only 'points' have pure edge or pure screw character

  Edge: **b** ⊥ **t** → two points A,C

  Screw: **b** || **t** → two points B,D.
- The region enclosed by the loop can be considered as the 'slipped region'.



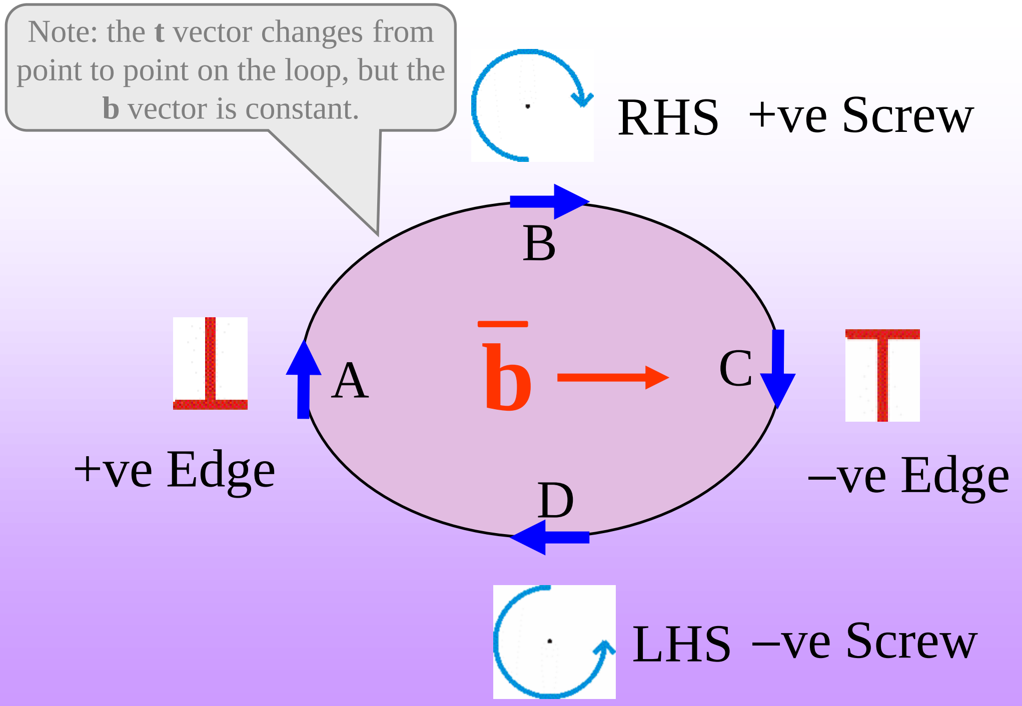
Vectors defining a dislocation

$\vec{b}$

$\vec{t}$

Red line is the loop

Slip Plane



Note: the **t** vector changes from point to point on the loop, but the **b** vector is constant.

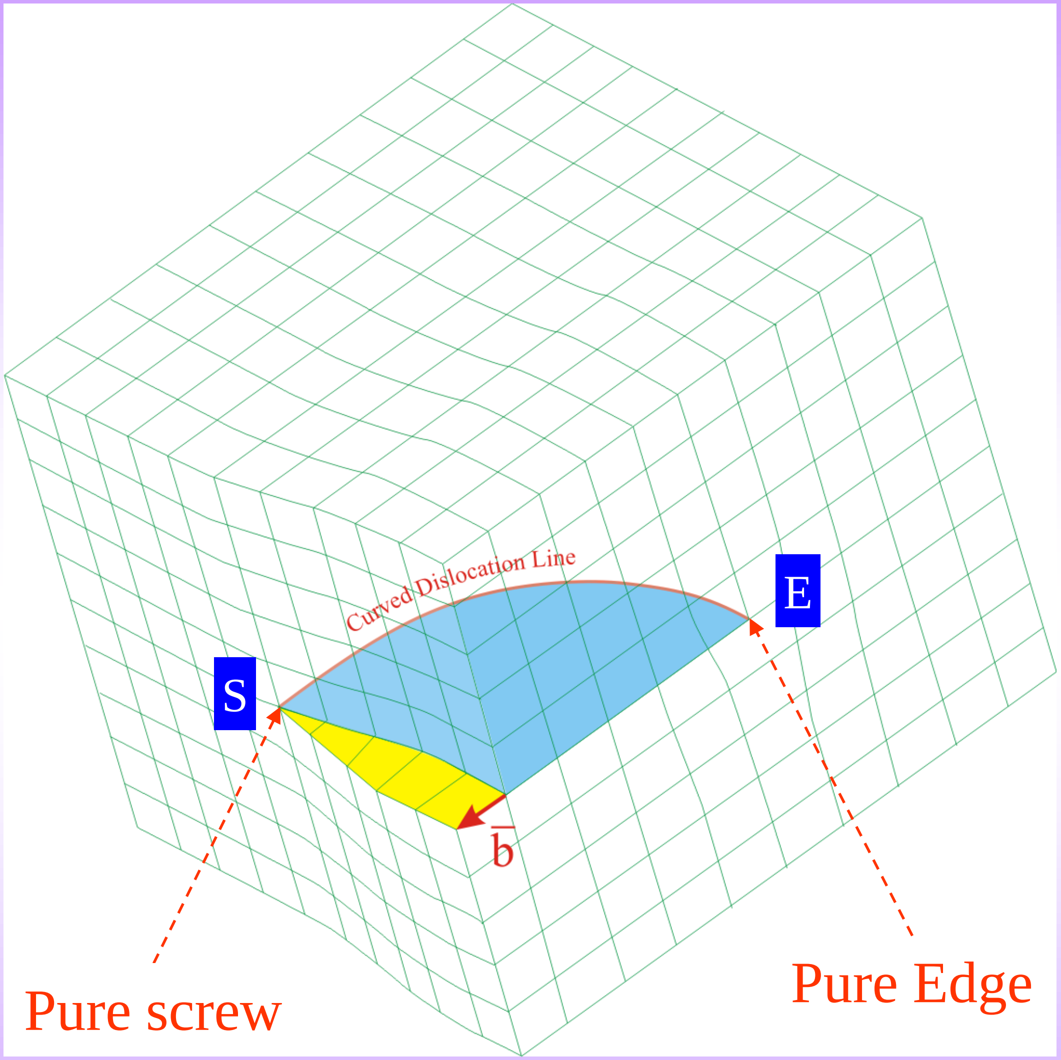
RHS +ve Screw

+ve Edge

–ve Edge

LHS –ve Screw

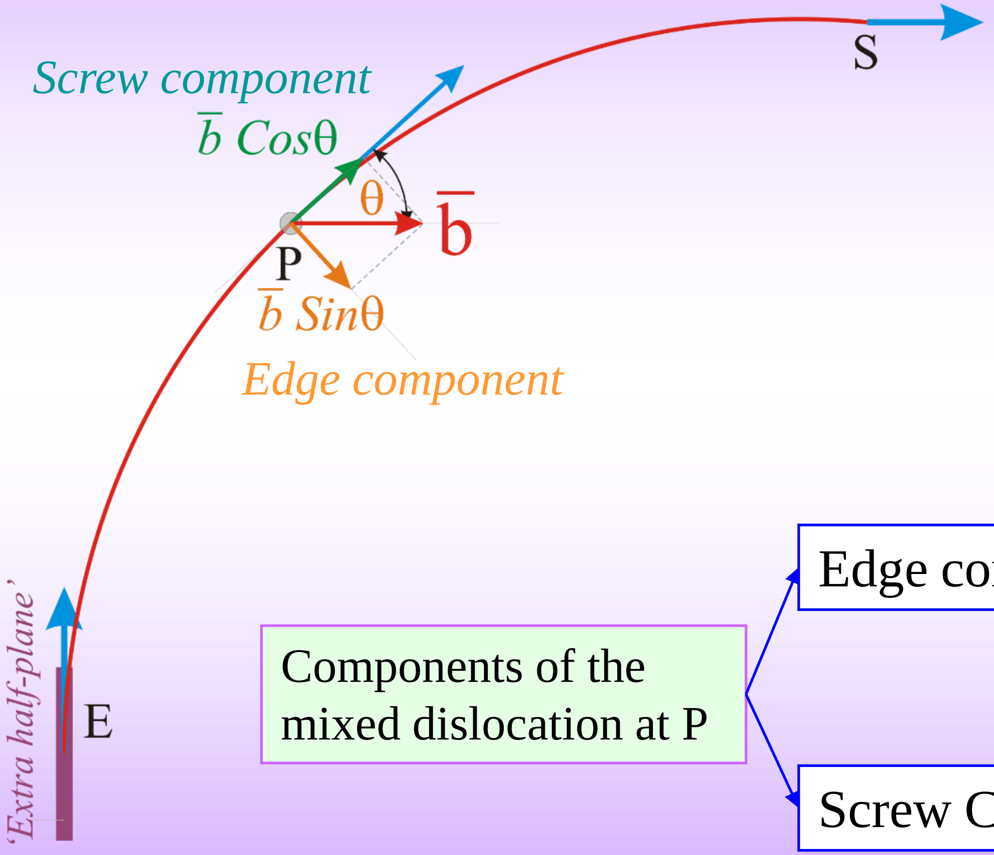
Let us consider a ‘quarter’ of a loop



Except for points S and E the remaining portion of the dislocation line has a mixed character

Edge and Screw components: the 'usual' way to get the effective Burgers vector

The **b** vector is resolved into components:
'parallel to **t**' → screw component and
'perpendicular to **t**' → edge component



Components of the mixed dislocation at P

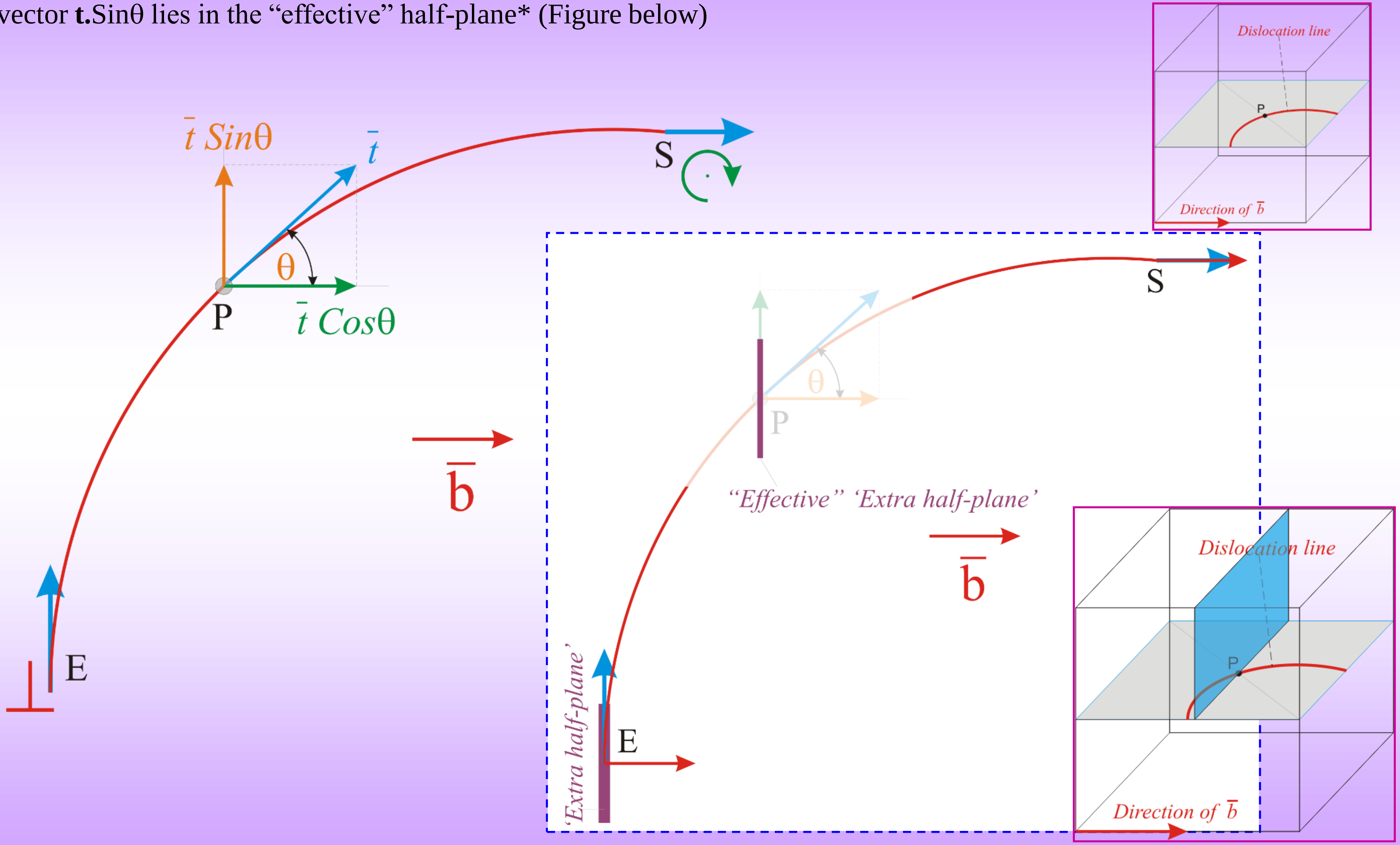
Edge component $\vec{b}\,Sin(\theta)$

Screw Component $\vec{b}\,Cos(\theta)$

Edge and Screw components: different way to visualize the orientation of the effective half-plane

Instead of resolving the **b** vector if the **t** vector is resolved to find the edge and screw components

For an edge dislocation the extra half-plane contains the **t** vector → by resolving the **t** vector the edge component of the **t** vector **t.**Sinθ lies in the "effective" half-plane* (Figure below)

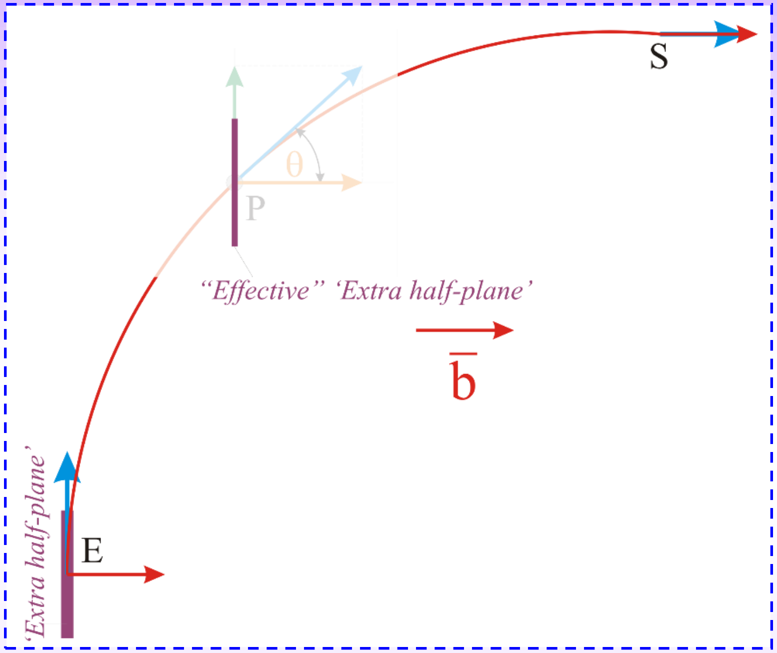


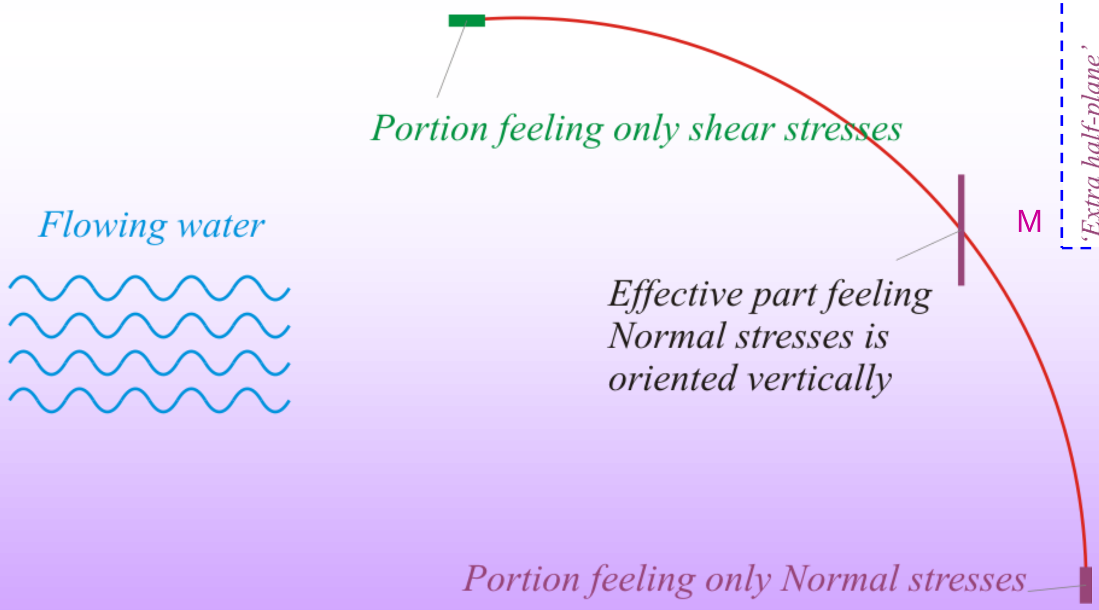
**Note: For a mixed dislocation there is no distinct 'half-plane'*

Edge and Screw components- the effective half-plane: a ‘crude’ anology to understand the orientation of the extra half plane

Assume water is flowing from left to right onto a rigid curved wall (in red colour below). The green portion of the wall ‘feels’ only shear stresses, while the maroon portion feels only normal stresses (of magnitude b).

A point M (in the curved segment) feels both normal and shear stresses. The effective part which feels normal stresses is oriented vertically with magnitude bSinθ.





Motion of Dislocations

- Two kinds of motion of a dislocation are possible: Glide and Climb.
- First we consider glide motion.
- Dislocations *may* move under an externally applied force (resulting in stress inside the material- often casually referred to 'applied stress').
- At the local level shear stresses on the slip plane can only drive dislocations.
- The minimum stress required to move a dislocation is called the Peierls-Nabarro (PN) stress or the Peierls stress or the Lattice Friction stress *(i.e the externally 'applied stress' may even be purely tensile but on the slip plane shear stresses must act in order to move the dislocation).*
- Dislocations may also move under the influence of other internal stress fields *(e.g. those from other dislocations, precipitates, those generated by phase transformations etc.).*
- Dislocations are attracted to free-surfaces (and interfaces with softer materials) and may move because of this attraction → this force is called the Image Force.
- *In any case the Peierls stress must be exceeded for the dislocation to move.*
- The value of the Peierls stress is different for the edge and the screw dislocations.
- The first step of plastic deformation can be considered as the step created when the dislocation moves and leaves the crystal.
  → "One small step for the dislocation, but a giant leap for plasticity".
- When the dislocation leaves the crystal a step of height 'b' is created → with it all the stress and energy stored in the crystal due to the dislocation is relieved.

Motion of Edge dislocation

- Conservative (*Glide*) — *Motion of dislocations on the slip plane*
- Non-conservative (*Climb**) — *Motion of dislocation ⊥ to the slip plane*

❑ For edge dislocation: as **b** ⊥ **t** → they define a plane → *the slip plane.*

❑ Climb involves addition or subtraction of a row of atoms below the half plane

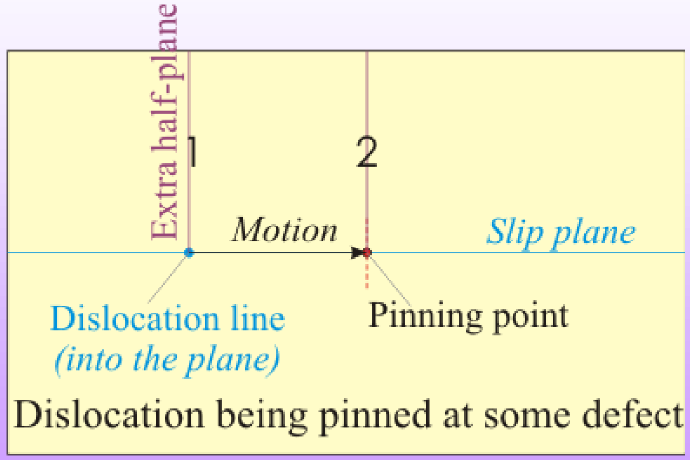
► +ve climb = climb up → removal of a plane of atoms

► –ve climb = climb down → addition of a plane of atoms.

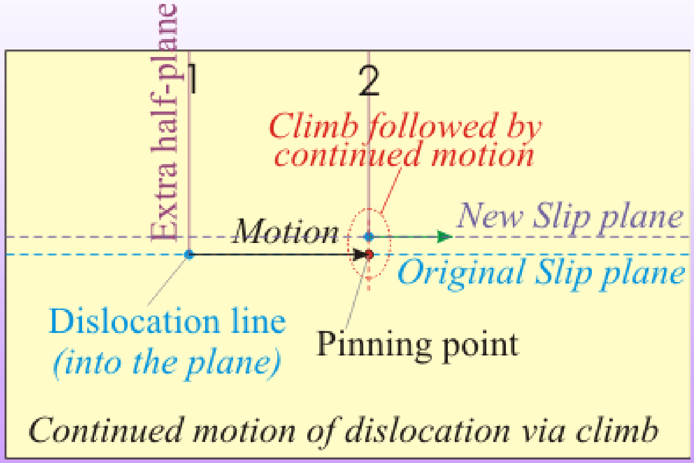
❑ Importance of climb: climb plays an important role in many ways.

▪ If an edge dislocation is 'stuck' at some obstacle on a *particular slip plane*, then it can continue to glide if climb can climb 'above' that slip plane. This way climb plays an important role in facilitating continued slip.

▪ Vacancy concentration in the crystal can decrease due to +ve climb.



