

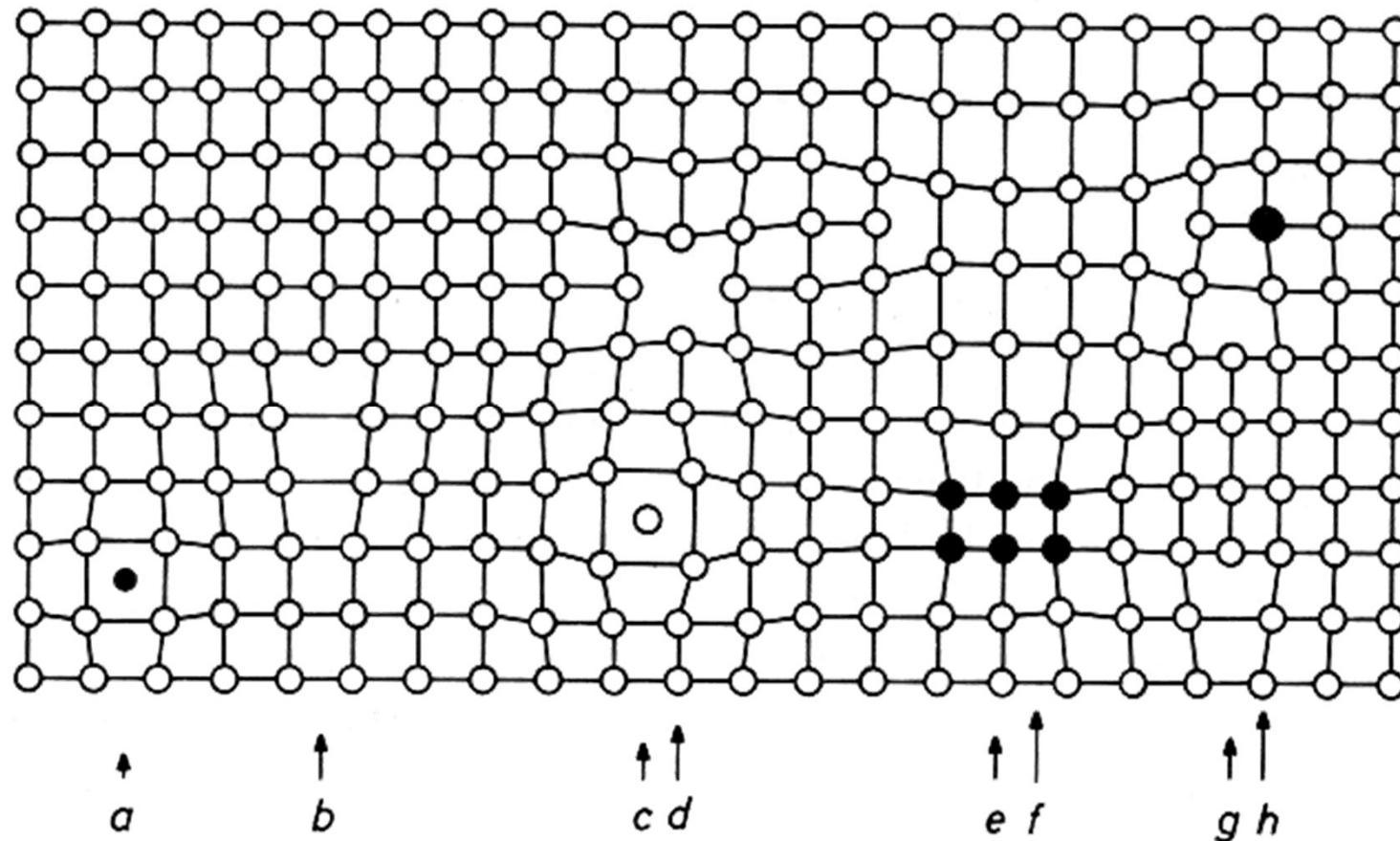
# Crystal Defects



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# Defects

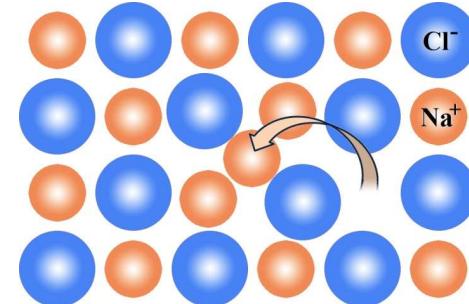
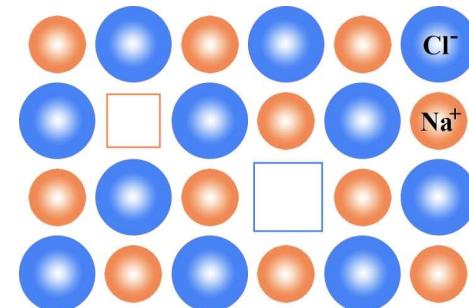
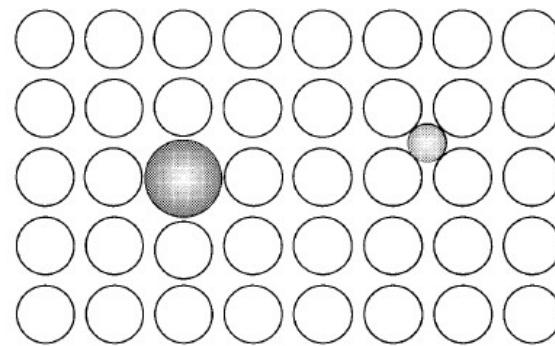
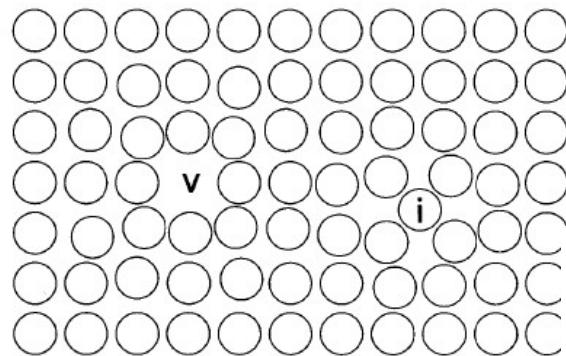