Dislocation being pinned at some defect

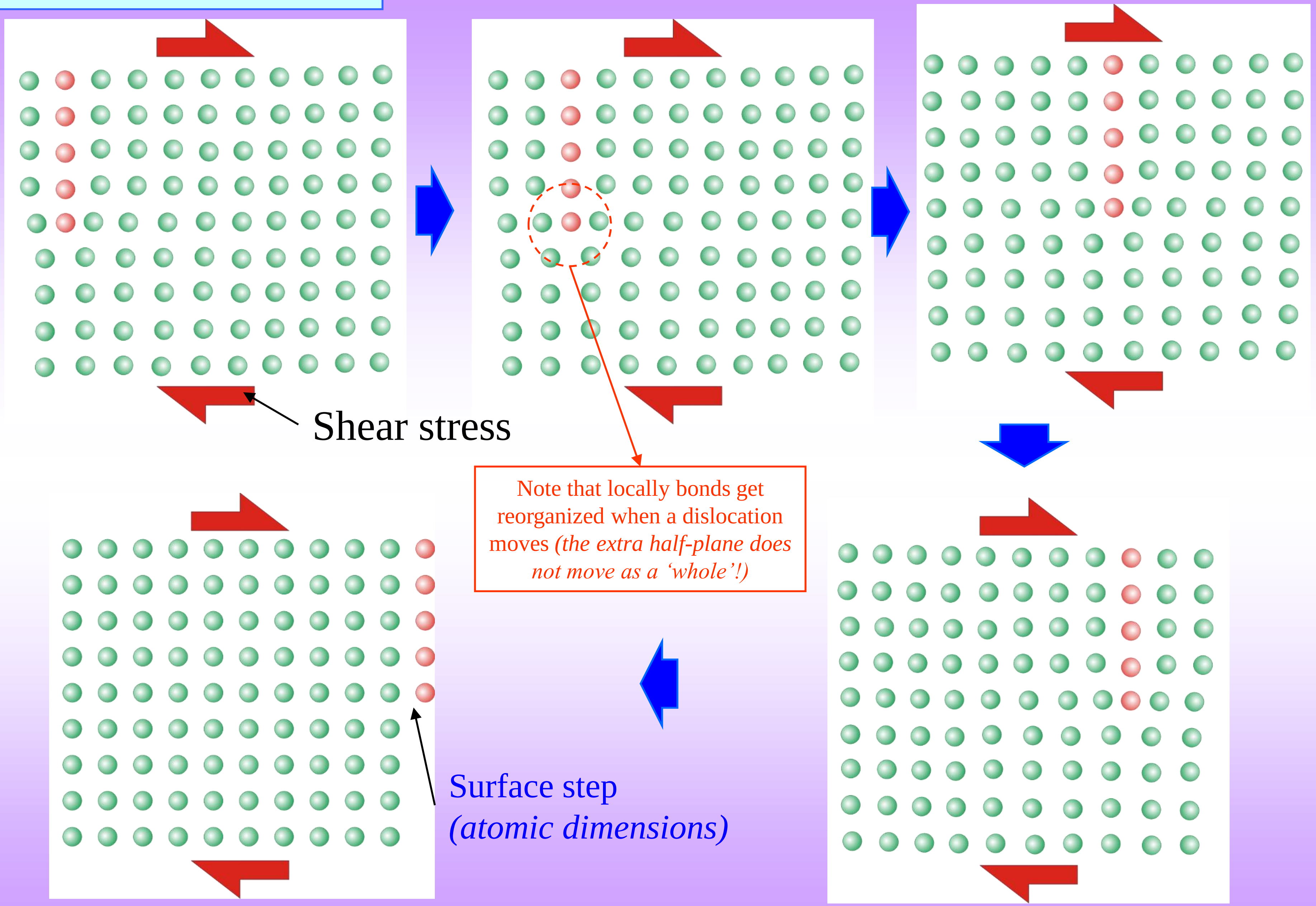


Continued motion of dislocation via climb

** There is even an interesting phenomenon called conservative climb!!*

Edge Dislocation Glide

Motion of an edge dislocation leading to the formation of a step (of 'b')

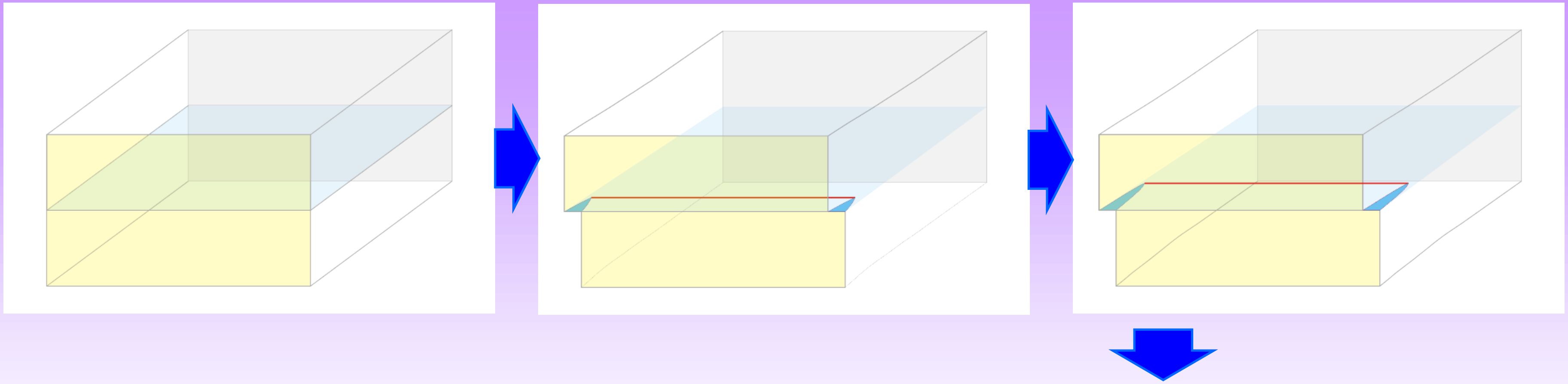


Shear stress

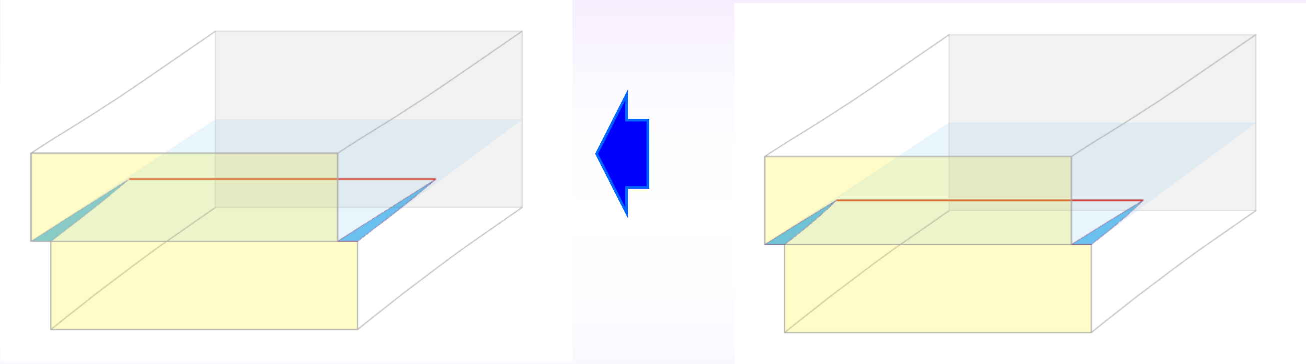
Note that locally bonds get reorganized when a dislocation moves *(the extra half-plane does not move as a 'whole'!)*

Surface step
(atomic dimensions)

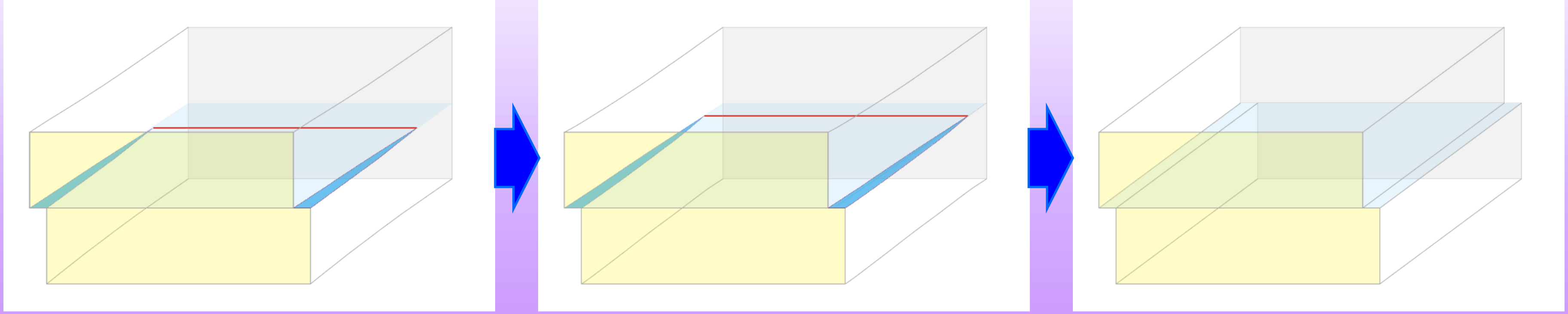
Graphics ➢ Motion of Edge Dislocation



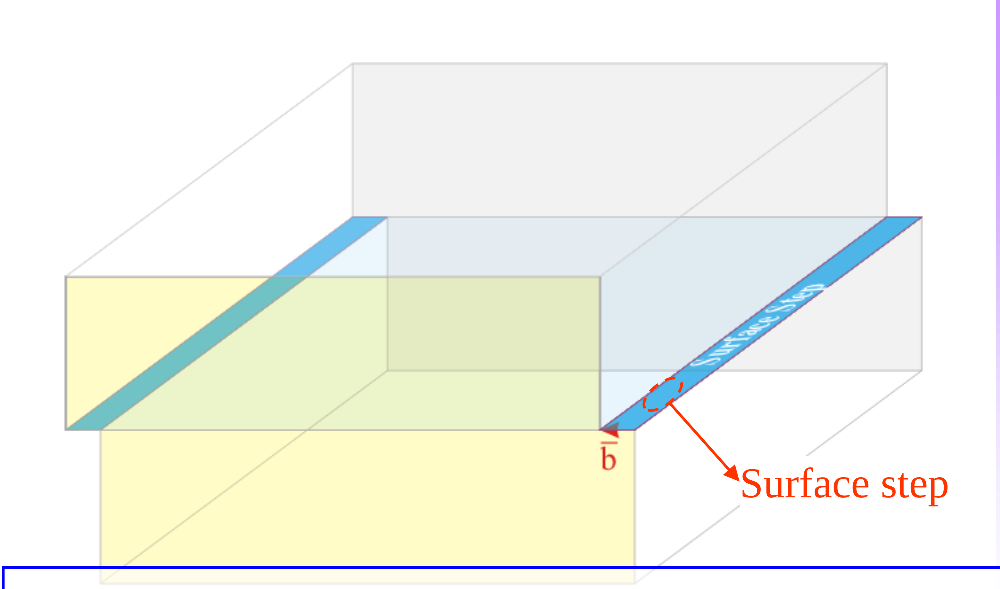
Motion of a screw dislocation leading to a step of **b**



Graphics ➤ Video: Motion of Screw Dislocation

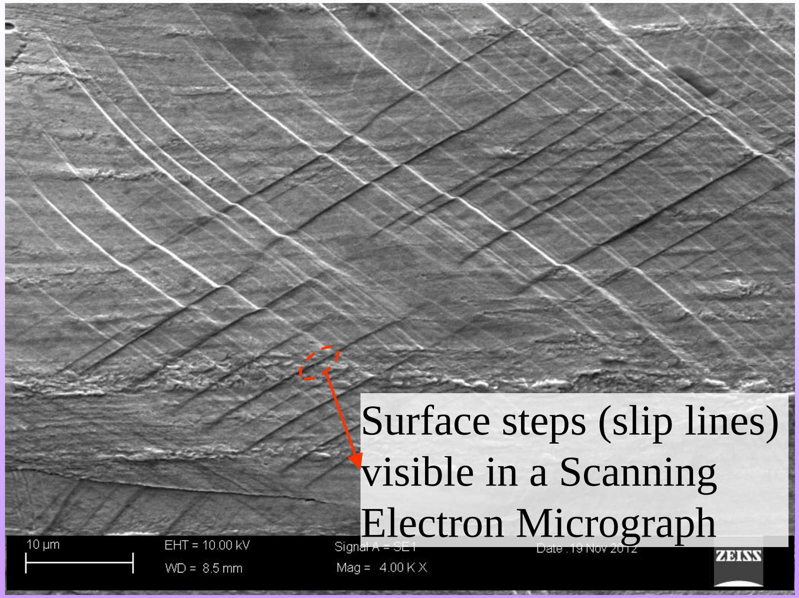


Note: Schematic diagrams

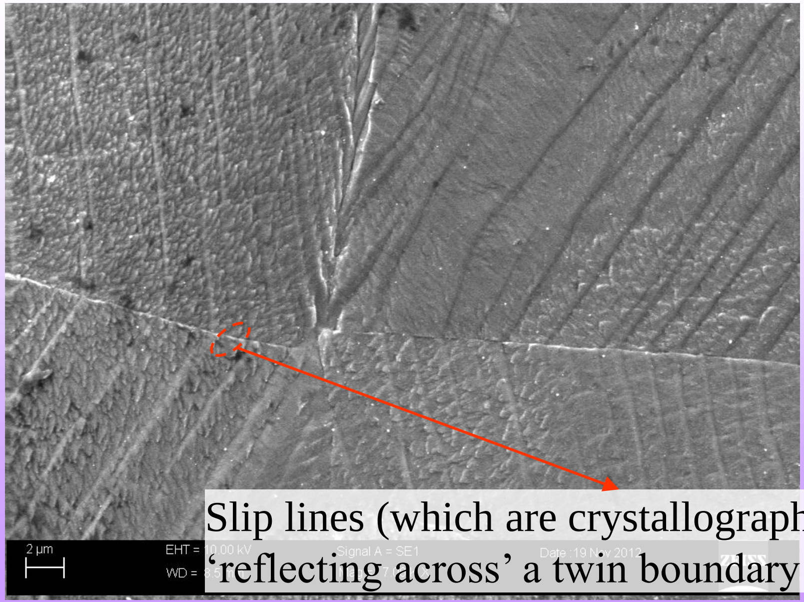


- When the dislocation leaves the crystal, the stress field associated with it is relieved.
- However, it costs some energy to create the extra surface corresponding to the step.

- Are these steps visible?
  These steps being of atomic dimensions are not visible in optical microscopes. However, if many dislocations operate on the same slip plane then a step of nb (n~ 100s-1000s) is created which can even be seen in an optical microscope *(called the slip lines)*.



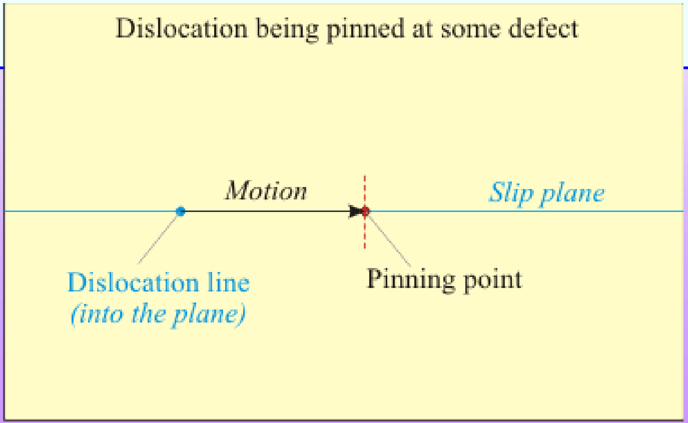
Surface steps (slip lines) visible in a Scanning Electron Micrograph

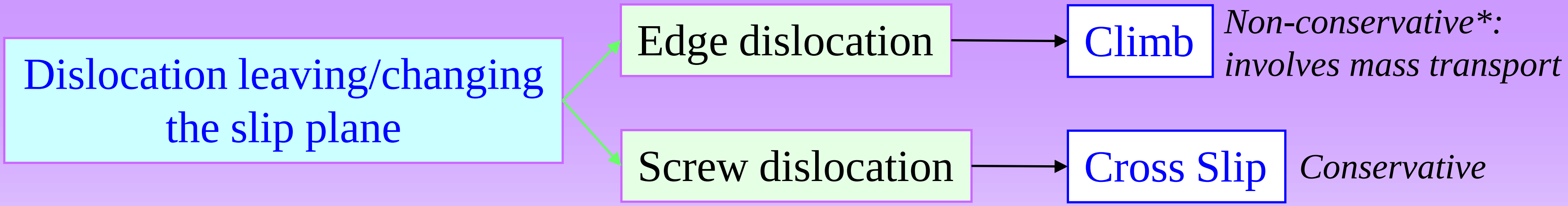


Slip lines (which are crystallographic markers) 'reflecting across' a twin boundary in Cu

Dislocations leaving the slip plane

- As it was observed the ‘first step’ of plastic deformation is the motion of a dislocation leaving the crystal (or to some other interface bounding the crystal) → leading to the formation of a step.
- For continued plastic deformation it is necessary that dislocations continue to move and leave the crystal. Hence, any impediments to the motion of a dislocation will lead to ‘hardening’ of the crystal and would ‘stall’ plastic deformation *(the pinning of a dislocation)*.
- Once a dislocation has been pinned it can either ‘break down the barrier’ or ‘bypass’ the barrier.
- Bypassing the barrier can take place by mechanisms like:
  ➢ Climb ➢ Cross Slip ➢ Frank-Read mechanism ….
- In climb and cross slip the dislocation leaves/changes its ‘current’ slip plane and moves to another slip plane thus avoiding the barrier
- However, these processes (climb and cross slip) can occur independent of the pinning of the dislocation!


Dislocation being pinned at some defect



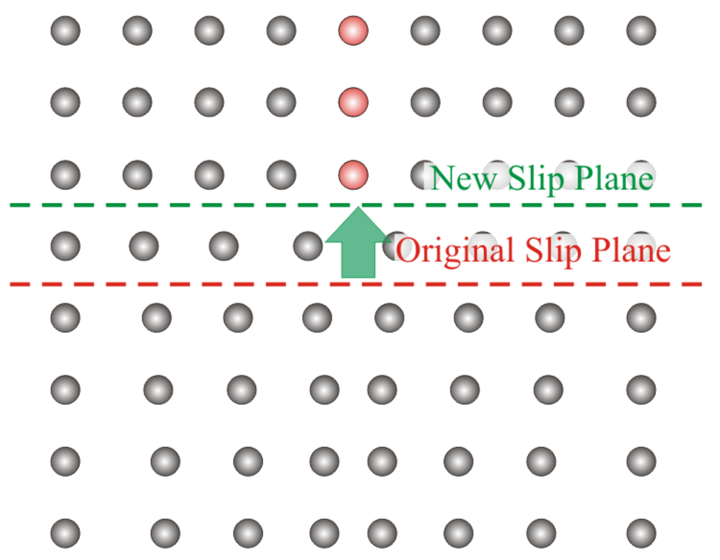
Dislocation leaving/changing the slip plane

Edge dislocation → Climb *Non-conservative*: involves mass transport*

Screw dislocation → Cross Slip *Conservative*

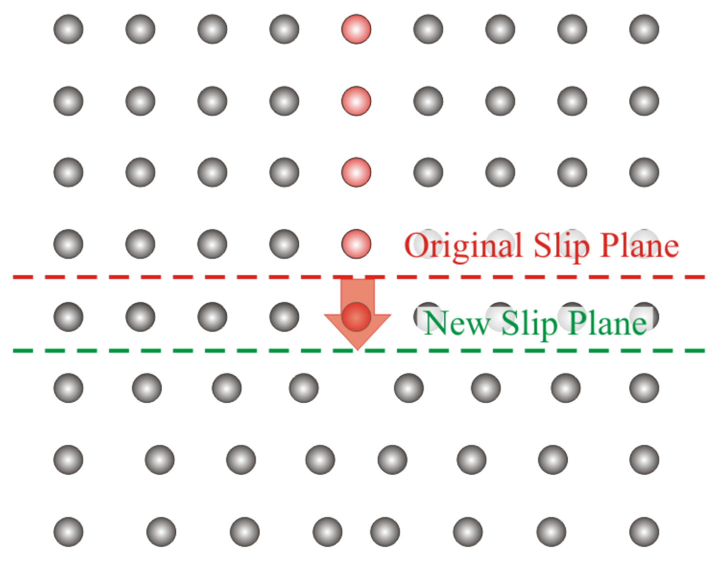
In climb an edge dislocation moves to an adjacent parallel plane, but in cross slip a screw dislocation moves to a plane inclined to the original plane.

Climb of an Edge Dislocation



Positive climb

Removal of a row of atoms



Negative climb

Addition of a row of atoms

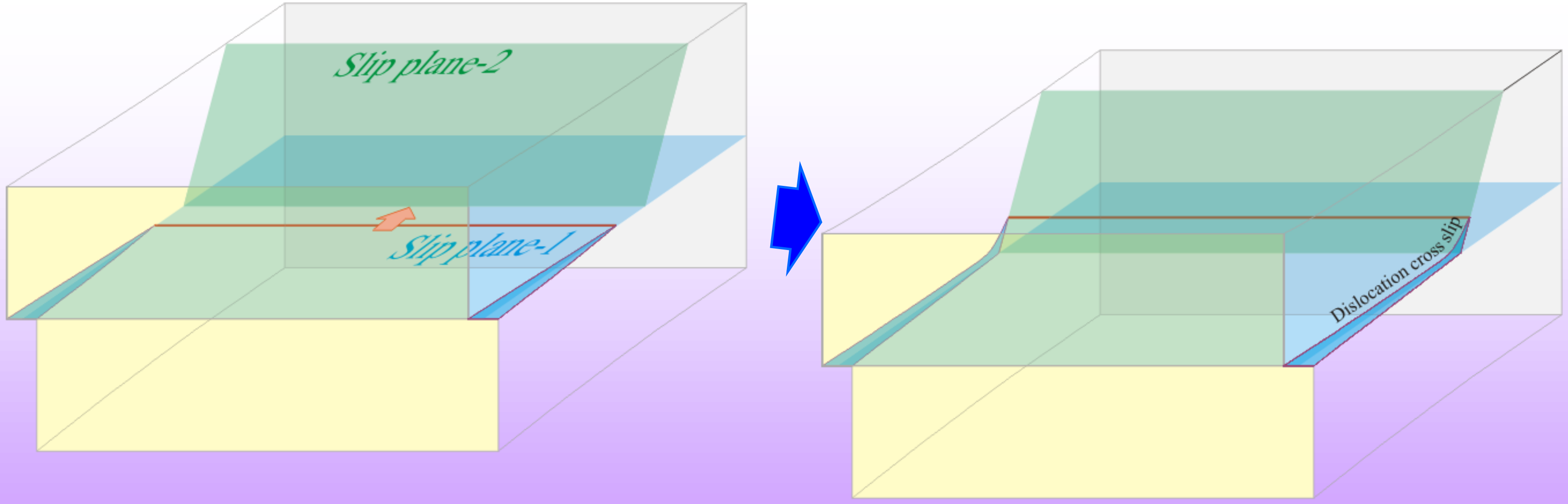
Removal of a row of atoms leads to a decrease in vacancy concentration in the crystal and negative climb leads to an increase in vacancy concentration in the crystal.

**Conservative climb is also possible!! → by motion of prismatic edge loop on the slip plane*

Screw dislocation: Cross Slip

- Let the dislocation be moving on SP1 (as the resolved shear stress is maximum on Slip Plane-1 (SP1)).
- The figures below show the cross slip of a screw dislocation line from SP1 to Slip plane-2 (SP2). This may occur if the dislocation is 'pinned' in slip plane-1.
- For such a process to occur the Resolved Shear Stress on SP2 should be at least greater than the Peierls stress

  (often stresses higher than the Peierls stress has to be overcome due to the presence of other stress fields).
- It is to be noted that SP1 & SP2 are (usually) crystallographically equivalent, i.e. if SP1 is $(111)_{\text{CCP Crystal}}$ then SP2 can be $(-111)_{\text{CCP Crystal}}$.



The dislocation is shown cross-slipping from the blue plane to the green plane

Funda Check

How does plastic deformation by slip occur?

- As we have seen *slip (a technical term)* is one of the many mechanisms by which plastic deformation can occur.

The first step of plastic deformation by slip (at the fundamental level) is the motion of a dislocation leaving the crystal.

- By externally applied force (or some other means!) stress has to be ‘generated’ within the crystal.
- The slip plane should feel shear stresses.
- The shear stress should exceed the ‘Critical Resolved Shear Stress (CRSS)’ or Peierls stress.
- The dislocation should leave the crystal creating a surface step of height ‘b’.

The process ahead of this which leads to an arbitrary shape change is complicated and we will deal with a part of it later.

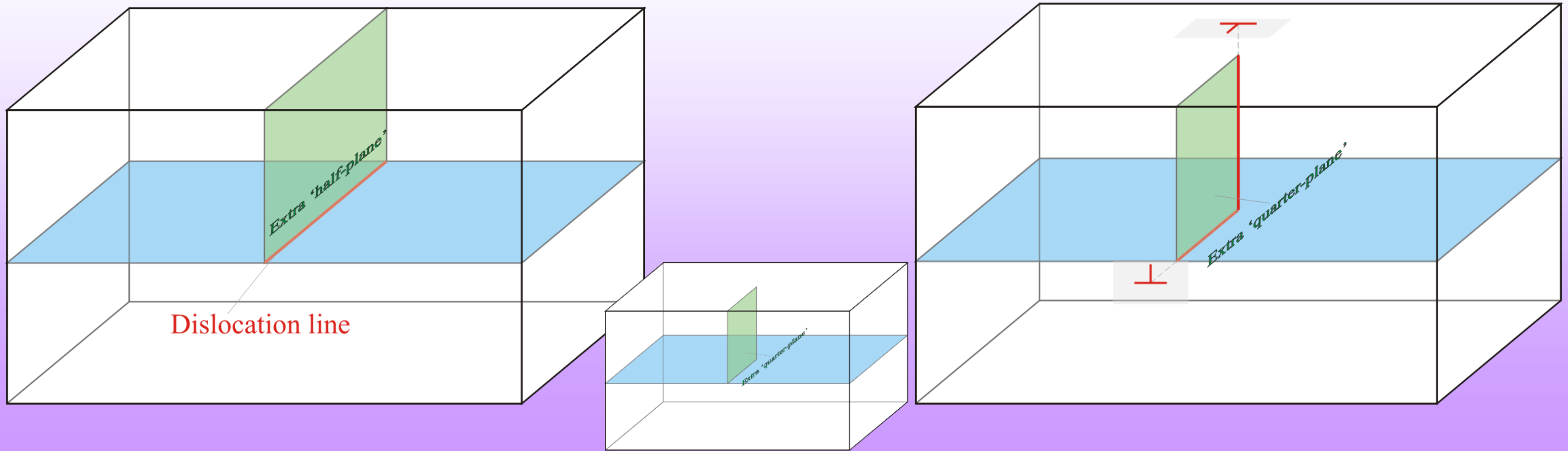
Where can a dislocation line end?

- Dislocation line cannot end inside the crystal *(abruptly)*
- The dislocation line:
  - Ends on a free surface of the crystal
  - Ends on an internal surface or interface
  - Closes on itself to form a loop
  - Ends in a *node*
- A *node* is the intersection point of more than two dislocations
- The vectoral sum of the Burgers vectors of dislocations meeting at a node = 0

Funda Check

What about the introduction of a quarter plane of atoms- doesn't the dislocation line end inside the crystal?

- As seen in the figure below there are two sections to the dislocation line ending on free surface of the crystal and hence not inside the crystal.

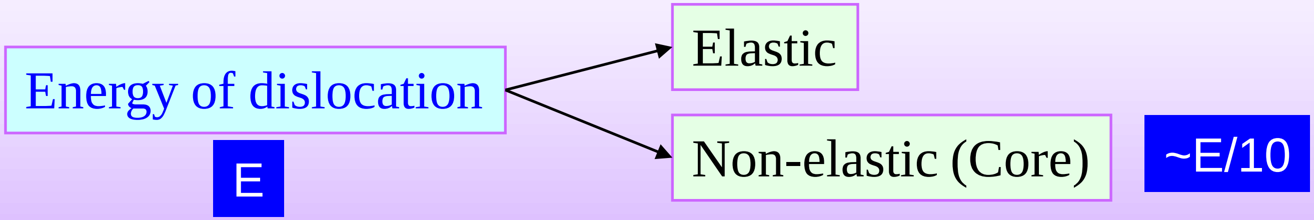


Positive and Negative dislocations

- As we have seen when there are two are more EDGE dislocations in a slip plane one of them is assigned a +ve sign and the other one a –ve sign *(done arbitrarily)*
- In the case of screw dislocations the Right Handed Screw (RHS) Dislocation is *Structurally Distinct* from the Left Handed Screw (LHS) Dislocations
  - In the case of RHS dislocation as a clockwise circuit (Burgers) is drawn then a helical path leads into the plane of the

Energy of dislocations

- The presence of a dislocation distorts the bonds and costs energy to the crystal. Hence, dislocations have distortion energy associated with them
- The energy is expressed as Energy per unit length of dislocation line
  → Units: [J/m]
- Edge → Compressive and tensile stress fields
  Screw → Shear stress fields
- The energy of a dislocation can approximately be calculated from linear elastic theory. The distortions are very large near the dislocation line and the linear elastic description fails in this region → called the Core of the dislocation *(estimates of this region range from b to 5b depending on the crystal in question)*. The structure and energy of the core has to be computed through other methods and the energy of the core is about 1/10 the total energy of the dislocation.
- The formula given below gives reasonable approximation of the dislocation energy.



Energy of dislocation

E

Elastic

Non-elastic (Core)

~E/10

Elastic Energy of a dislocation / unit length →

$$E_d \sim \frac{1}{2} G b^2$$

G → (μ) shear modulus
b → |**b**|

- ☐ As it costs energy to put a dislocation in a crystal:
  - ➢ Dislocations tend to have as small a **b** as possible
  - ➢ There is a line tension associated with the dislocation line
  - ➢ Dislocations may dissociate into Partial Dislocations to reduce their energy

$$E_d \sim \frac{1}{2} G b^2 \Rightarrow$$

Dislocations will have as small a **b** as possible

Dislocations
(in terms of lattice translation)

- Full — **b** → Full lattice translation
- Partial — **b** → Fraction of lattice translation

Another formula for the energy (Edge dislocation)

$$E_d^{edge} \sim \frac{Gb^2}{4\pi(1-\nu)}\left[2+\ln\left(\frac{\gamma_0}{b}\right)\right]$$

γ_0 - size of the control volume ~ 70b

Core contribution

$$E_d^{screw} \sim \frac{Gb^2}{4\pi}\left[2+\ln\left(\frac{\gamma_0}{b}\right)\right]$$

Dissociation of dislocations

- Dislocations may dissociate to reduce their energy

Consider the reaction*: $2\mathbf{b} \rightarrow \mathbf{b} + \mathbf{b}$

Change in energy:

Initial energy before splitting into partials: $G(2b)^2/2 = 2Gb^2$

Energy after splitting into partials: $2[G(b)^2/2] = G(b)^2$

Reduction in energy $= 2Gb^2 - Gb^2 = Gb^2$.

$\Rightarrow$ The reaction would be favorable.

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* Note that this example is considered for illustration purpose only *(here a full dislocation is not splitting into partials)*

Stress Fields of Dislocations

The self stresses

Edge dislocation

- An edge dislocation in an infinite body has compressive stress field above *(the region of the extra half-plane)* and tensile stress field below *(the region of the missing half-plane)* the slip plane
- These stress fields will be altered in a finite body
- Asymmetric position of the dislocation in the crystal will also alter the stress field described by the standard equations *(as listed below)*
- The core region is ignored in these equations *(which hence have a singularity at* $x = 0, y = 0$*)* (Core being the region where the linear theory of elasticity fails)
- Obviously a real material cannot bear such ‘singular’ stresses
- The interaction of the stress fields of the dislocations with: (i) those originating from externally applied forces and (ii) other internal stress fields → determines the motion of dislocation → leading to many aspects of mechanical behaviour of materials

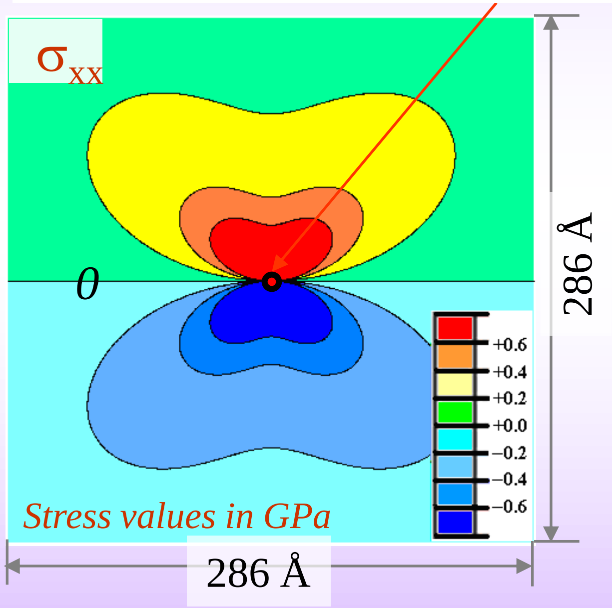
$$\left.\begin{aligned}
\sigma_{xx} &= \frac{Gb}{2\pi(1-\nu)}\,\frac{y(3x^2+y^2)}{(x^2+y^2)^2}\\
\sigma_{yy} &= \frac{-Gb}{2\pi(1-\nu)}\,\frac{y(x^2-y^2)}{(x^2+y^2)^2}\\
\sigma_{xy} = \tau_{xy} &= \frac{-Gb}{2\pi(1-\nu)}\,\frac{x(x^2-y^2)}{(x^2+y^2)^2}
\end{aligned}\right\}\ \text{stress fields}$$

The material is considered isotropic (two elastic constants only- E & ν or G & ν)
→ in reality crystals are anisotropic w.r.t *to the elastic properties*

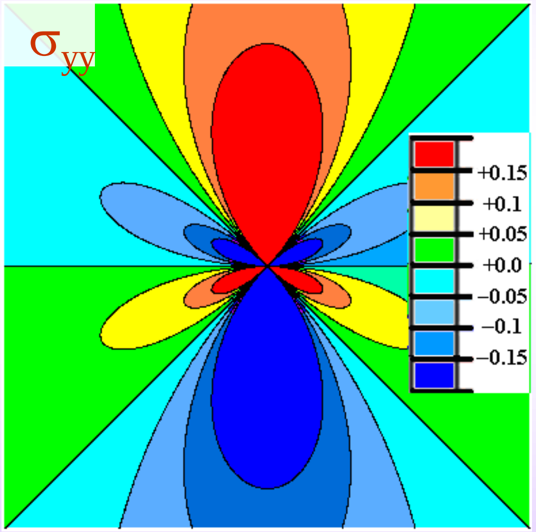
Edge dislocation

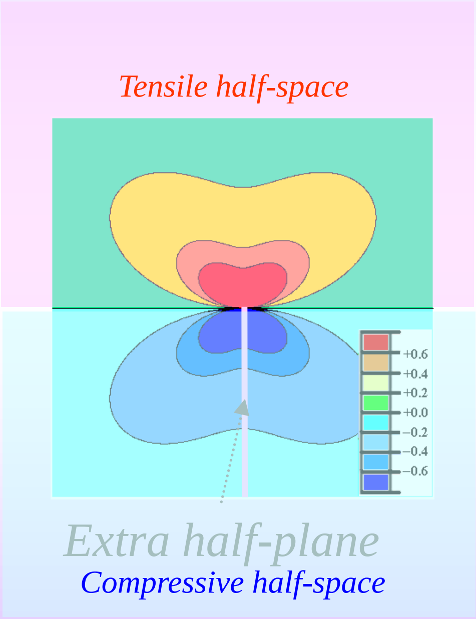
- Note that the region near the dislocation has stresses of the order of GPa
- These stresses are the self stresses of the dislocation and a straight dislocation line cannot move under the action of self stresses alone *(in an infinite body)*
- *A dislocation interacts with other defects in the material via these 'long range' stress fields*

Position of the Dislocation line → into the plane



Stress values in GPa





$$\sigma_{xx} = \frac{Gb}{2\pi(1-\nu)}\,\frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$

$$\sigma_{yy} = \frac{-Gb}{2\pi(1-\nu)}\,\frac{y(x^2-y^2)}{(x^2+y^2)^2}$$

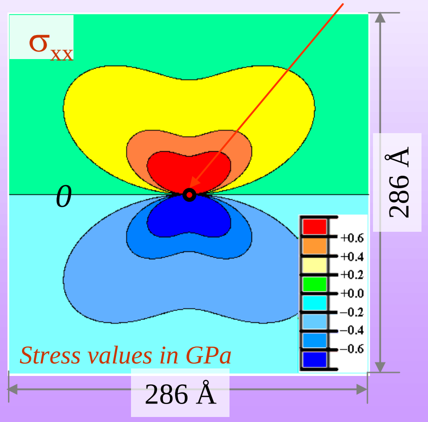
Assumptions:
Iso-stress contours, infinite body, straight edge dislocation along 'z', plane strain condition, core of dislocation ignored (i.e. the equations should not be used close to the dislocation line– in the range of 'b' to '5b')

➢ *Material properties used in the plots are in the last slide*

Funda Check

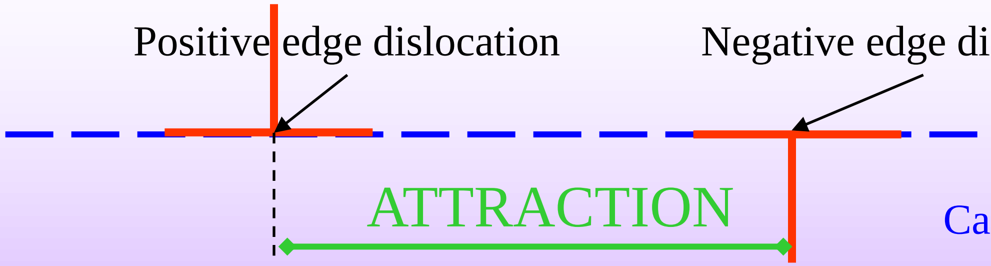
Note that the stresses near the dislocation line reaches values in GPa. Yield stress is usually in 100s of MPa. How does a material not yield under the effect of such high stresses?

- The predominant mechanism of plastic deformation is slip, which involves motion of a large number of dislocations (ultimately leaving interfaces).
- The stresses described here are due to the ‘dislocation itself’ (the causative agent for plastic deformation by slip) and they are the *elastic stress fields* associated with the dislocation.



Interaction between dislocations

- Here we only consider elastic interactions between edge dislocations on the same slip plane.
- This can lead to Attractive and Repulsive interactions.
- To understand these interaction we need to consider Positive and Negative edge dislocations. If a single edge dislocation is present in a material it can be called either positive or negative. If two (or more) dislocations are present on the same slip plane, with the extra half-plane on two different sides of the slip plane, then one of them is positive and the other negative.
- The picture (region of attraction and repulsion) gets a little 'detailed' if the two dislocations are arbitrarily oriented. [See Stress Fields of Dislocations]

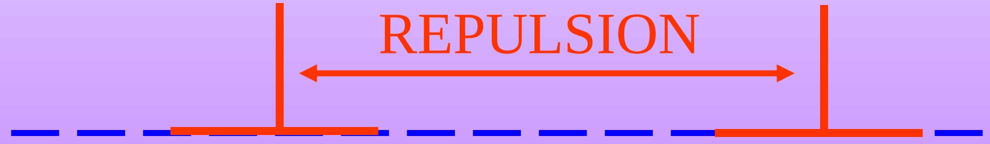


Positive edge dislocation

Negative edge dislocation

ATTRACTION

Can come together and cancel one another



REPULSION

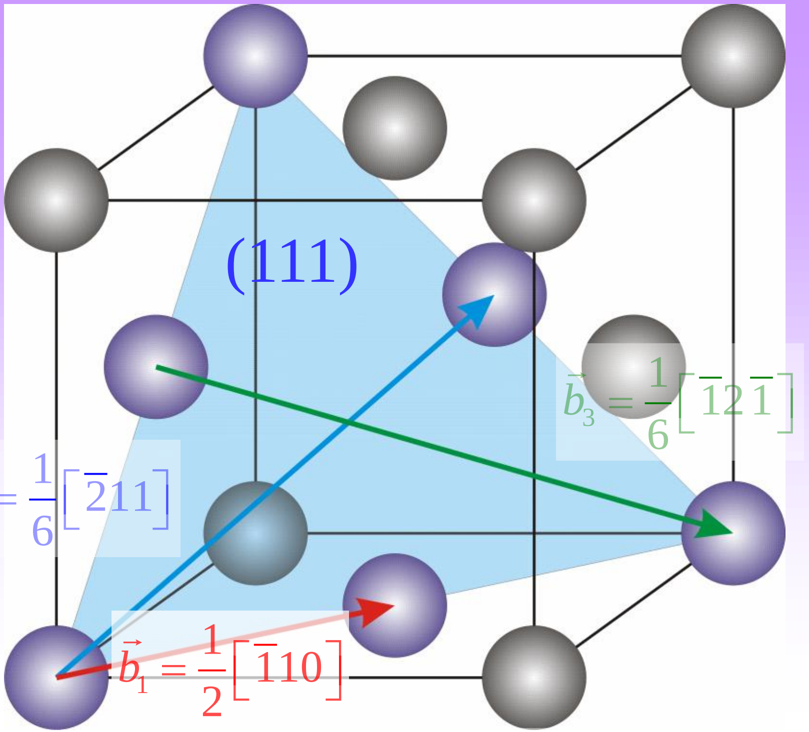
Dislocations in CCP Crystals

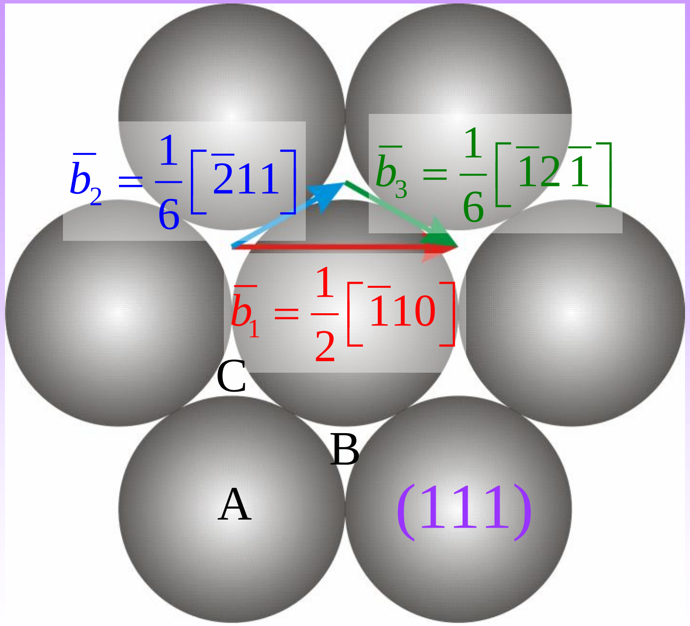
Figures in coming slides

- Slip system → <110>, {111}.
- Perfect dislocations can split into partials *(Shockley partials considered first)* to reduce their energy. As we shall see, this can be best understood with edge dislocation, where two atomic planes form the perfect (full) dislocation and when these two atomic planes separate we form partials (each partial has one atomic plane).
- The dissociation into partials leaves a Stacking Fault* between the two partials on the slip plane.
- The two partials repel each other and want to be as far as possible → but this leads to a larger faulted area (leading to an increase in energy) → depending on the stacking fault energy there will be an equilibrium separation between the partials.
- The Shockley partial has Burgers vector of the type: (1/6) [211] type.
  This is an important vector in the CCP crystals, as vectors of this family connect B site to C site and vice-versa.
- For a pure edge dislocation in a CCP crystal the ‘extra half-plane’ consists of two atomic planes. The partial dislocations consist of one ‘extra’ atomic plane each (but the Burgers vector of the partial is not perpendicular to the dislocation line- as in the case of the perfect edge dislocation).