- Perfection is a myth
- But one can be perfectly imperfect
- Batman and Superman analogy
- Crystal = Lattice + Motif
- Lattice is infinite
- Crystal has finite dimensions
- Missing bonds at edges in 2D and surfaces in 3D

- Missing atoms at lattice points
- Vacancies
- Remember the length scale
- Unit cell at Angstrom level
- Crystal at micron to meter level
- Single versus polycrystal
- Grain boundaries as interfaces

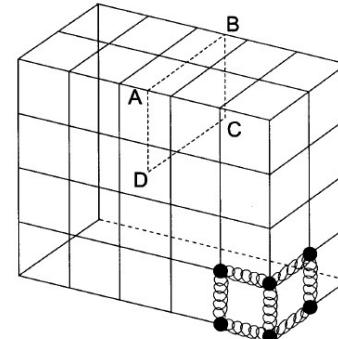
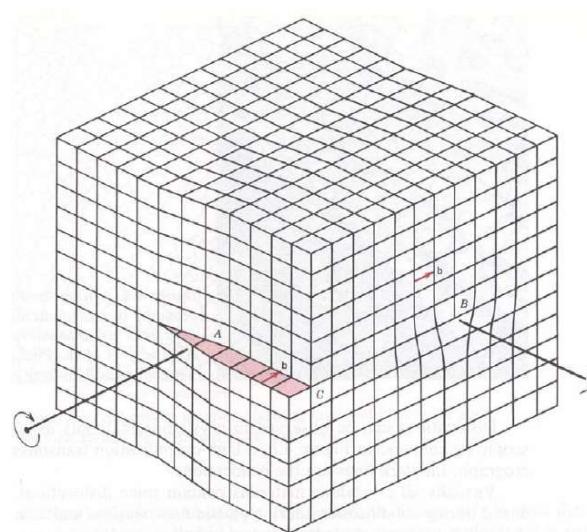
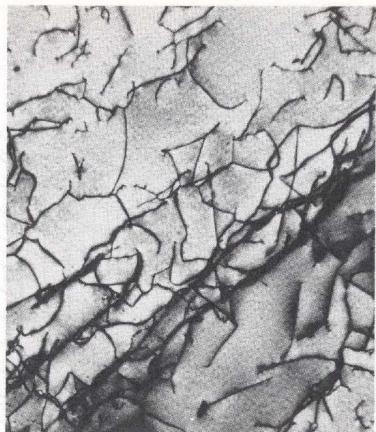
# Dimensionality of Defects

- 0, 1, 2, 3 dimensional defects in crystalline materials
- 0-D or Point defects
  - vacancies
  - interstitials, substitutional atoms

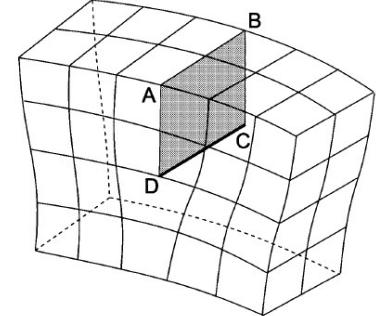


# Dimensionality of Defects

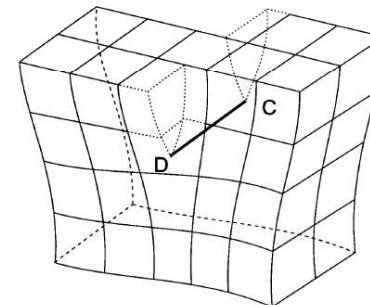
- 1-D or Line defects  
dislocations  
disclinations



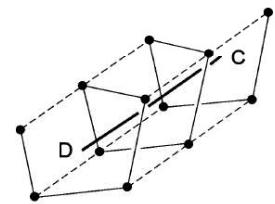
(a)



(b)



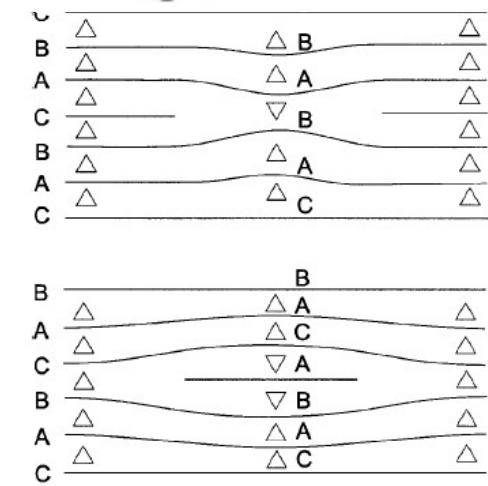
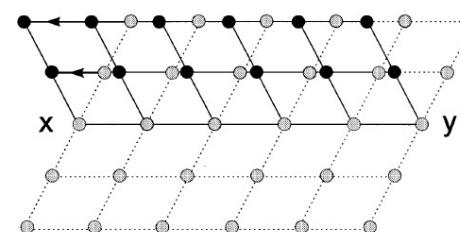
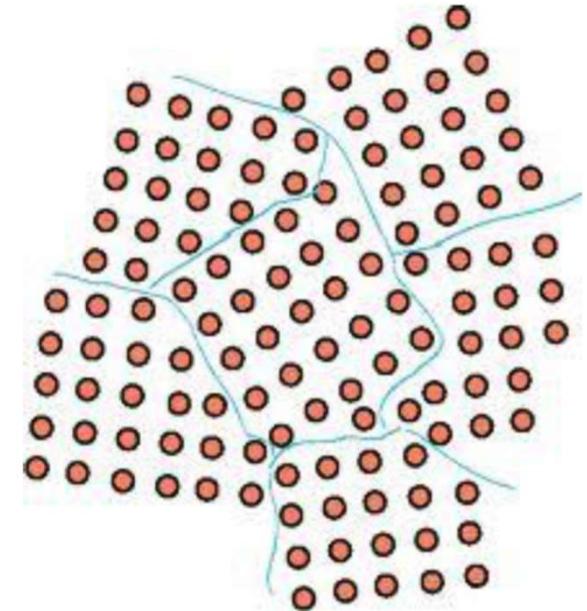
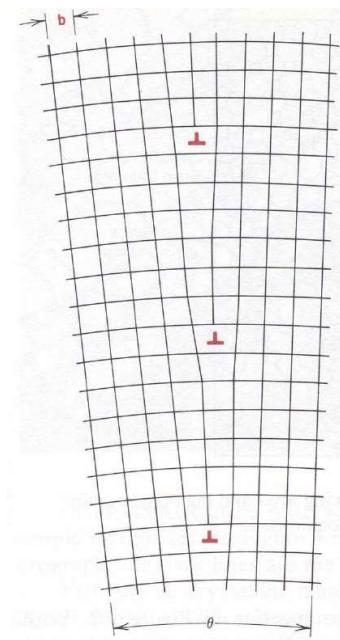
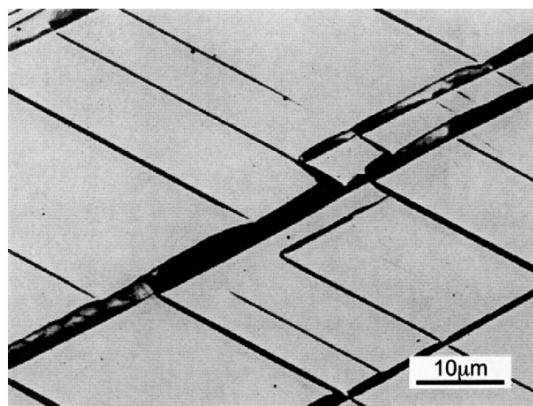
(c)



(d)

**Figure 1.18** (a) Model of a simple cubic lattice; the atoms are represented by filled circles, and the bonds between atoms by springs, only a few of which are shown; (b) positive edge dislocation  $DC$  formed by inserting an extra half-plane of atoms in  $ABCD$ ; (c) left-handed screw dislocation  $DC$  formed by displacing the faces  $ABCD$  relative to each other in direction  $AB$ ; (d) spiral of atoms adjacent to the line  $DC$  in (c).

- 2-D or Planar defects
- surfaces
- grain boundaries
- twin boundaries
- stacking faults