CCP

Perfect Edge Dislocation and Shockley Partials



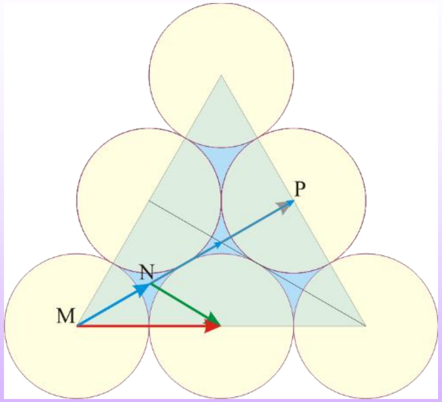


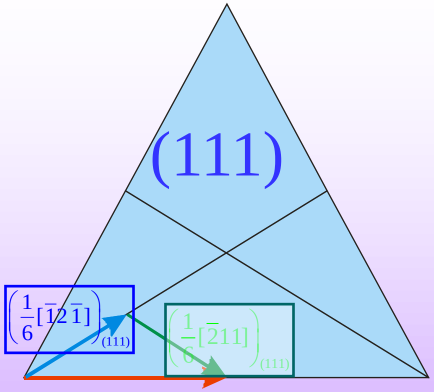
(111)
Slip plane

Some of the atoms are omitted for clarity, Full vectors $[\bar{2}11]$ *(blue vector) &* $[\bar{1}2\bar{1}]$ *(green vector) shown in the left figure*

$$\boxed{\left(\frac{1}{2}[\bar{1}10]\right)_{(111)}} \longrightarrow \boxed{\left(\frac{1}{6}[\bar{1}2\bar{1}]\right)_{(111)}} + \boxed{\left(\frac{1}{6}[\bar{2}11]\right)_{(111)}}$$

Shockley Partials





$$|\vec{b}_2| = \left(\frac{\sqrt{\bar{1}^2+2^2+\bar{1}^2}}{6}\right)^2 = \left(\frac{\sqrt{6}}{6}\right)^2 = \frac{1}{6}$$

$(b_2^2 + b_3^2) = 1/6 + 1/6 = 1/3$

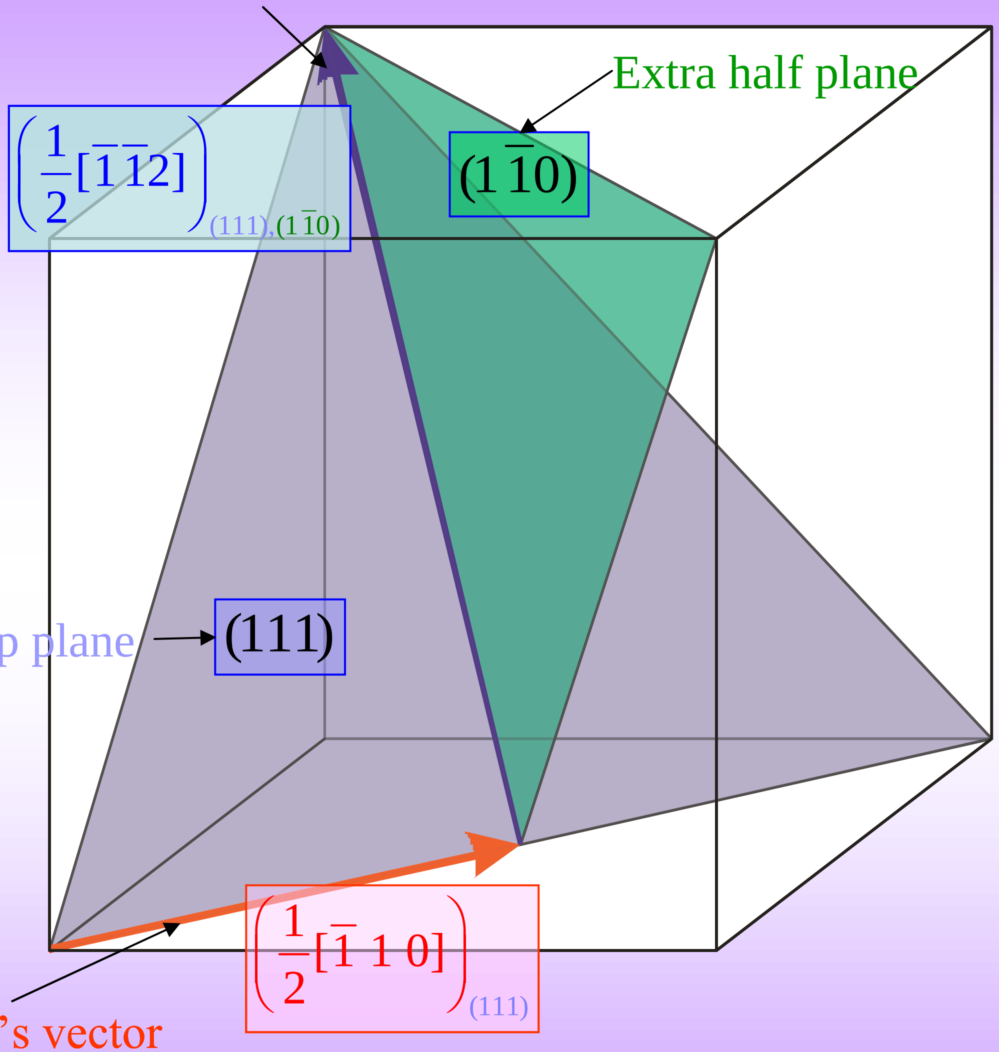
$$\boxed{\begin{array}{c} b_1^2 > (b_2^2 + b_3^2) \\ \frac{1}{2} > \frac{1}{3} \end{array}}$$

Energy of the dislocation is proportional to b^2*.*
As the energy of the system is reduced on dissociation into partials the perfect dislocation will split into two partials.

Pure edge dislocation

CCP

Dislocation line vector



$\left(\frac{1}{2}[\bar{1}\bar{1}2]\right)_{(111),(1\bar{1}0)}$

Extra half plane

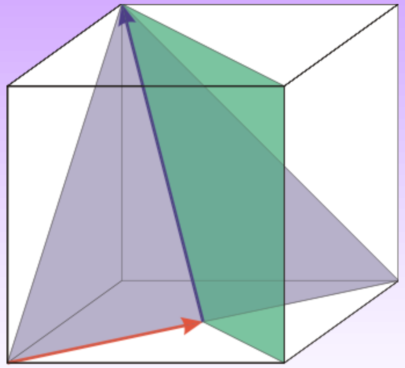
$(1\bar{1}0)$

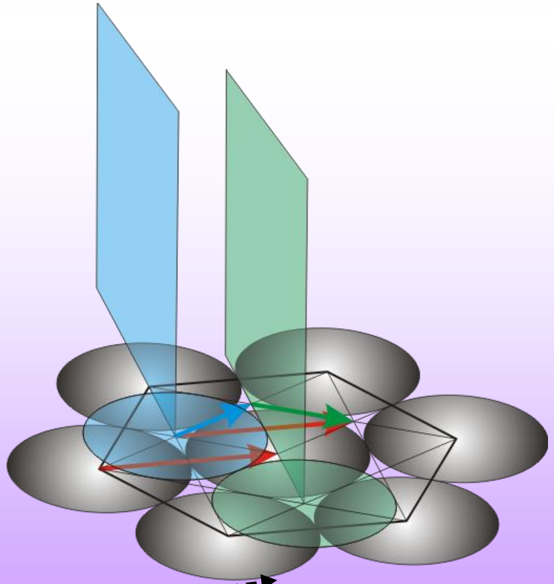
Slip plane

(111)

Burger's vector

$\left(\frac{1}{2}[\bar{1}\,1\,0]\right)_{(111)}$

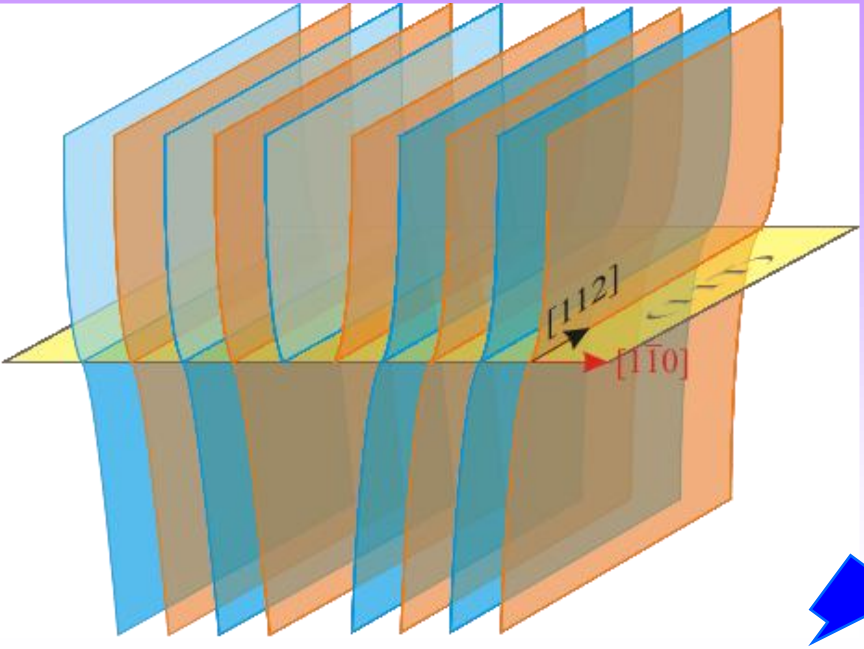




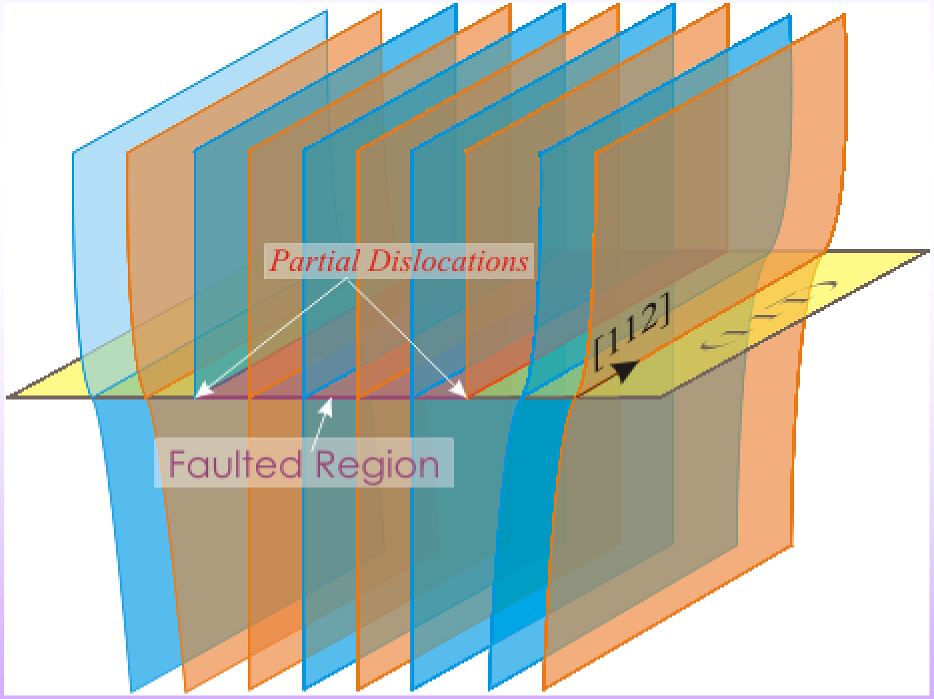
The extra- "half plane" consists of two 'planes' of atoms!

One crystal plane is 'lattice plane' decorated with two atomic planes.

Shockley Partials



Perfect edge dislocation ('full' Burgers vector) with two atomic 'extra-half' planes



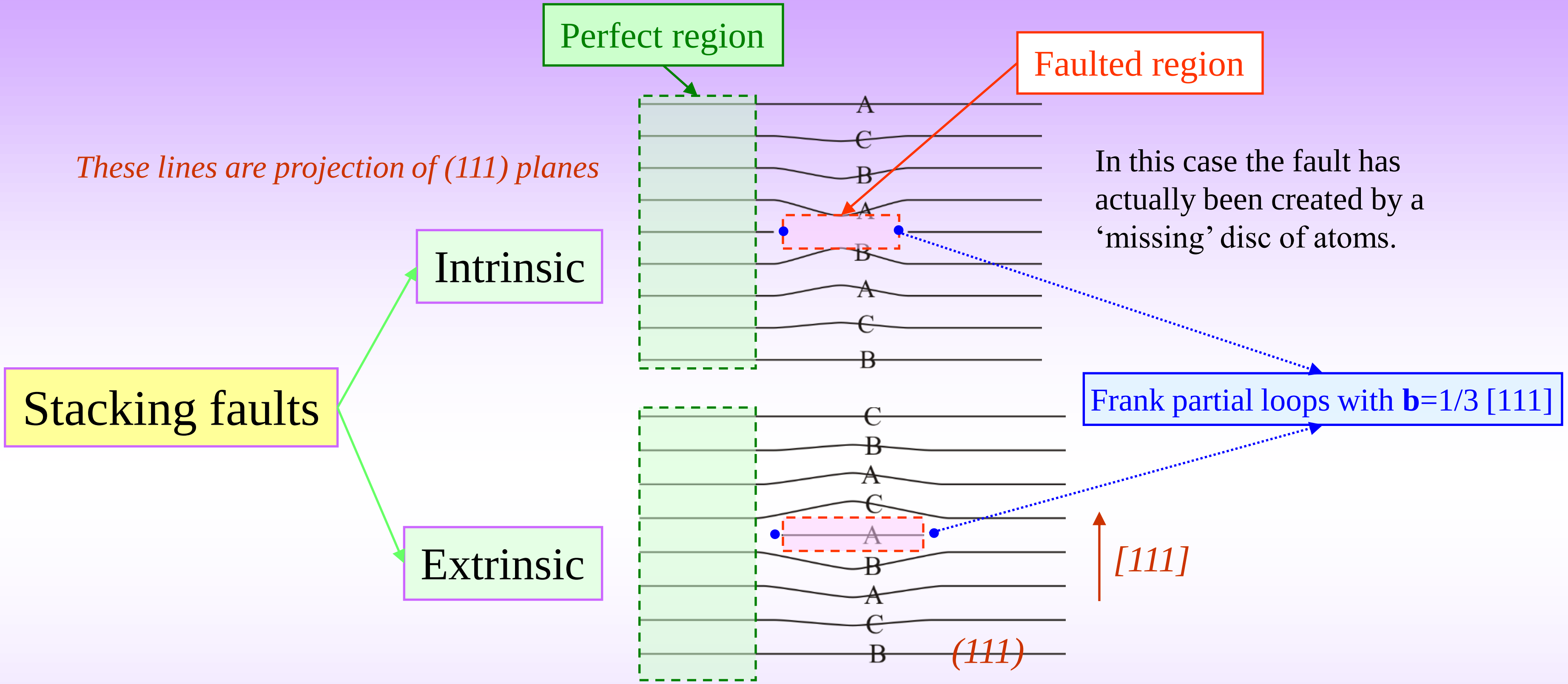
Partial dislocations: each with one atomic 'extra-half' plane

Dislocation loops and Frank Partial dislocations

- ❑ Formed by insertion or removal of a disc of atoms from the (111) plane.
- ❑ The (111) crystal plane consists of three atomic planes and the lattice translation vector along [111] has a magnitude of √3 (the distance between the atomic planes along [111] is √3/3). The packing along this direction is: ABCABCABC…
- ❑ ➢ Removal of a disc → Intrinsic fault
  ➢ Insertion of a disc → Extrinsic fault
- ❑ $\mathbf{b}_{\text{Frank Partial}} = [111]/3$
- ❑ As **b** is not on a slip plane (a member of the {111} family) the dislocation cannot move conservatively (i.e. without mass transport) → is a Sessile Dislocation (as opposed to a Glissile dislocation (which can move, e.g. the Shockley partials)).
- ❑ Excess vacancies (quenched-in or formed by irradiation) can form an intrinsic fault (these may have hexagonal shape in some cases).
- ❑ This shows that a dislocation loop can have a completely edge character; but never a completely screw character.

Frank partial dislocation loop bounding a stacking fault in CCP crystal

This shows that pure edge dislocation loop can exist (but a pure screw loop cannot exist)



Perfect region

Faulted region

These lines are projection of (111) planes

In this case the fault has actually been created by a ‘missing’ disc of atoms.

Stacking faults

Intrinsic

Extrinsic

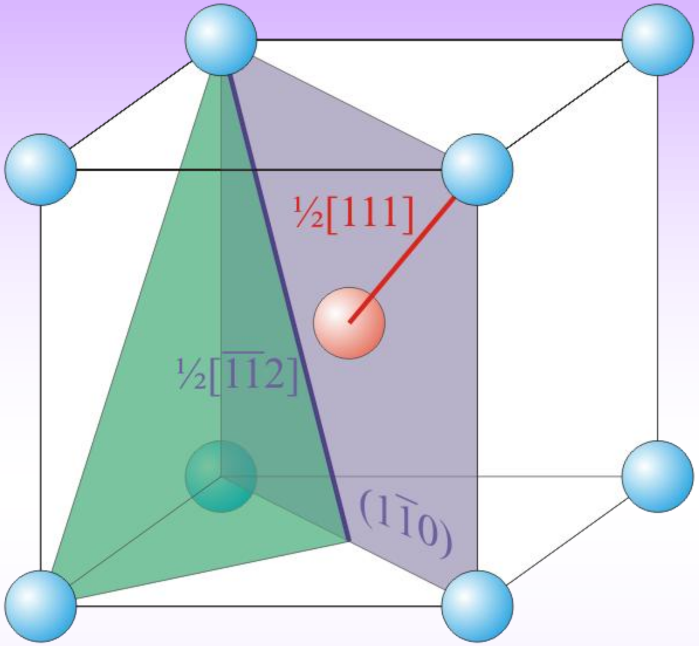
Frank partial loops with **b**=1/3 [111]

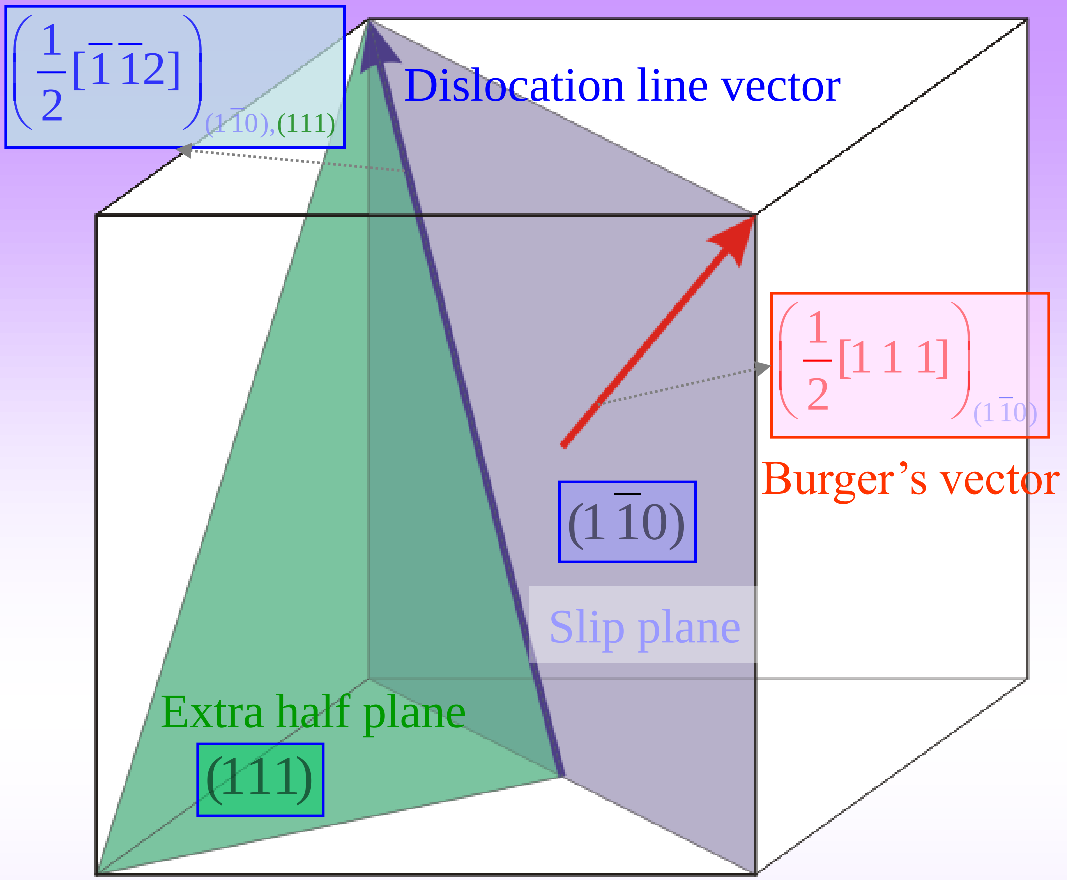
[111]

(111)

Two breaks introduced into the stacking sequence

BCC Pure edge dislocation




$\left(\frac{1}{2}[\bar{1}\,\bar{1}2]\right)_{(1\bar{1}0),(111)}$

Dislocation line vector

$\left(\frac{1}{2}[1\,1\,1]\right)_{(1\bar{1}0)}$

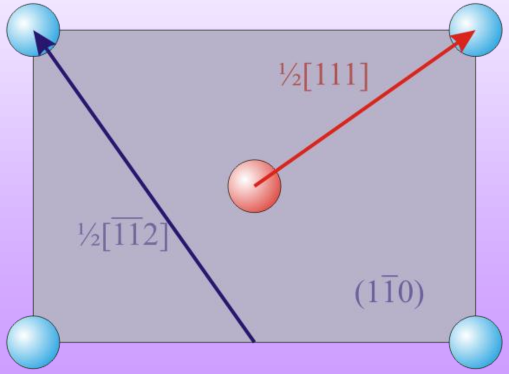
Burger's vector

$(1\,\bar{1}0)$

Slip plane

Extra half plane

(111)



Dislocations in Ionic crystals

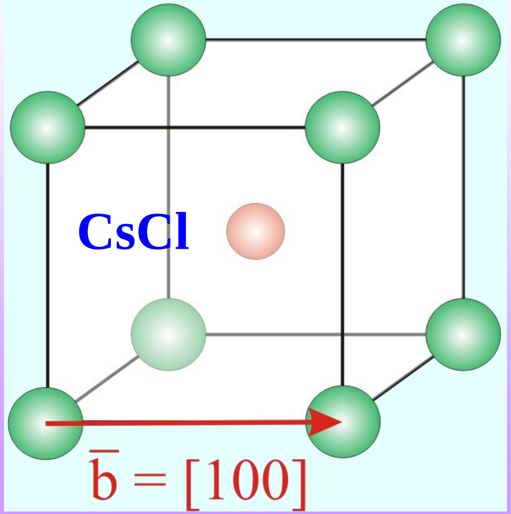
- In ionic crystals if there is an extra half-plane of atoms contained only atoms of one type then the charge neutrality condition would be violated→ this is an unstable condition.
- This implies that Burgers vector has to be a full lattice translation vector:

  CsCl → **b = <100>** *Cannot be ½<111>*

  NaCl → **b = ½ <110>** *Cannot be ½<100>*.
- This makes Burgers vector large in ionic crystals:

  Cu → |**b**| = 2.55 Å

  NaCl → |**b**| = 3.95 Å.
- A large value for Burgers vector implies a higher Peierls stress. It so happens that the stress required to propagate cracks in such materials is lower (i.e. $\sigma_f < \sigma_y$) and hence ionic materials are very brittle (at low temperatures).



Formation of dislocations (in the bulk of the crystal)

- ❑ Due to accidents in crystal growth from the melt.*
- ❑ Mechanical deformation of the crystal.
- ❑ Nucleation of dislocation.
  - ➢ Homogenous nucleation of a dislocation required high stresses (~G/10).
  - ➢ Stress concentrators in the crystal can aid the process.
- ❑ Dislocation density increases due to plastic deformation mainly by multiplication of pre-existing dislocations.

Typical values of Dislocation Density

- ❑ Dislocation density refers to the length of dislocation lines in a volume of material → hence the units are [m/m^3]
  (it is better not to cancel the 'm' in the numerator and the denominator and write as /m^2 as the units m/m^3 is more physical!).
- ❑ Annealed crystal: dislocation density (ρ) ~ $10^6 – 10^{10}$ m/m^3.
- ❑ Cold worked crystal: ρ ~ $10^{12} – 10^{14}$ m/m^3.
- ❑ As the dislocation density increases the crystal becomes stronger (more about this later).

Note: in this context it is noteworthy that screw dislocations can actually play a role in crystal growth → Constructive role of dislocations

Burgers vectors of dislocations in cubic crystals

Crystallography determines the Burgers vector
fundamental lattice translational vector lying on the slip plane

Monoatomic FCC	½<110>
Monoatomic BCC	½<111>
Monoatomic SC	<100>
NaCl type structure	½<110>
CsCl type structure	<100>
DC type structure	½<110>

A rule of thumb can be evolved as follows:

"Close packed volumes tend to remain close packed,
close packed areas tend to remain close packed &
close packed lines tend to remain close packed"

Close packed in this context implies 'better bonded'

Slip systems

- A combination of a slip direction (**b**) lying on a slip plane is called a slip system. This is described in terms of a family of directions and a family of planes.
- In close packed crystals it is a close packed direction lying on a close packed plane.
- In BCC crystals there are many planes with similar planar atomic density → there is no clear choice of slip plane. Hence, the slip lines are wavy.
- There might be more than one *active* slip system in some crystals *(e.g. BCC crystals below).*
  → *the active slip system gives rise to plastic deformation by slip.*
- Even if there is only one slip system is active at low temperature, more slip systems may become active at high temperatures → polycrystalline materials which are brittle at room temperature may become ductile at high temperatures.

Crystal	**Slip plane(s)**	**Slip direction**
FCC	{111}	<110>
HCP	(0001)	<11$\bar{2}$0>
BCC *Not close packed*	{110}, {112}, {123}	<111>

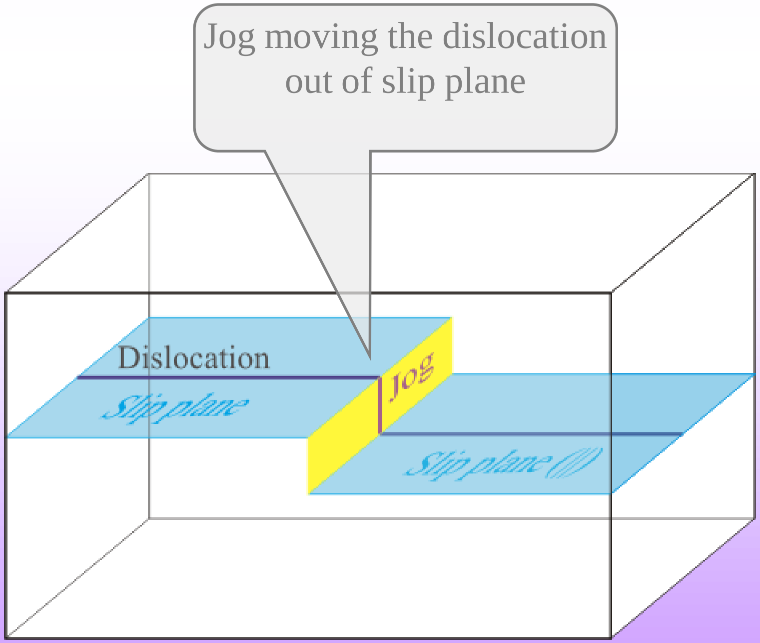
Anisotropic slip behaviour

No clear choice of slip plane
⇒ Wavy slip lines

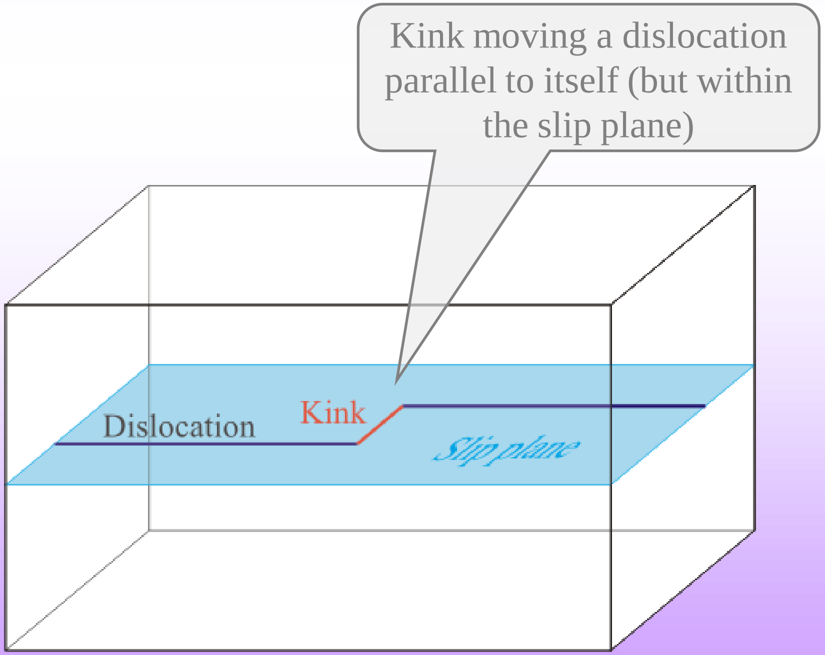
Jogs and Kinks

Defect in a defect!

- A straight dislocation line can have a break in it of two types:
  - A jog moves it out of the current slip plane *(→ to a parallel one)*
  - A kink leaves the dislocation on the slip plane.
- The Jog and the Kink can be considered as a defect in a dislocation line *(which itself is a defect →* *hence these are defects in a defect)*.
- Jogs and Kinks can be produced by intersection of straight dislocations.



Jogs



Kinks

- ☐ Jogs and Kinks in a screw dislocation will have edge character.
- ☐ Jog in a Edge dislocation has Edge character and Kink in a edge dislocation has screw character.

Jogs and Kinks: Character Table

	Edge dislocation	Screw Dislocation
Jog	Edge character	Edge character
Kink	Screw Character	Edge character

Jogs

- ☐ The presence of a jog in a dislocation line increases the energy of the crystal.
- ☐ The energy of a jog per unit length is less than that for the dislocation (as this lies in the distorted region near the core of the dislocation).
- ☐ This energy is about 0.5-1.0 eV ($\sim 10^{-19}$ J) for metals.

$$E_{Jog} = \alpha G b_1^2 b_2$$

- $\mathbf{b}_1 \rightarrow$ Burgers vector of the dislocation
- $b_2 \rightarrow$ Length of the jog
- $\alpha \rightarrow$ Constant with value $\in$ (0.5-1.0)

Dislocation-Dislocation Interactions

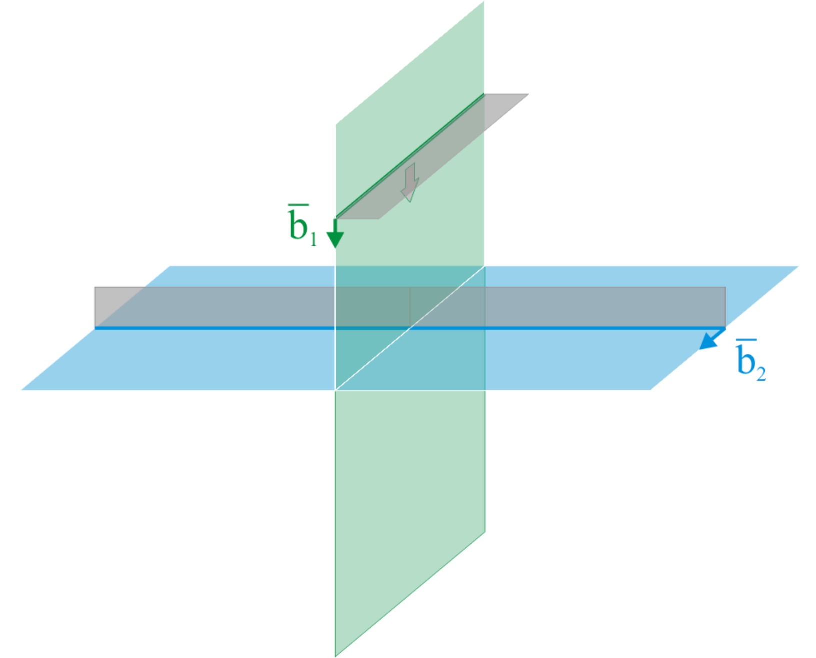
- Two straight dislocation can intersect to leave Jogs and Kinks in the dislocation line
- These extra segments in a dislocation line cost energy and hence require work done by the external force ⇒ lead to hardening of the material
  (Additional stress as compared to the stress required to glide the dislocation line is required to form the Jog/Kink)
- Four types of interactions are considered next.

1

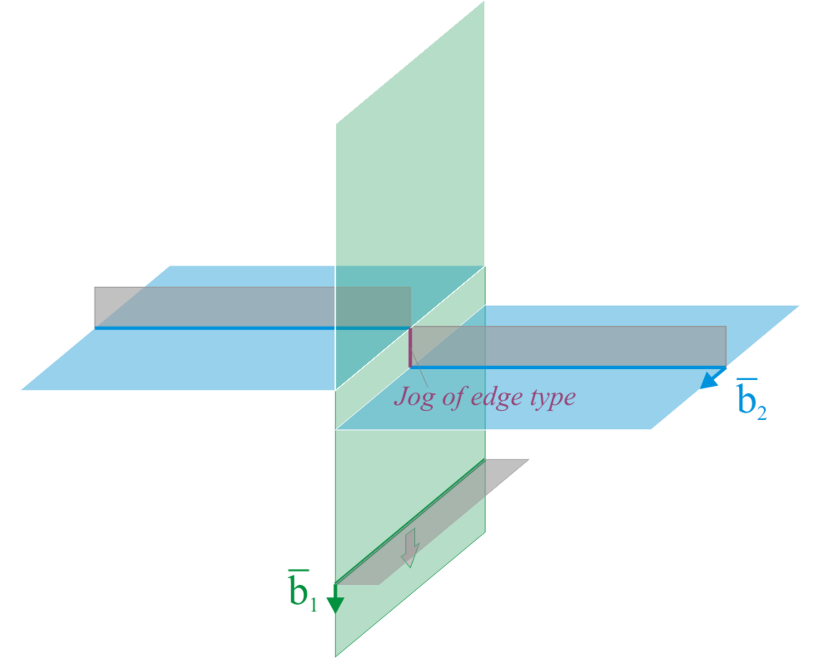
Edge-Edge Intersection

Perpendicular Burgers vector

- The jog has edge character and can glide *(with Burgers vector =* $\boldsymbol{b}_2$*)*
- The length of the jog = $\mathbf{b}_1$
- Edge Dislocation-1 *(Burgers vector* $\mathbf{b}_1$*)* → Unaffected as $\mathbf{b}_2$ is $\parallel$ $\mathbf{t}_1$ *(line vector)*
- Edge Dislocation-2 *(Burgers vector* $\mathbf{b}_2$*)* → Jog (Edge character) → Length $|\mathbf{b}_1|$



Intersection between two edge dislocations producing a Jog



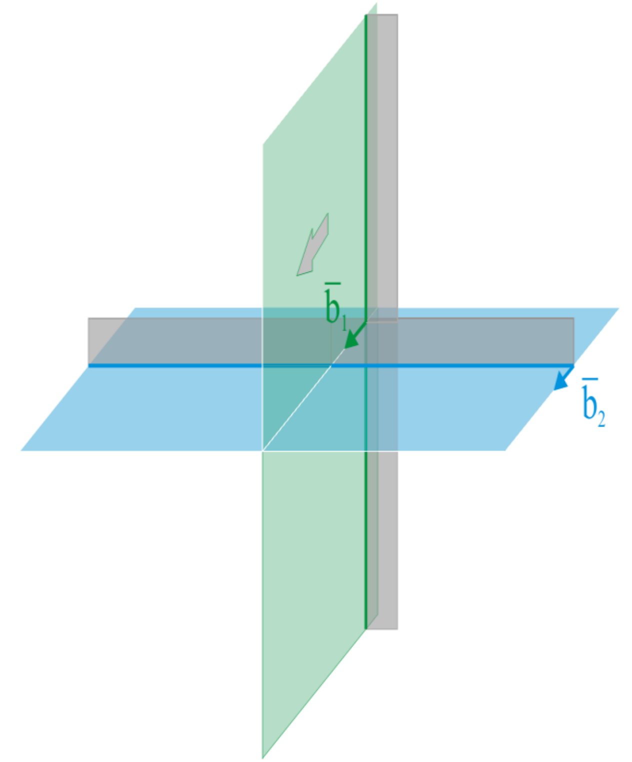
Intersection between two edge dislocations producing a Jog

2

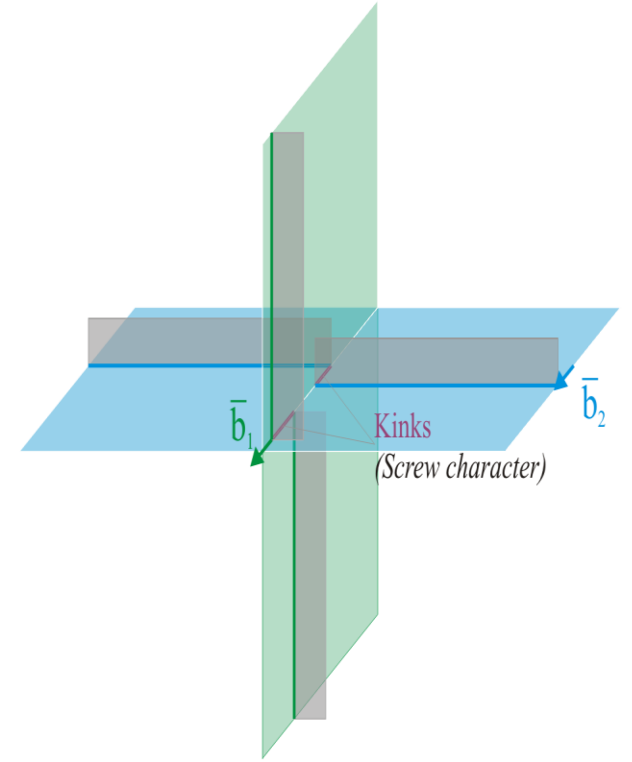
Edge-Edge Intersection

Parallel Burgers vector

- Both dislocations are kinked
- Edge Dislocation-1 *(Burgers vector* $\mathbf{b}_1$*)* → Kink (Screw character) → Length $|\mathbf{b}_2|$
- Edge Dislocation-2 *(Burgers vector* $\mathbf{b}_2$*)* → Kink (Screw character) → Length $|\mathbf{b}_1|$
- The kinks can glide



Intersection between two edge dislocations



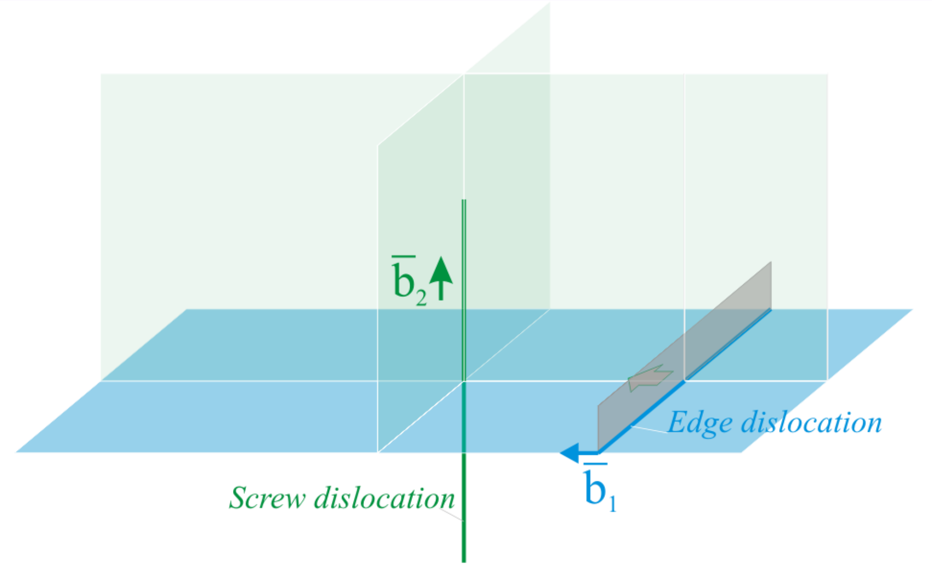
Intersection between two edge dislocations

3

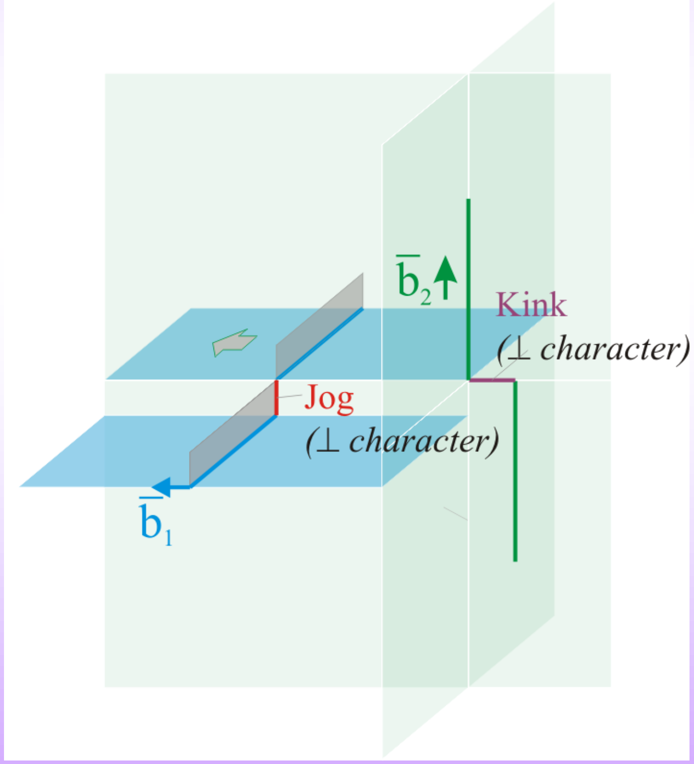
Edge-Screw Intersection

Perpendicular Burgers vector

- Edge Dislocation *(Burgers vector* $\mathbf{b}_1$*)* → Jog (Edge Character) → Length $|\mathbf{b}_2|$
- Screw Dislocation *(Burgers vector* $\mathbf{b}_2$*)* → Kink (Edge Character) → Length $|\mathbf{b}_1|$



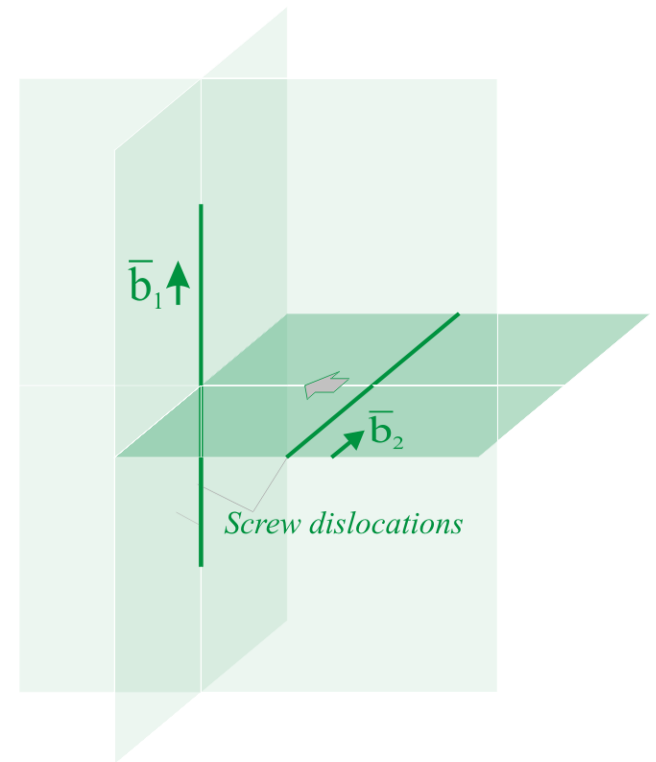
Intersection between an edge & a screw dislocation