- 3-D or Volume defects
  - voids
  - precipitates
  - twins

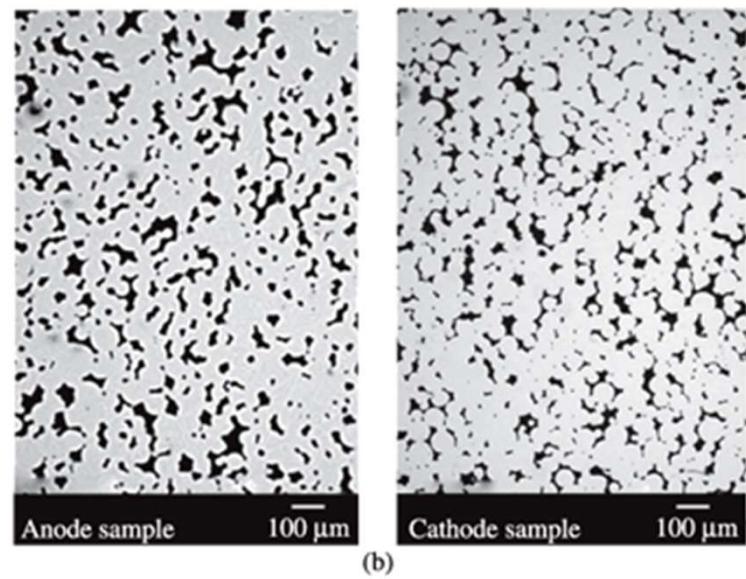
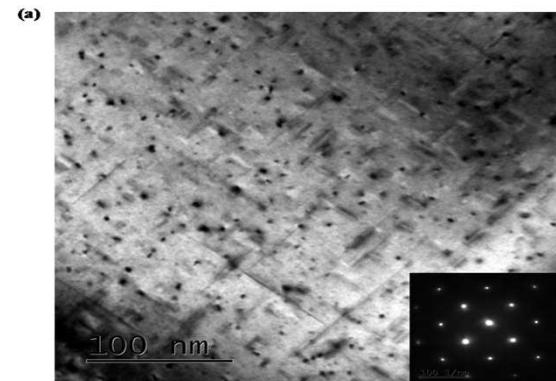
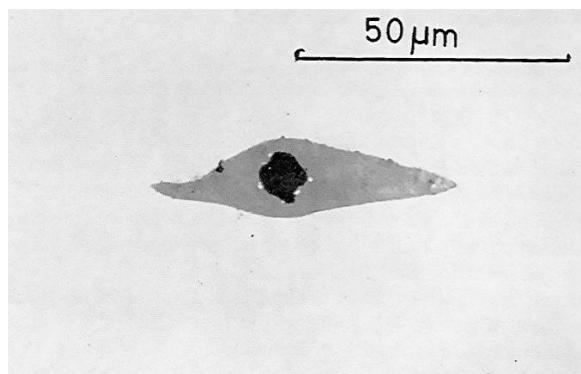


Figure 7. Micrographs of the section of the samples produced without vibration during the powder filling step, sintered at 1423 K for 3600 seconds and compressed at (a) 300 MPa and (b) 600 MPa.



# Inteinsic and Extrinsic PD

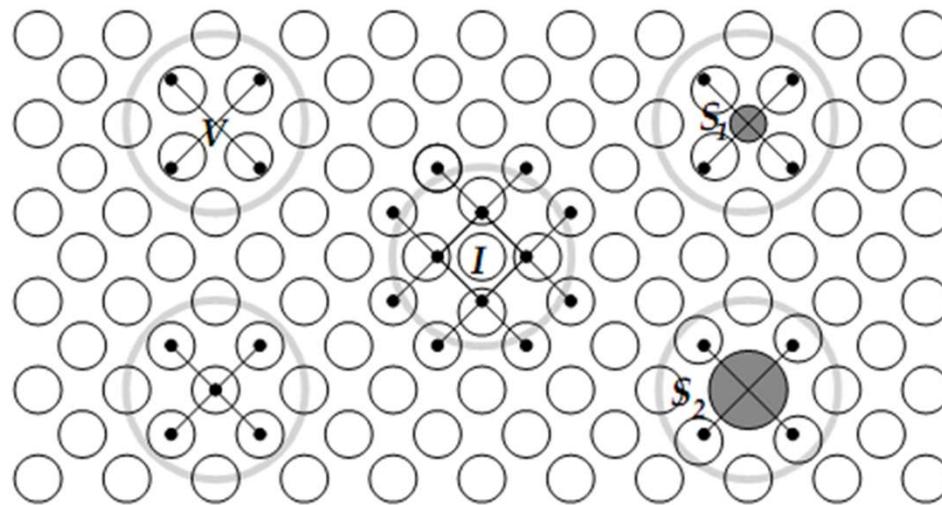
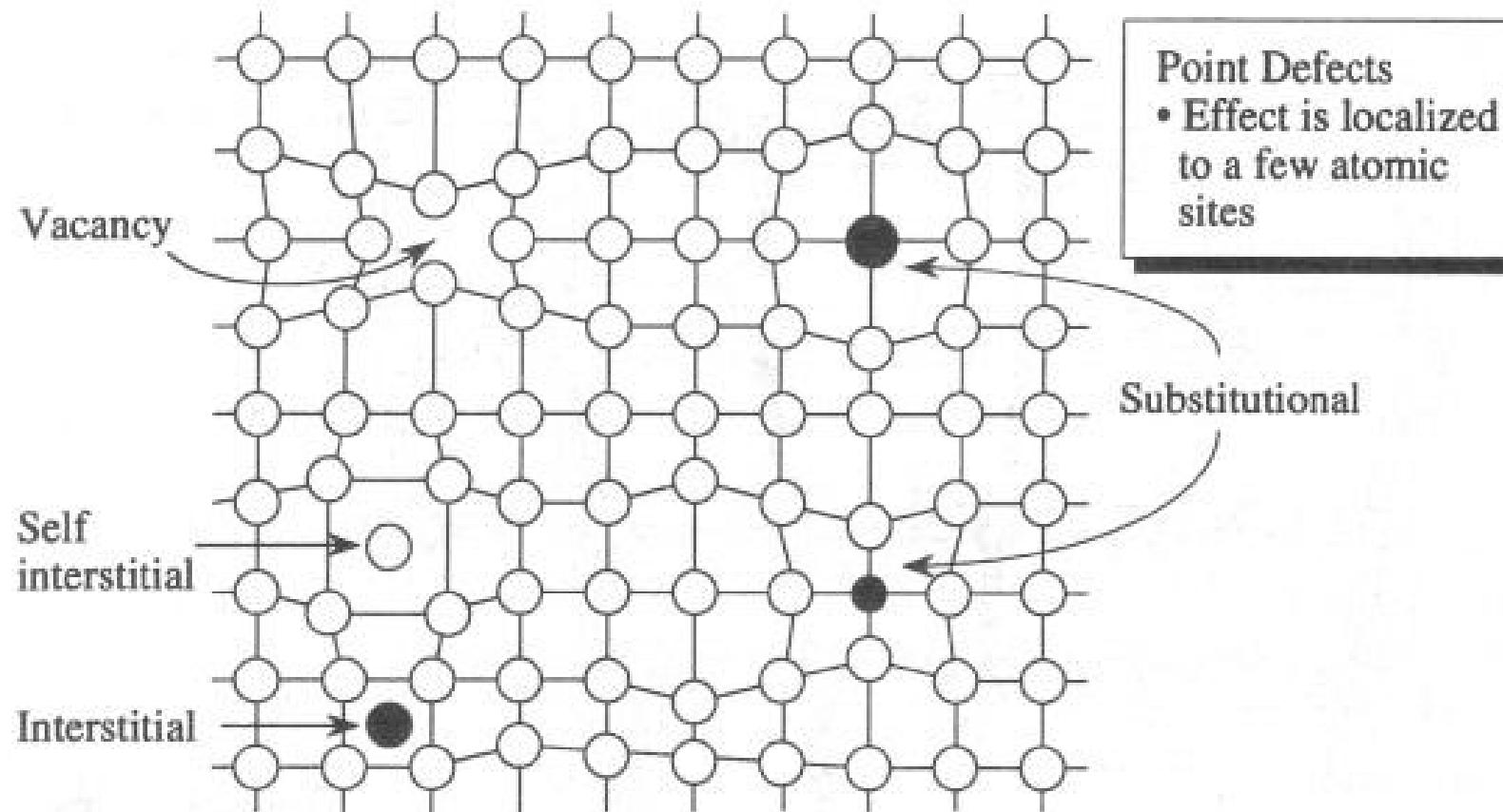