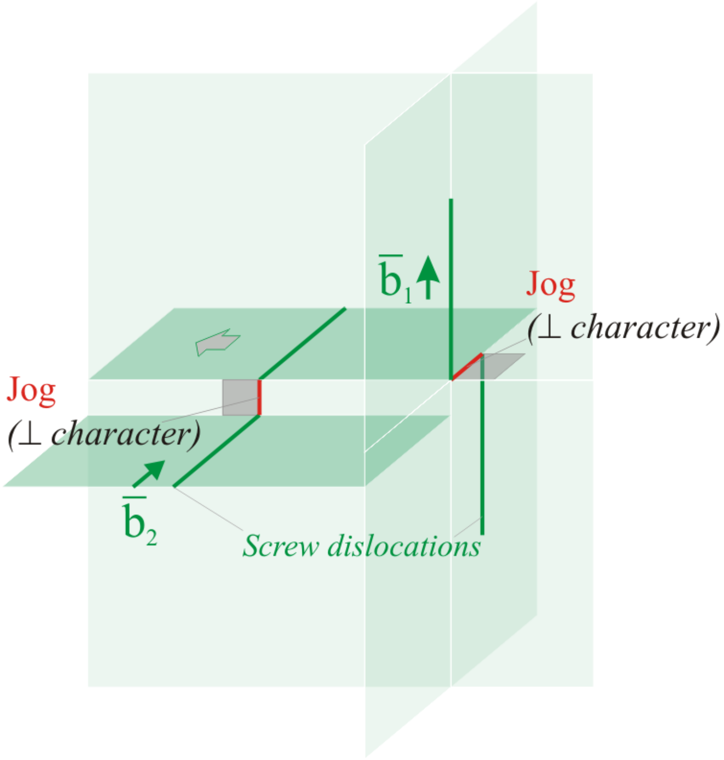
4 Screw -Screw Intersection

Perpendicular Burgers vector

- Important from plastic deformation point of view
- Screw Dislocation *(Burgers vector* $\mathbf{b}_1$*)* → Jog (Edge Character) → Length $\mathbf{b}_2$
- Screw Dislocation *(Burgers vector* $\mathbf{b}_2$*)* → Jog (Edge Character) → Length $\mathbf{b}_1$
- Both the jogs are non conservative
  (i.e. cannot move with the dislocations by glide)



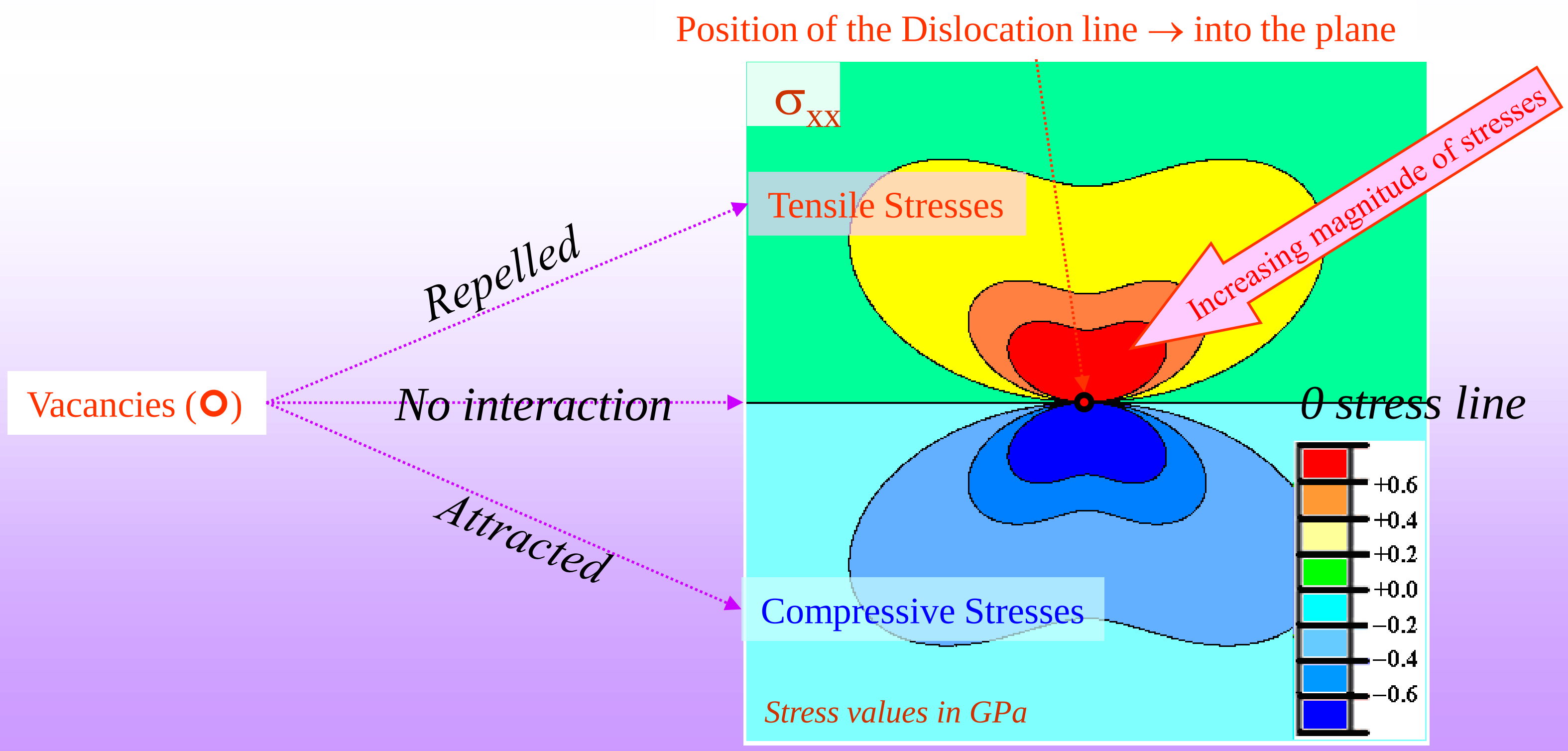
Intersection between two screw dislocations



Dislocation-Point defect Interactions

- The stress field of a dislocation can interact with the stress field of point defects.
- Defects associated with tensile stress fields are attracted towards the compressive region of the stress field of an edge dislocation *(and vice versa)*.
- Solute atoms can segregate in the core region of the edge dislocation *(formation of the Cottrell atmosphere)* → higher stress is now required to move the dislocation *(the system is in a low energy state after the segregation and higher stress is required to 'pull' the dislocation out of the energy well).*
- Higher free-volume at the core of the edge dislocation aids this segregation process.
- Defects associated with shear stress fields (having a non-spherical distortion field; e.g. interstitial carbon atoms in BCC Fe) can interact with the stress field of a screw dislocation.

- Vacancies are attracted to the compressive regions of an edge dislocation and are repelled from tensile regions. This is due to stress gradients (i.e. increasing stress as we move closer to the dislocation line).
- The behaviour of substitutional atoms smaller than the parent atoms is similar to that of the vacancies.
- Larger substitutional atoms are attracted to the tensile region of the edge dislocation and are repelled from the compressive regions.
- Interstitial atoms (associated with compressive stress fields) are attracted towards the tensile region of the edge dislocation and are repelled from the compressive region of the stress field.

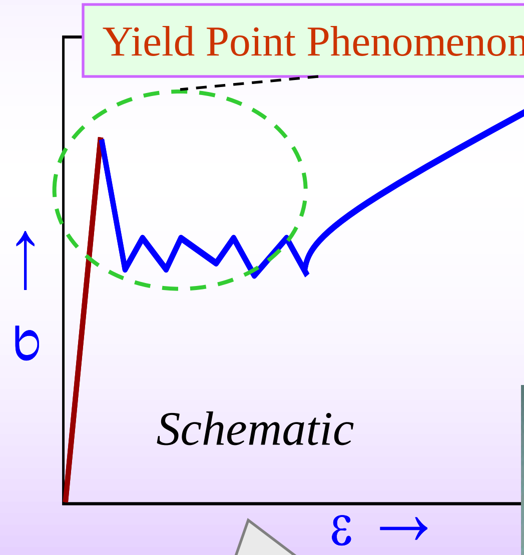


Summary of edge dislocation - point defect interactions

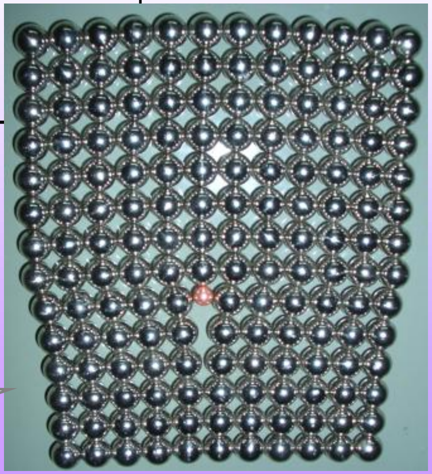
Point Defect	Tensile Region	Compressive Region
Vacancy	Repelled	Attracted
Interstitial *(of size larger than the void)*	Attracted	Repelled
Smaller substitutional atom	Repelled	Attracted
Larger Substitutional atoms	Attracted	Repelled

Yield Point Phenomenon

- ❑ The interaction of interstitial carbon atoms with edge dislocations *(interaction of stress fields of dislocations with solute atoms)* → leading to their segregation to the core of the edge dislocations (forming a Cottrell atmosphere) is responsible for the Yield Point Phenomenon seen in the tensile test of mild steel specimens.
- ❑ In Yield point phenomenon, there is a yield drop (when the dislocation breaks free of Cottrell atmosphere) followed by serrated yielding (due to repeated 'pinning' of edge dislocations by carbon atoms).

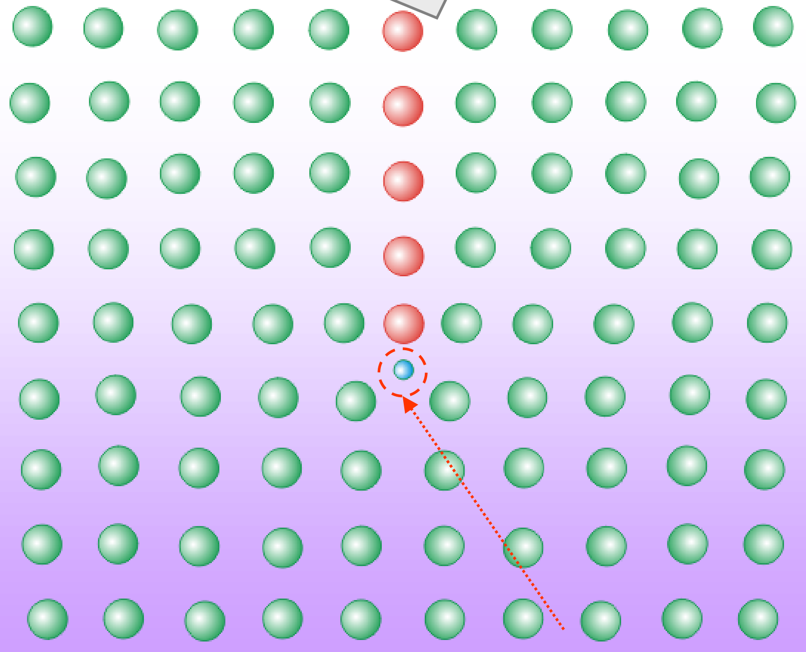


More about this in the chapter on plasticity



Model made of magnetic balls *(core segregation)*

This is low energy state as compared to a isolated interstitial atom and a isolated dislocation.



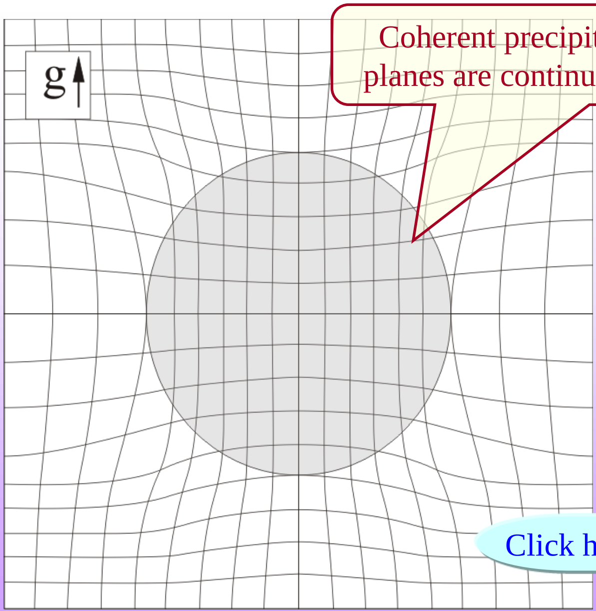
Interstitial Atom at the core

Dislocation-Precipitate Interactions

- Dislocations can interact with the stress fields of precipitates.
- Moving dislocations can:

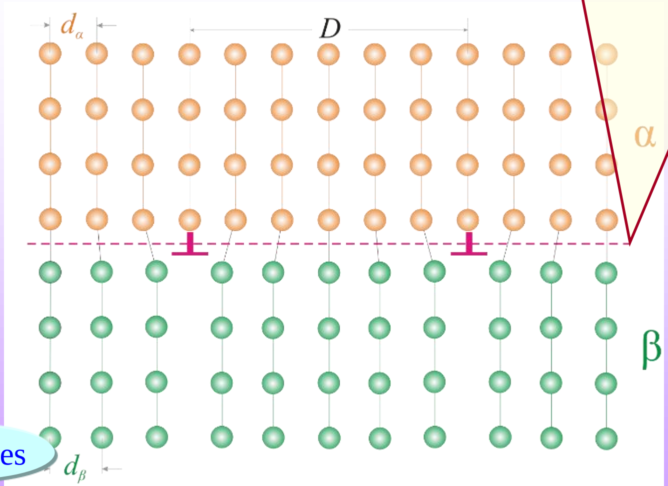
  A ◘ glide through coherent precipitates* → shearing the precipitate.

  B ◘ bow around incoherent precipitates, leaving loops as they bypass two precipitates which act like pinning centres for the dislocations *(→ leading to an increase in the dislocation density).*
- Both these processes need an application of higher stresses (assuming an harder precipitate) → lead to the strengthening of the material.
- Semi-coherent precipitates have interfacial misfit dislocations which partially relieve the coherency strains. *(These dislocations are structural dislocations).*



Coherent precipitate- note that the lattice planes are continuous across the precipitate

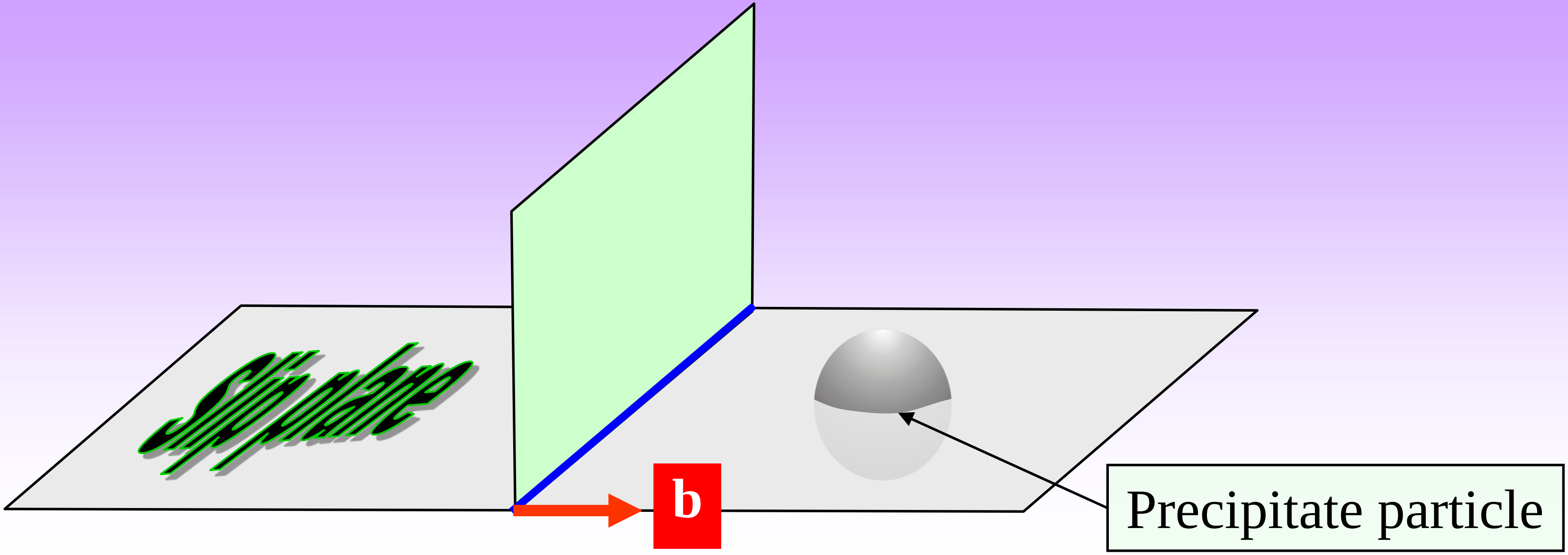
Semi-Coherent interface

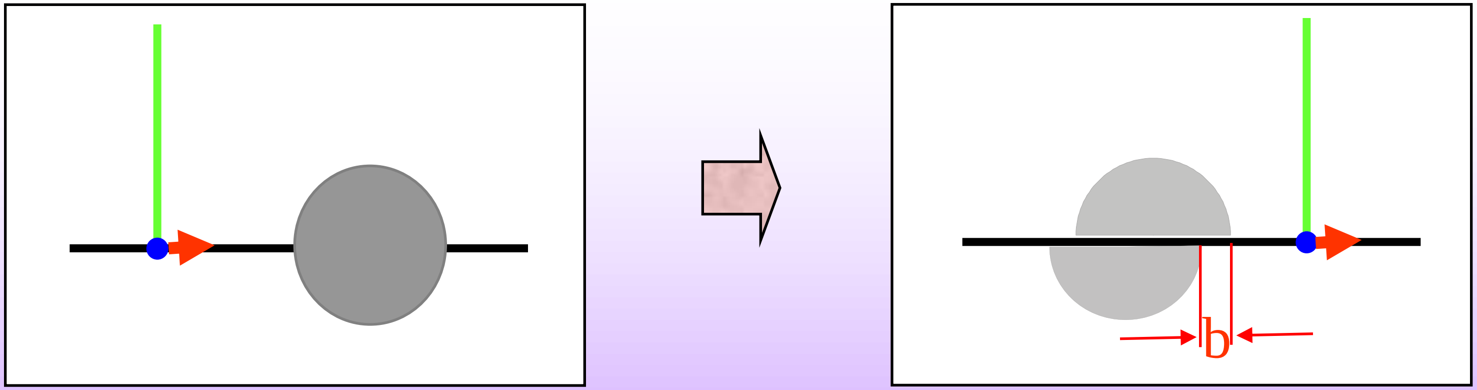


Click here to know more about interfaces

* *Though the word coherent is used as an adjective for the precipitate- actually what is meant is that the interface is coherent (or semi-coherent if we talk about a semi-coherent precipitate)*

A ◘ Glide through coherent precipitates





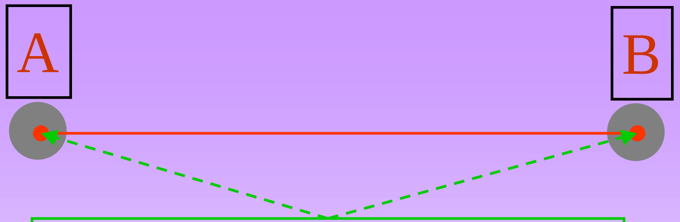
B ◘ Bow around incoherent precipitates

Double Ended Frank-Read Source

- ❑ A dislocation can be pinned between two incoherent precipitate particles (or in other ways), thus hindering the motion of the dislocation.
- ❑ For motion of the dislocation, leading to plasticity the dislocation has to bypass the pinned segment, under the action of the applied stress (shear stress on the slip plane drives the motion).
- ❑ The dislocation takes a series of configurations (as shown the in the figures) under the action of the applied stress → leading to the formation of a dislocation loop *(leaving the original pinned segment)*.
- ❑ This leads to an increase in dislocation density *(one of the mechanisms by which dislocation density increases with plastic deformation)*.
- ❑ As the original segment is retained the 'source' (Frank-Read source) can operate repeatedly forming a loop each time.
- ❑ As the preexisting loops would oppose the formation of the next loop (repulsive stresses-dislocations of the same sign), higher stresses are required to operate the source each time.
- ❑ Till the formation of the half-loop (semi-circle), increasingly higher stresses are required. After this the process occurs downhill in stresses.
- ❑ The maximum stress (τ_{max}) required to operate the source thus corresponds to the formation of the half-loop (with radius r_{min}).

$$\tau_{\max} \sim \frac{Gb}{2r_{\min}}$$

Initial configuration

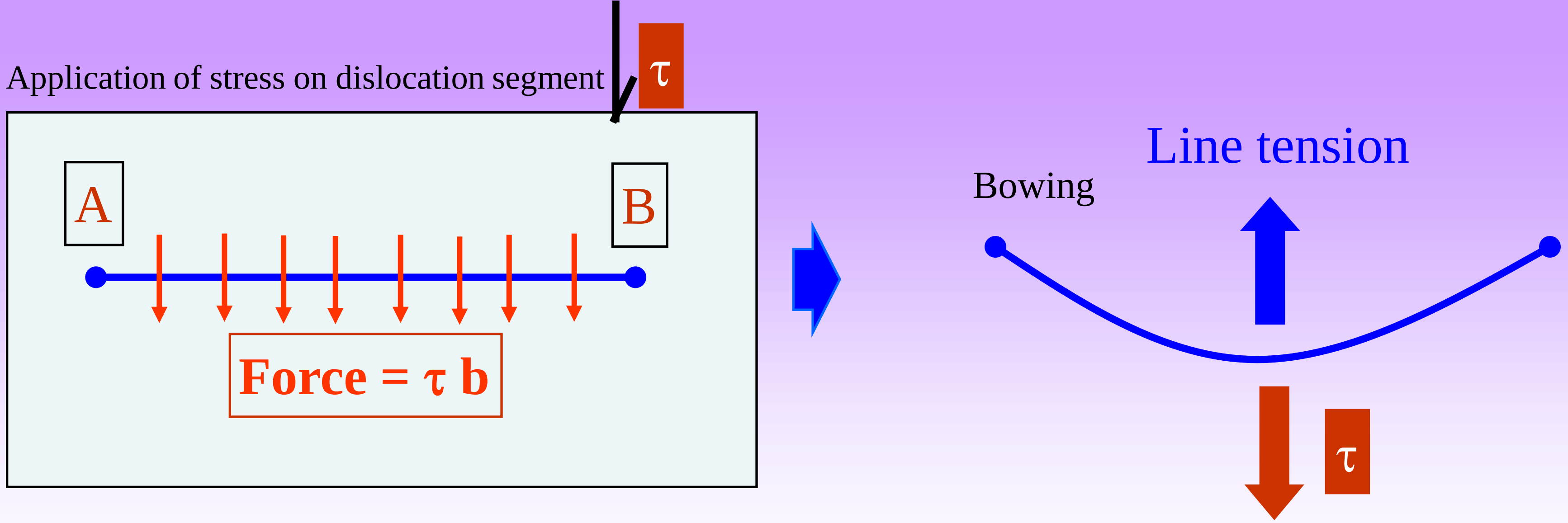


Dislocation line segment pinned at A and B by precipitates*

*** Pinning could (also) be caused by:**

- Dislocation in the plane of the paper intersects dislocations in other planes
- Anchored by impurity atoms or precipitate particles
- Dislocation leaves the slip plane at A and B

Application of stress on dislocation segment



- *As the dislocation line gets curved the energy of the system increases ⇒ work has to be done by external stresses to cause this extension.*
- *Line tension (opposes the shear stress on the slip plane (τ). At a given stress there might be a balances of forces leading to a curved geometry of the dislocation line.*
- *Further extension of the dislocation line occurs by increasing the stress.*

$$\text{Force on dislocation line} = \tau\, b\, ds$$

$$\text{Dislocation energy / length} = \ \gamma \sim \frac{1}{2} G b^2$$

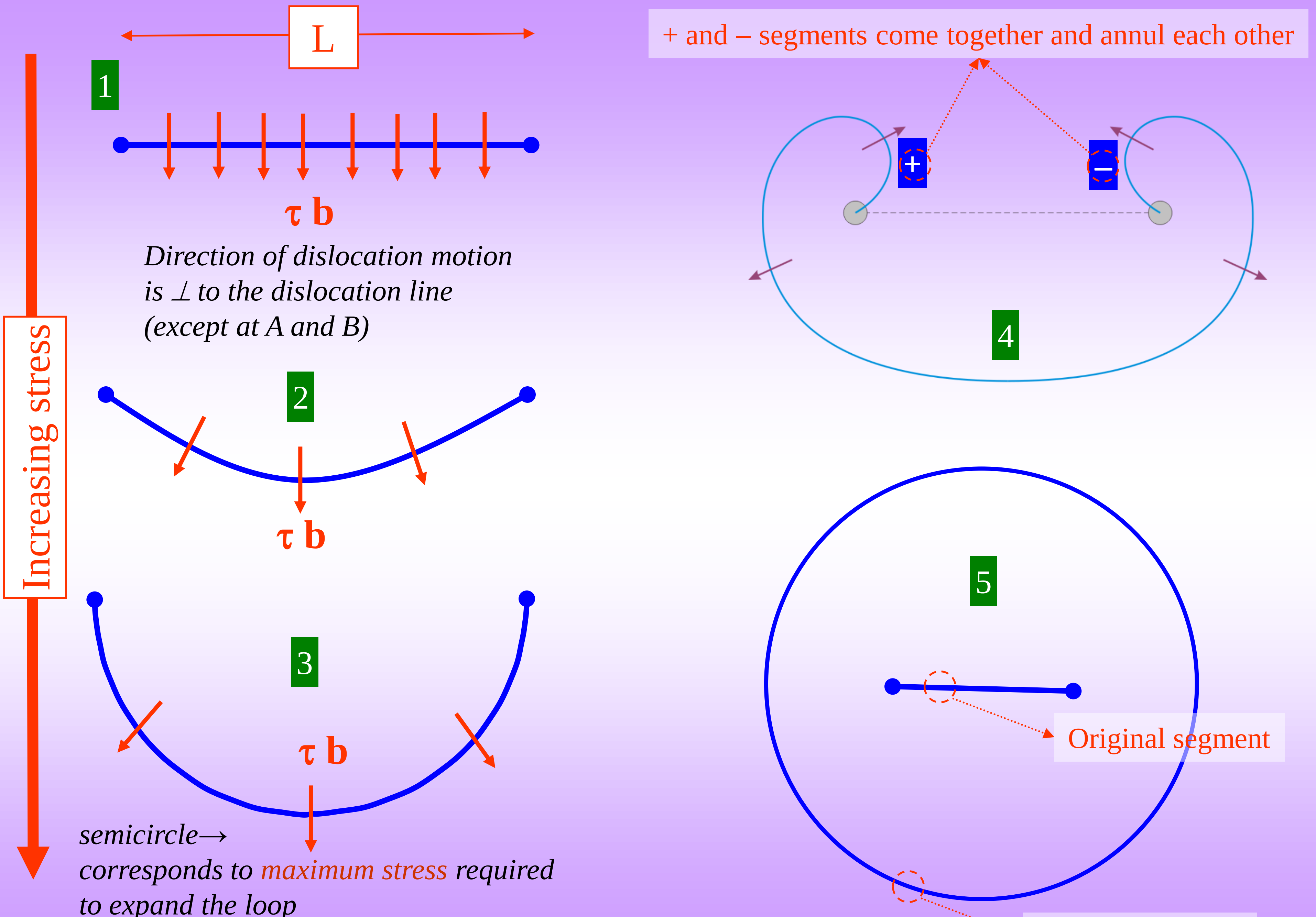
$$\text{Line tension force} = 2\,\gamma \sin\left(\frac{d\theta}{2}\right) \sim \gamma\, d\theta$$

For equilibrium in curved configuration →

$$\gamma\, d\theta = \tau\, b\, ds$$

$$\tau \sim \frac{Gb}{2r}$$

$$\tau_{max} \Rightarrow r_{min}$$



+ and – segments come together and annul each other

Direction of dislocation motion
is ⊥ to the dislocation line
(except at A and B)

semicircle→
corresponds to maximum stress required
to expand the loop

Original segment

New loop created

After this decreasing stress is required to expand the loop

Frank-Read dislocation source →

- Can operate from a single source producing a loop each time
- This loop produces a slip of 1**b** each time on the slip plane
- The maximum value of shear stress required is when the bulge becomes a semi-circle ($r_{min} = L/2$) → $\tau_{max} \sim Gb/L$

  ⇒ $\tau\downarrow$ as $L\uparrow$ i.e. The longest segments operate first

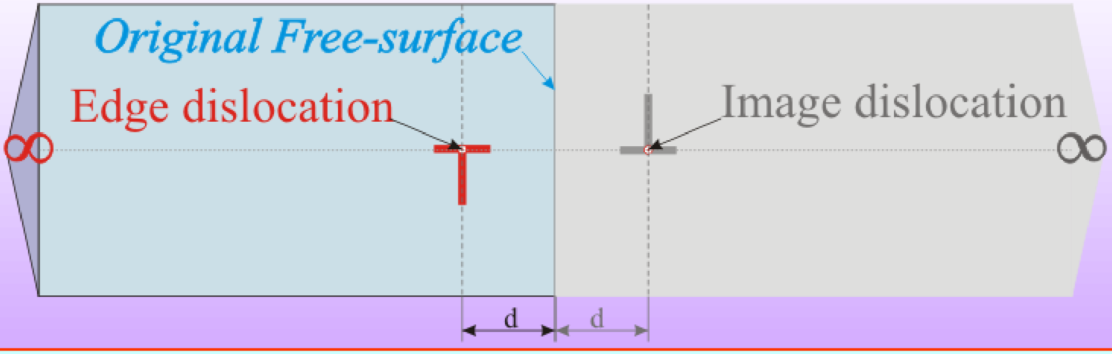
  ► When the long segments get immobilized shorter segments operate with increasing stress

  ⇒ *work hardening*
- If the dislocation loops keep piling up on the slip plane the back stress will oppose the applied stress
- When the *back-stress* > τ_{max} the source will cease to operate
- Double ended F-R sources have been observed experimentally they are not frequent ⇒ other mechanisms must exist

$\tau_{max} = \alpha Gb/L$ α = 0.5 for edge dislocations and α = 1.5 for screw dislocations.

Dislocation- Free surface Interaction → Concept of Image Forces

- A dislocation near a free surface (in a semi-infinite body) experiences a force towards the free surface, which is called the image force. This is a type of Configurational Force *(i.e. force experienced when the energy is lowered by a change in configuration of a system)*
- The force is called an 'image force' as the force can be calculated assuming an negative hypothetical dislocation on the other side of the surface *(figure below).* The force of attraction between the dislocations (+ & –) is gives the image force. The material properties are identical throughout.
- If the image force exceeds the Peierls stress then the dislocation can spontaneously leave the crystal, without application of external stresses!
- Hence, regions near a free surface and nano-crystals can become spontaneously dislocation free. In nanocrystals due to the proximity of more than one surface, many images have to be constructed and the net force is the superposition of these image forces.

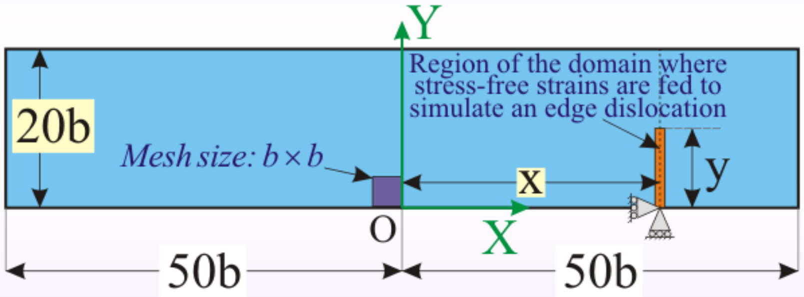


$$F_{image} = \frac{-Gb^2}{4\pi(1-\nu)d}$$

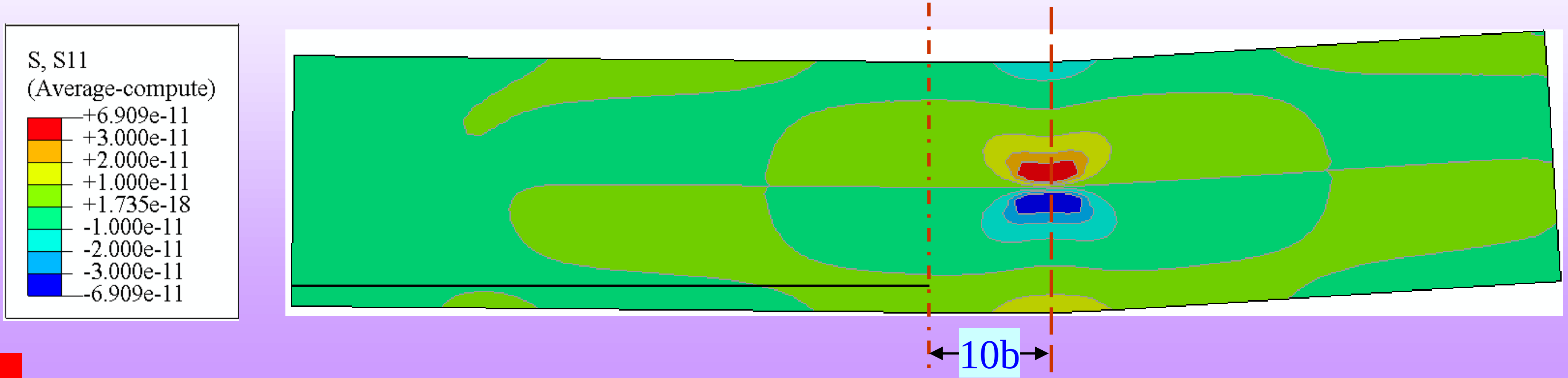
A hypothetical negative dislocation is assumed to exist across the free-surface for the calculation of the force (attractive) experienced by the dislocation in the proximal presence of a free-surface

Domain deformations in Nanocrystals in the presence of dislocations

- Dislocation near a free surface in a semi-infinite body can deform the surface. This is a small deformation as shown in the figure below for the case of an edge dislocation.
- In nanocrystals *(e.g. the kind shown in the figure below)* the domain can bend/buckle in the presence of dislocations *(the figure shows the effect of an edge dislocation in a plate → a screw dislocation leads to the twisting of - for example - a cylindrical domain)*
- This is elastic deformation in the presence of dislocations in a nanomaterial!
  - Hence, we can have *reversible plastic deformation due to elasticity!!!*



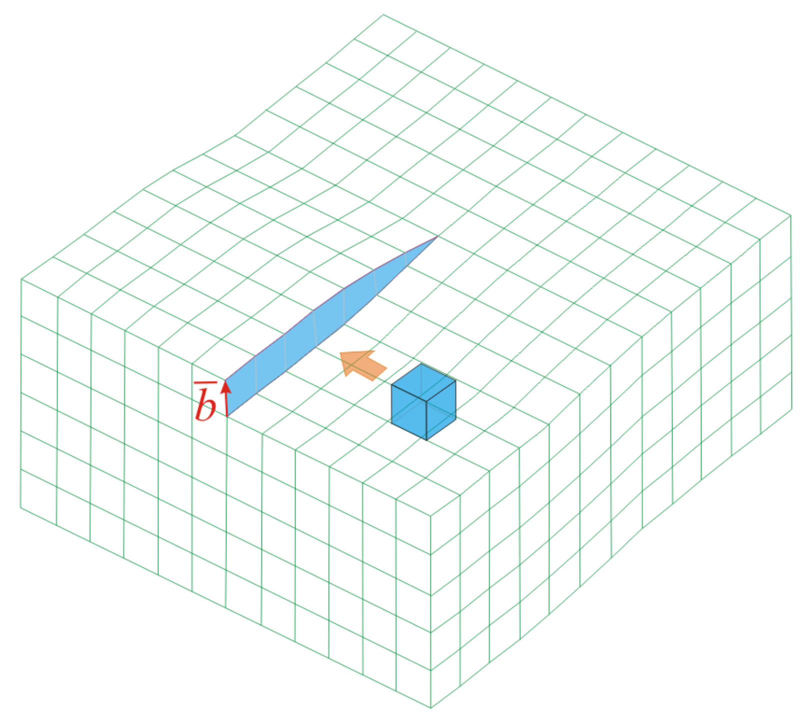
Dislocation in a thin 'plate' of Al leading to its bending

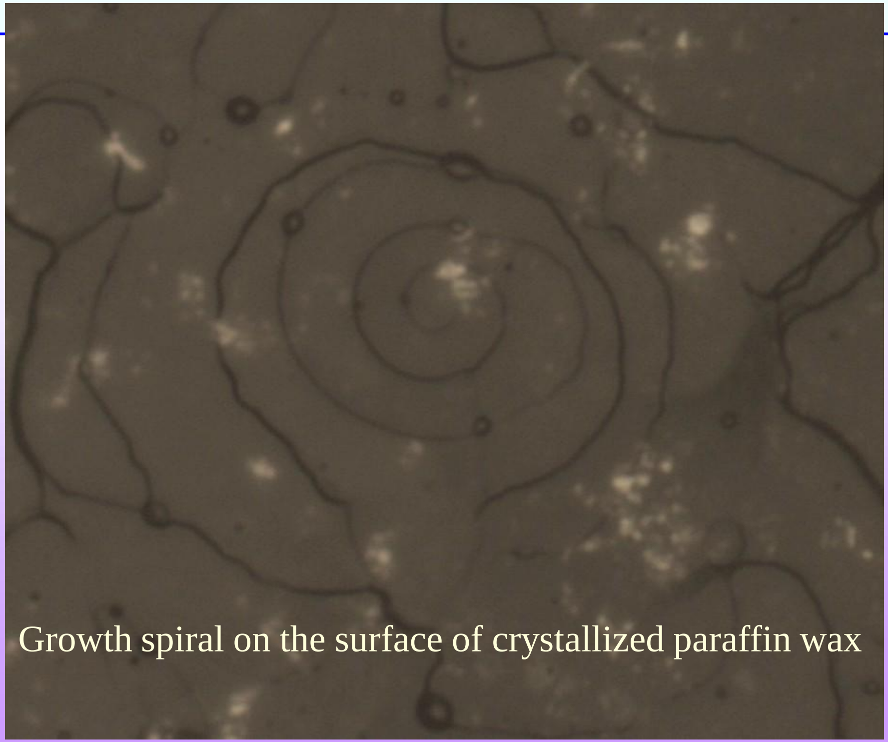


Role of dislocations in crystal growth

Constructive role of dislocations!

- Crystals grown under low supersaturation (~1%) the growth rate is considerably faster than that calculated for an ideal crystal
- In an ideal crystal surface the difficulty in growth arises due to difficulty in the nucleation of a new monolayer
- If a screw dislocation terminates on the surface of a crystal then addition of atoms can take place around the point where the screw dislocation intersects the surface *(the step)* → leading to a spiral (actually spiral helix) growth staircase pattern





Growth spiral on the surface of crystallized paraffin wax

Role of dislocations in phase transformation

- Dislocations can act as heterogeneous nucleation sites during phase transformation.
  - Dislocations may dictate the orientation and morphology of the second phase.
- The stain associated with the dislocation may be partly relieved by the formation of a second phase.
- The strain associated with the transformation (the Eshelby strain) may be accommodated by plastic flow (mediated by dislocations).

Mental Picture of a dislocation

Let us consider the various ways of understanding the dislocation
→ The different perspectives

- ☐ Association with translational symmetry
- ☐ As a line defect
- ☐ Distortion of bonds → region of high energy
- ☐ Increase in entropy of the system
- ☐ Free volume at the core → pipe diffusion
- ☐ Core of dislocation & its geometry → Peierls Stress
- ☐ Stress & Strain fields
- ☐ Interaction with other defects
- ☐ Role in slip
- ☐ Role as a structural defect

Funda Check

Why are dislocations non-equilibrium defects?

$\Delta G = \Delta H - T\Delta S$ ← +ve for dislocations

- It is clear from the above equation that if a configuration* gives an entropy benefit (i.e. ΔS is positive); then that state will be stabilized at some temperature (even if the enthalpy cost is very high for that configuration)
- In the present case: it costs an energy of $\sim Gb^2/2$ per unit length of dislocation line introduced into the crystal; but, this gives us a configurational entropy benefit (as this dislocation can exist in many *equivalent* positions in the crystal)
- This implies that there must be temperature where dislocations can become stable in the crystal (ignoring the change in the energy cost with temperature for now)
- *Unfortunately this temperature is above the melting point of all known materials*
- Hence, dislocations are not stable thermodynamic defects in materials

► The energy required to create Kinks and Jogs of length ‘b’ is **$\sim Gb^3/10$**
→ these can be created by thermal fluctuations

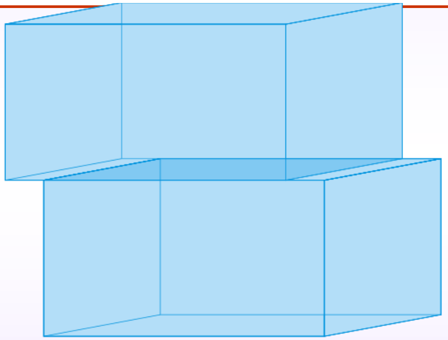
* *Including positional, electronic, rotational & vibrational multiplicity of states*

Funda Check

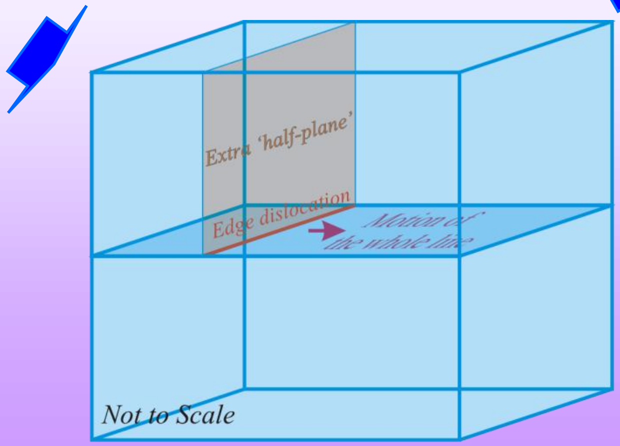
How are crystals weakened?