Figure 9.1. Illustration of point defects in a two-dimensional square lattice.  $V$  = vacancy,  $I$  = interstitial,  $S_1$ ,  $S_2$  = substitutional impurities of size smaller and larger than the host atoms, respectively. In all cases the defects are surrounded by a faintly drawn circle which includes their nearest neighbors. In the lower left corner an ideal atom and its nearest neighbors are shown for comparison, also surrounded by a faint circle of the same radius. The thin lines and small dots in the neighborhood of defects serve to identify the position of neighboring atoms in the ideal, undistorted crystal.

- Inherent point defects are intrinsic
- Those generated by doping or external stimuli are extrinsic



# Vacancies

- Free energy of formation of an uncharged vacancy

- $G_F = H_F - T^*S_F$

- $H_F = E_F$ , formation energy

$$G = G_0 + G_F + G_C$$

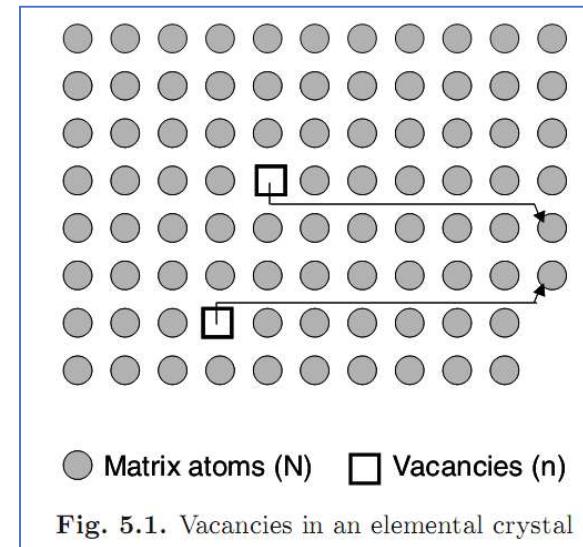


Fig. 5.1. Vacancies in an elemental crystal

- $G_0$  is Gibbs energy of perfect lattice,  
 $G_F = n^*G_f$  and  $G_C = -T^*S_F$  where  $S_F$  is configurational entropy of vacancies,  $n$  is no. of vacancies