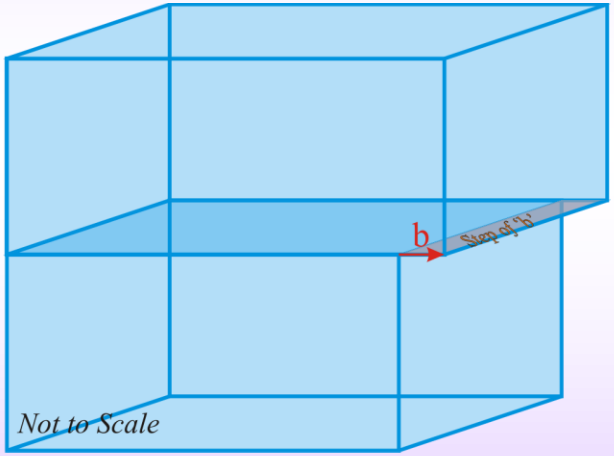
The two step process

- As we have seen the process of sliding (by shear) of an ‘entire plane’ of atoms can be reduced to a *‘line-wise’* process by dislocations
  ► this leads to a shear stress reduction of a few orders of magnitude
- This problem can be further broken down (in dimension and energy) to the formation and migration of kink pairs along the dislocation line *(usually occurs to screw components of dislocations in BCC metals)*
  ► this can further lead to the reduction in stress required for dislocation motion



Shearing of a whole part of a crystal with respect to another





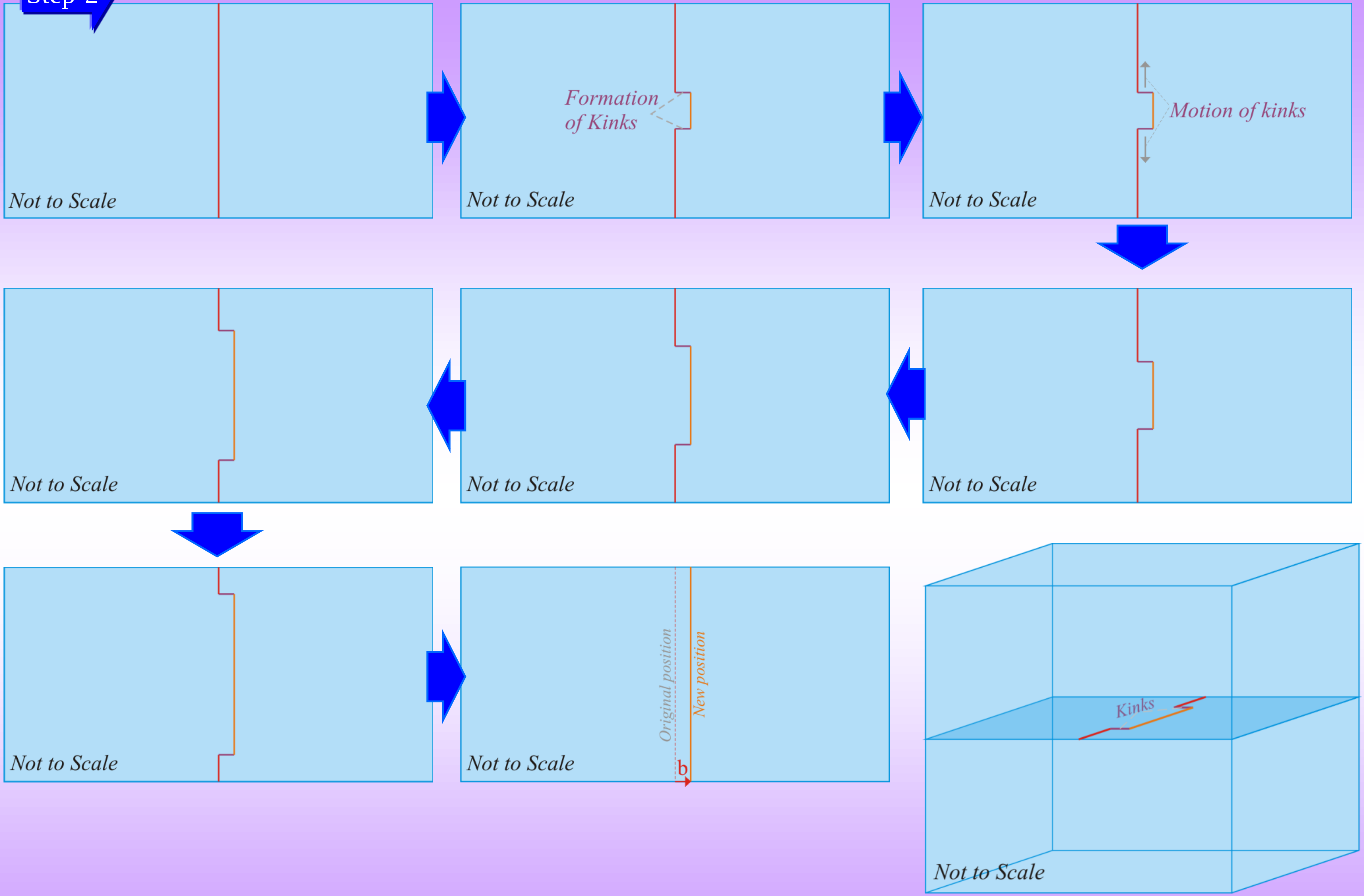
Step-1

Motion of dislocation line
→ leaving the crystal

Continued…

Step-2

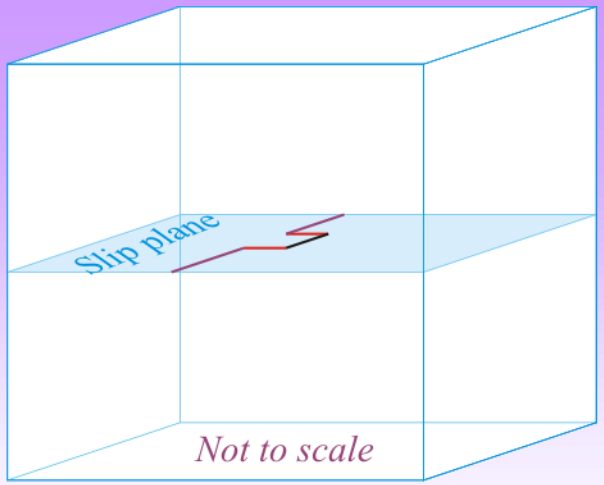
Further break up of the motion of the dislocation

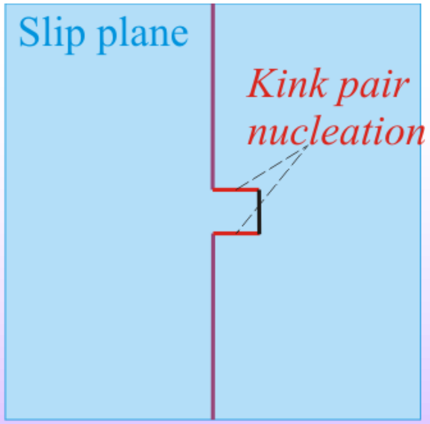


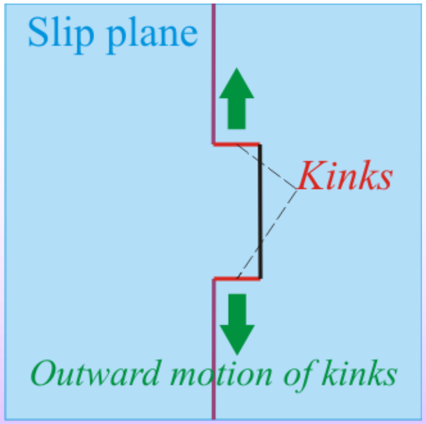
- In BCC metals and Ge thermally assisted formation of kink pairs can cause slip at stresses $\tau < \tau_{PN}$

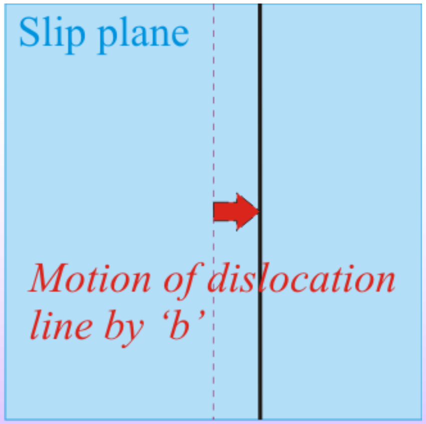
Continued…

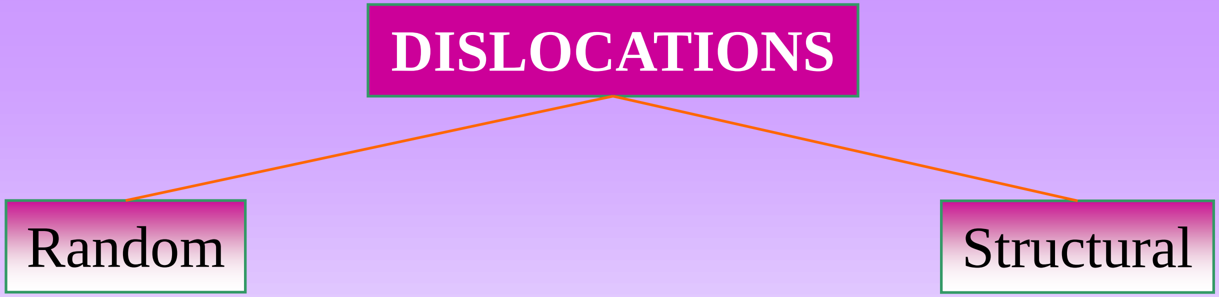
More views


Slip plane
Not to scale


Slip plane
Kink pair
nucleation


Slip plane
Kinks
Outward motion of kinks


Slip plane
Motion of dislocation
line by 'b'



DISLOCATIONS

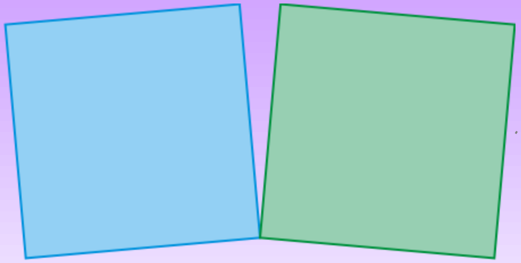
Random

Structural

Distinct from ‘Geometrically Necessary Dislocations’ (GND)

- As mentioned before: Structural defects play a very different role in material behaviour as compared to “Random Statistical Defects” *(non-structural)*
- Structural dislocations may be associated with a boundary and hence their role in plasticity may be very different from random (“statistically stored”) dislocations
- Often a related term- Geometrically Necessary Dislocations is used in literature *(we have intentionally avoided the use of the term here)*
- Structural dislocations include:
  - Dislocations at low angle grain boundaries (will be discussed along with other 2D defects)
    → responsible for a tilt or twist
  - Dislocation at semi-coherent interfaces
    → responsible for matching misfit (between adjacent crystals)

Accommodated by an array of edge dislocations



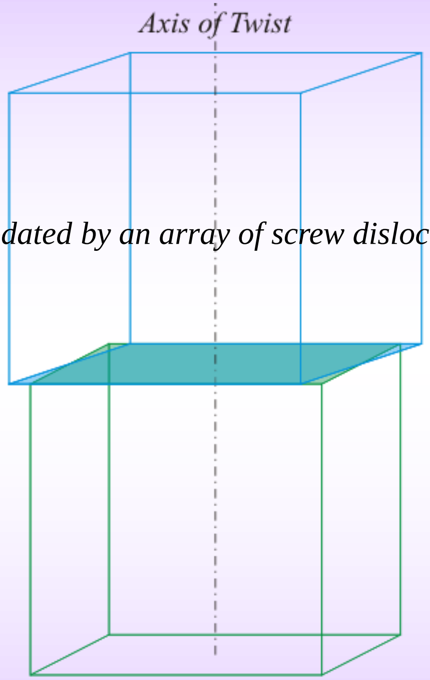
Tilt

Structural dislocations can accommodate

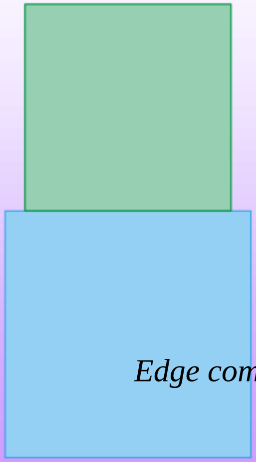
between two crystals

Twist

Accommodated by an array of screw dislocations



Misfit



Edge component relieves misfit strain

More on some of this in the chapter on 2D defects

Funda Check

What determines the Burgers vector?

- There are two distinct questions we can ask:
  Q1➢ If you already have a dislocation how to determine the Burgers vector?
  Q2➢ What determines the Burgers vector?
- The answer to Q1 is by constructing a Burgers circuit
- The answer to Q2 is: Crystallography → the Burgers vector is the shortest lattice translation vector (for a perfect/full dislocation)

Solved Example

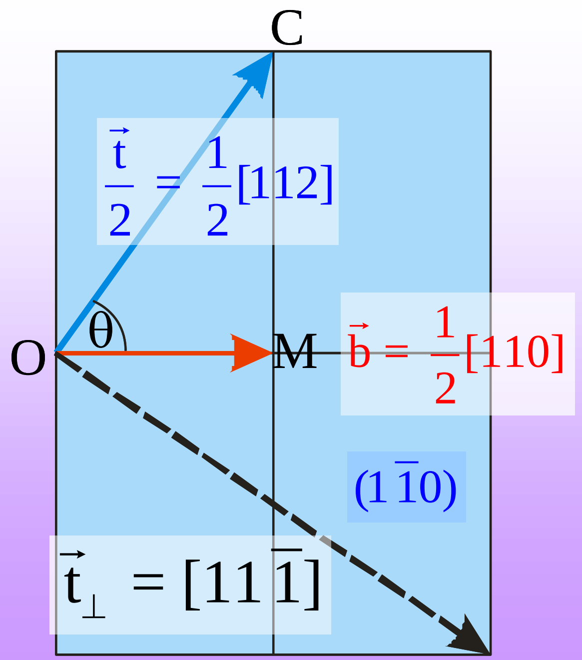
In a cubic crystal a dislocation line of mixed character lies along the [112] direction. Burgers vector = ½[110]. What are the edge and screw components of the Burgers vector? Which is the slip plane?

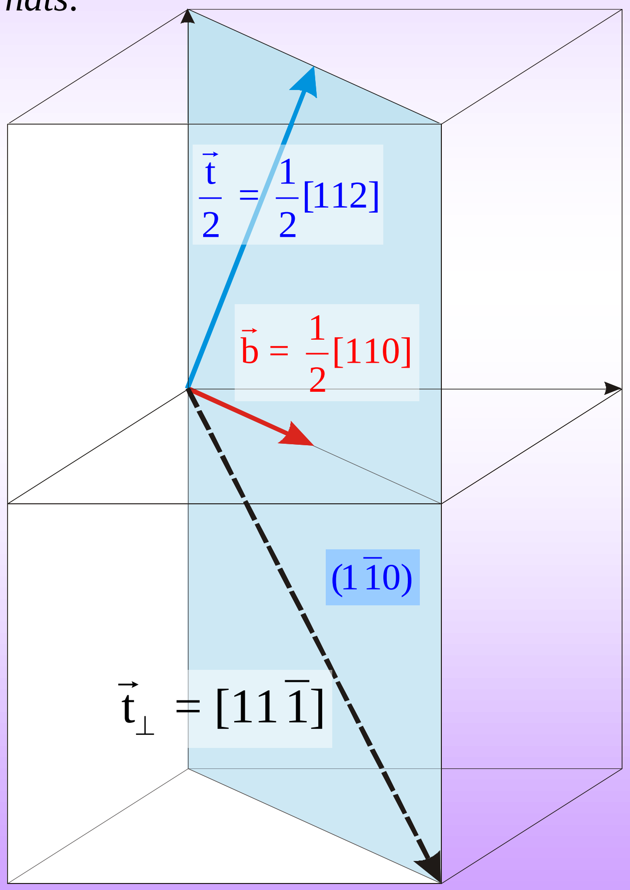
Given: $\vec{b} = \frac{1}{2}[110],\ \vec{t} = [112]$

$\vec{t}_\perp$ refers to the direction perpendicular to $\vec{t}$ and unit vectors are shown by *hats*.

$$\vec{b} = \frac{1}{2}[110],\ |\vec{b}| = \frac{\sqrt{2}}{2} = \frac{1}{\sqrt{2}},\ \hat{b} = \frac{1}{\sqrt{2}}[110]$$

$$\vec{t} = [112],\ |\vec{t}| = \sqrt{6},\ \hat{t} = \frac{1}{\sqrt{6}}[112].\ (\vec{t}' = \frac{1}{2}[112],\ |\vec{t}'| = \frac{\sqrt{6}}{2} = \sqrt{\frac{3}{2}}).$$





Slip plane contains both $\vec{b}$ & $\vec{t}$. Let slip plane (hkl).

Applying Wiess zone law:

(on [110]) On $\vec{b} \rightarrow h + k = 0$

(on [112]) On $\vec{t} \rightarrow h + k + 2l = 0 \quad \Rightarrow l = 0,\ h = -k \Rightarrow$ the slip plane $(s) = (1\bar{1}0)$

For the screw segment of a dislocation: $\vec{b} \parallel \vec{t}$

For the edge segment of the dislocation: $\vec{b} \perp \vec{t}$

Looking at the figure: $\mathrm{Cos}\,\theta = \dfrac{1/\sqrt{2}}{\sqrt{6}/2} = \dfrac{1}{\sqrt{3}}$, $\mathrm{Sin}\,\theta = \dfrac{\sqrt{2}}{\sqrt{3}}$, $\theta = 54.73^o$

Let the direction $\perp$ to $\vec{t}$ be $\vec{t}_\perp = [uvw]$. This direction lies on $(1\bar{1}0)$ plane and is $\perp$ to $\vec{t}$.

Applying Weiss zone law for these conditions:

$u - v = 0,\ u + v + 2w = 0,\ \Rightarrow u = -w,\ u = v \Rightarrow \vec{t}_\perp$ is of the form $[uu\bar{u}]$

$$\Rightarrow \vec{t}_\perp = [11\bar{1}],\ \hat{t}_\perp = \frac{1}{\sqrt{3}}[11\bar{1}]$$

$$\left|\vec{b}_\parallel\right| = \vec{b}.\vec{t} = \frac{1}{2}\big([110].[112]\big)\cos\theta = \frac{1}{2}\sqrt{2}\,\frac{1}{\sqrt{3}} = \frac{1}{\sqrt{6}},\ \vec{b}_\parallel = \left|\vec{b}_\parallel\right|.\hat{t} = \frac{1}{\sqrt{6}}.\frac{1}{\sqrt{6}}[112] = \frac{1}{6}[112]$$

$$\left|\vec{b}_\perp\right| = \vec{b}.\vec{t}_\perp = \frac{1}{2}\big([110].[11\bar{1}]\big)\cos(90-\theta) = \frac{1}{2}\sqrt{2}\sqrt{\frac{2}{3}} = \frac{1}{\sqrt{3}},\ \vec{b}_\perp = \left|\vec{b}_\perp\right|.\hat{t}_\perp = \frac{1}{\sqrt{3}}.\frac{1}{\sqrt{3}}.[11\bar{1}] = \frac{1}{3}[11\bar{1}]$$

Solved Example

In a CCP crystal is the dislocation reaction shown below feasible energetically?
What is the significance of the vectors on the RHS of the reaction?

$$\frac{1}{2}[110] \to \frac{1}{6}\left[21\bar{1}\right] + \frac{1}{6}[121]$$

This is of the form $b_1 \to b_2 + b_3$

The dislocation reaction is feasible if: $b_1^2 > b_2^2 + b_3^2$

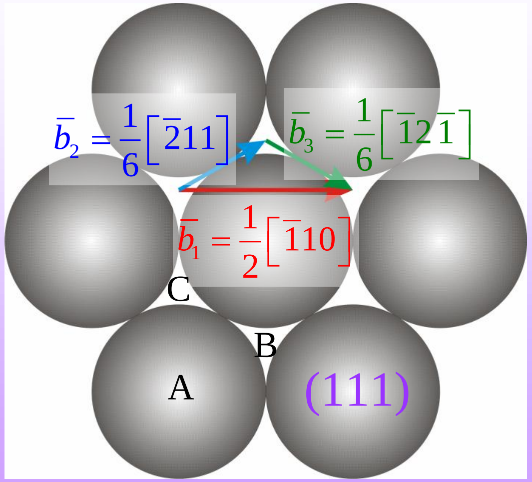
As the energy of a dislocation (per unit length of the dislocation line is proportional to b^2

$$|b_1|^2 = \left(\frac{\sqrt{1^2+1^2}}{2}\right)^2 = \frac{1}{2} \qquad |b_2|^2 = \left(\frac{\sqrt{2^2+1^2+\bar{1}^2}}{6}\right)^2 = \frac{1}{6} \qquad |b_3|^2 = \left(\frac{\sqrt{1^2+2^2+1^2}}{6}\right)^2 = \frac{1}{6}$$

$$\frac{1}{2} > \frac{1}{6} + \frac{1}{6} \quad \left(= \frac{1}{3}\right)$$

$\Rightarrow$ the dislocation reaction is feasible *(i.e. the full dislocation can lower its energy by splitting into partials)*

The vectors on the RHS lie on the (111) close packed plane in a CCP crystal and they connect B to C sites and C to B sites respectively. Equivalent vectors *(belonging to the same family)* are shown in the figure on the right.



Solved Example

What is the image force experienced by an edge dislocation at a distance of 100b from the free surface of an semi infinite Al crystal? Is this force sufficient to move the dislocation given that the Peierls Force (= Peierls Stress × b) = 2.5 × 10^{-4} N/m

Data for Al:

- a_0 = 4.04 Å, Slip system: <110>{111}, b = √2a_0/2 = 2.86 Å, G = 26.18 GPa, ν = 0.348

$$F_{\text{Image}} = \frac{-Gb^2}{4\pi(1-\nu)d}$$

$$F_{\text{Image}} = \frac{-Gb^{\cancel{2}}}{4\pi(1-\nu)100\cancel{b}}$$

–ve sign implies an attraction towards the free surface

$$F_{\text{Image}} = \frac{-(26.18\times10^{9})(2.86\times10^{-10})}{4\pi(1-0.348)(100)} = 9.1\times10^{-3}\ N/m$$

As $F_{\text{image}} > F_{\text{Peierls}}$ ⇒ that the dislocation will spontaneously move to the surface *(creating a step)* under the action of the image force, without the application of an externally applied stress.

Solved Example

Compute the individual number of slip systems for <111> {110}.

For each of the individual directions in the family, we have to locate all the planes such that the dot product between the direction and plane is zero.

Direction	Planes (including –ves of planes)	No.	Including negative of direction	No.
[111]	(1–10), (10–1), (01–1) – ve of above: (–110), (–101), (0–11)	6	×2 *(for [–1–1–1])*	12
[–111]	(110), (101), (01–1) – ve of above: (–1–10), (–10–1), (0–11)	6	×2 *(for [1–1–1])*	12
[1–11]	(110), (10–1), (011) – ve of above: (–1–10), (–101), (0–1–1)	6	×2 *(for [–11–1])*	12
[11–1]	(–110), (101), (011) – ve of above: (1–10), (–10–1), (0–1–1)	6	×2 *(for [–1–11])*	12
			Total	48