$$\frac{\partial G_0}{\partial n} = 0$$

$$\frac{\partial G_F}{\partial n} = G_f$$

$$\frac{\partial G}{\partial n} = G_f - T \frac{\partial S_F}{\partial n}$$

$$S_F = k_B \ln(P)$$

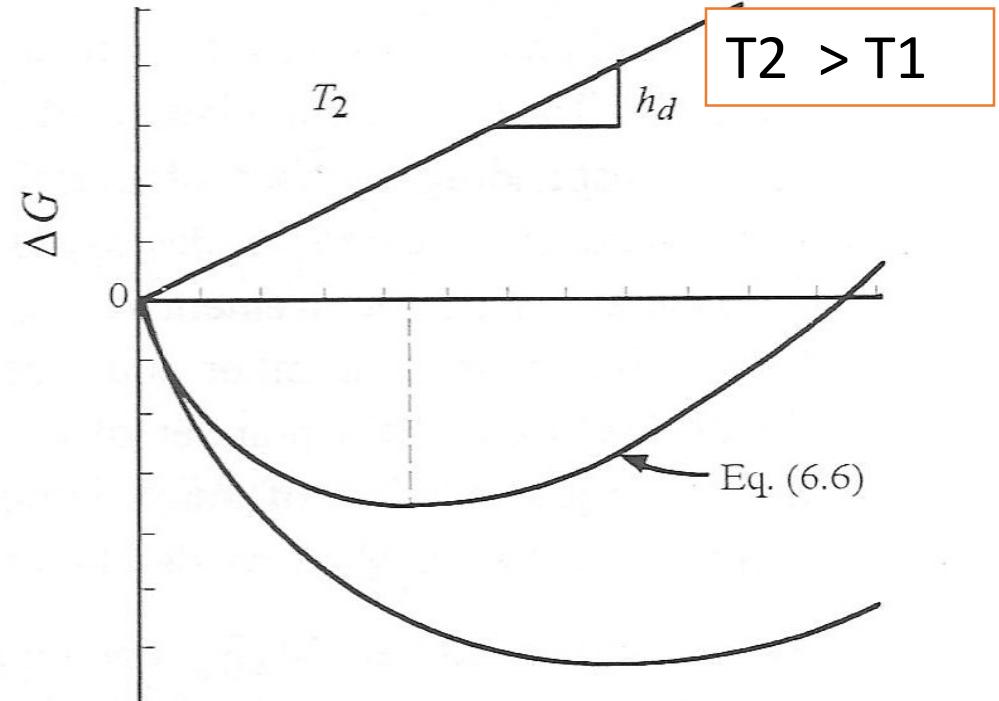
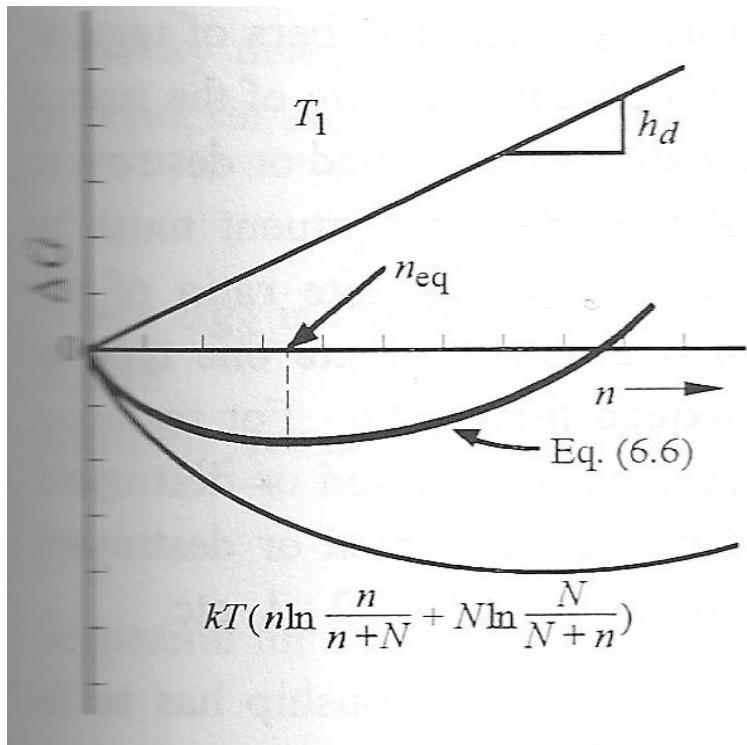
$$P = \frac{N!}{(N-n)!n!}$$

$$c_v = \frac{S_F}{k_B} * \exp\left(\frac{-H_F}{k_B T}\right)$$

- Energy of vacancy = 1eV
- Energy of divacancy higher >2 \* energy of single vacancy
- At temperature close to melting point for metals

$$C_v = 10^{-4} \text{ to } 10^{-3}$$

$$C_{2v} = 10^{-6} \text{ to } 10^{-5}$$



- A material with point-defects has higher enthalpy compared to when there is no point-defect
- $\Delta H$  is positive
- But due to large number of ways available for distributing the point-defects in the lattice, the configuration entropy is large
- Leads to large positive  $\Delta S$  and hence large  $T\Delta S$  which finally
- $\Delta G$  becomes negative
- System is at equilibrium with point-defects even though it takes energy to form them

In this case the system is Entropically stable



**Table 5.1.** Monovacancy properties of some metals.  $C_{1V}^{eq}$  is given in site fractions

Metal	$H_{1V}^F/\text{eV}$	$S_{1V}^F/k_B$	$C_{1V}^{eq}$ at $T_m$	Method(s)
Al	0.66	0.6	$9.4 \times 10^{-4}$	DD + PAS
Cu	1.17	1.5	$2 \times 10^{-4}$	DD + PAS
Au	0.94	1.1	$7.2 \times 10^{-4}$	DD
Ag	1.09	—	$1.7 \times 10^{-4}$	DD
Pb	0.49	0.7	$1.7 \times 10^{-4}$	DD
Pt	1.49	1.3	—	RQ
Ni	1.7	—	—	PAS
Mo	3.0	—	—	PAS
W	4.0	2.3	$1 \times 10^{-4}$	RQ + TEM



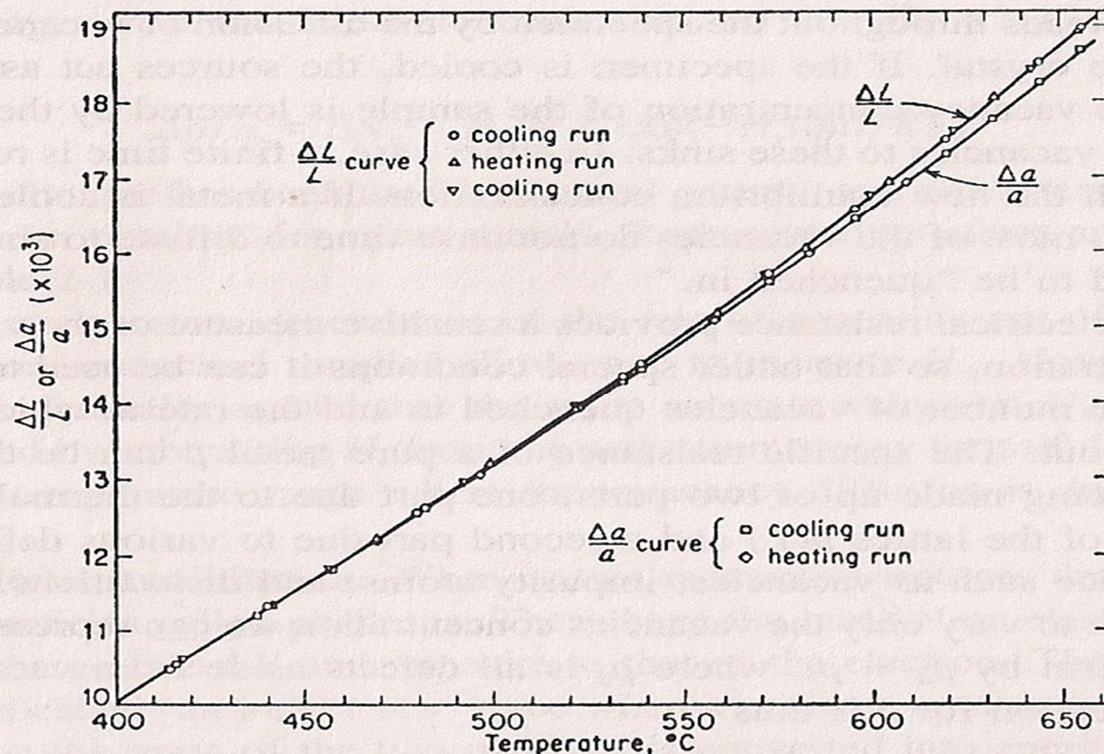
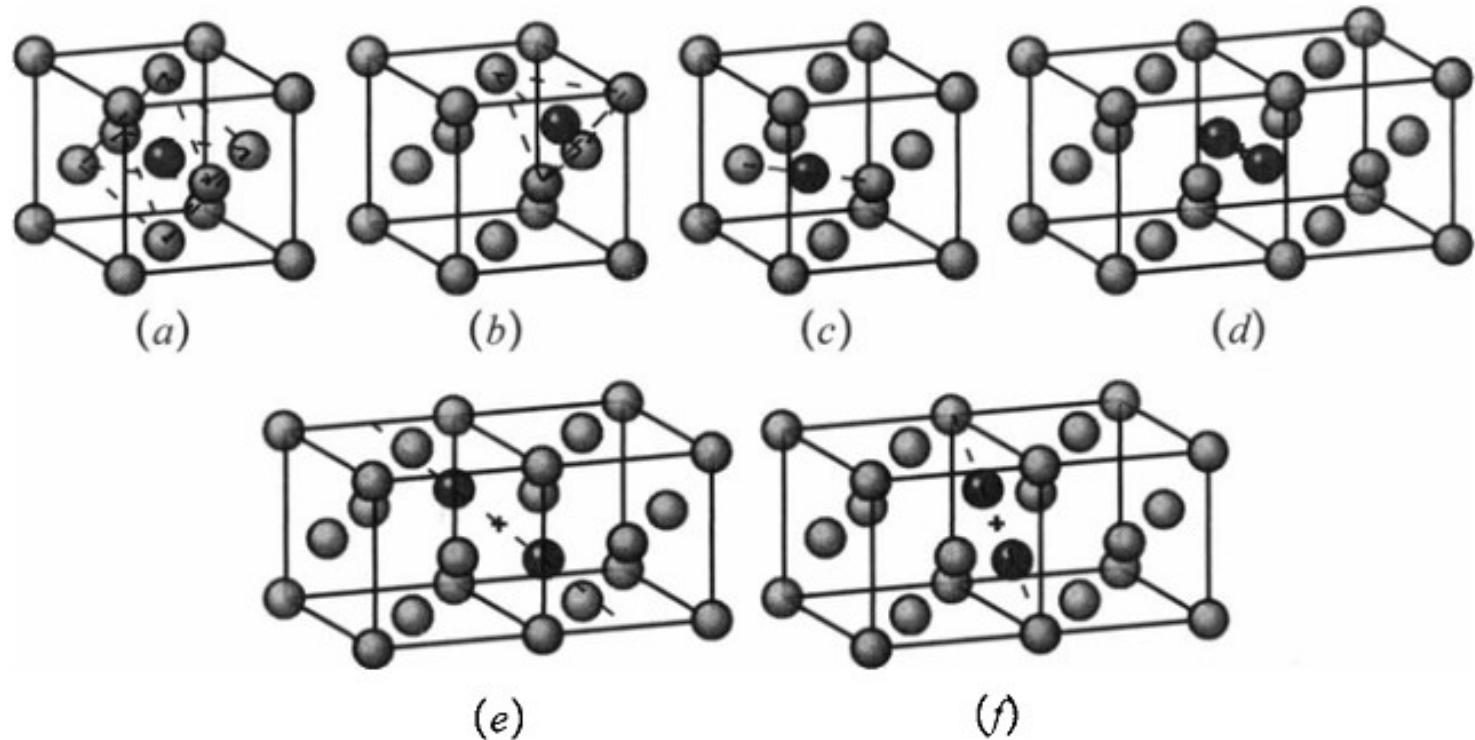


Fig. 2-15—Length change and lattice parameter change vs. temperature for aluminum, taking  $\Delta L/L$  and  $\Delta a/a$  to be zero at 20° C. The difference between the two lines is directly proportional to the concentration of vacant atomic sites. [From R. Simmons, R. Balluffi, *Phys. Rev.*, 117 (1960) 52.]

## Self interstitial



**Figure 8.5:** Geometric configurations for a self-interstitial defect atom in an f.c.c. crystal:  
**(a)** octahedral site, **(b)** tetrahedral site, **(c)**  $\langle 110 \rangle$  crowdion, **(d)**  $\langle 100 \rangle$  split dumbbell,  
**(e)**  $\langle 111 \rangle$  split, **(f)**  $\langle 110 \rangle$  split crowdion [2].



Formation enthalpy of a self-interstitial is considerably higher in closed packed structures (CCP/FCC and HCP) than that of a vacancy

$$H^F_I \approx (2 \text{ to } 3) \times H^F_V$$

Therefore, at thermal equilibrium

$$\Rightarrow C_{eq,V}^{eq} \ggg C_{eq,I}^{eq}$$

$H^F_I$  : Enthalpy of interstitial formation

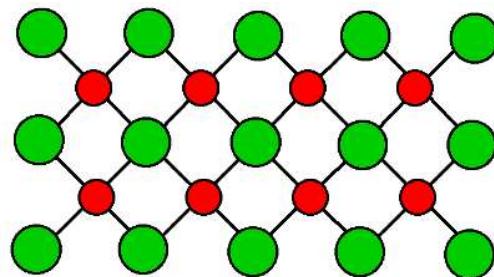
$H^F_V$  : Enthalpy of vacancy formation

Vacancies are dominant point defects in HCP and FCC

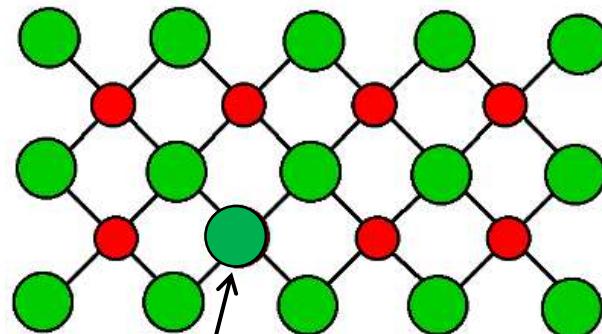


# Anti-site defect

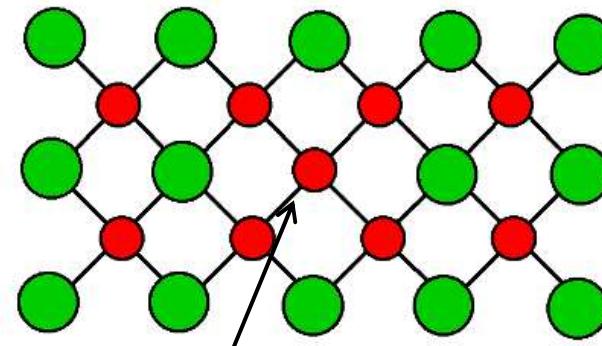
- Occurs in ordered alloys (consisting of more than one metals)
- Covalent compounds



(a) perfect lattice



(g)  $B_A$  antisite defect



(h)  $A_B$  antisite defect



# Intrinsic point defects in ionic compounds

## ➤ Frenkel defect

- Total number of lattice sites remain conserved
- Can occur on either one of the anion sub-lattice or cation sub-lattice
- Cations are smaller than anions and hence easier to be accommodated in interstitial sites

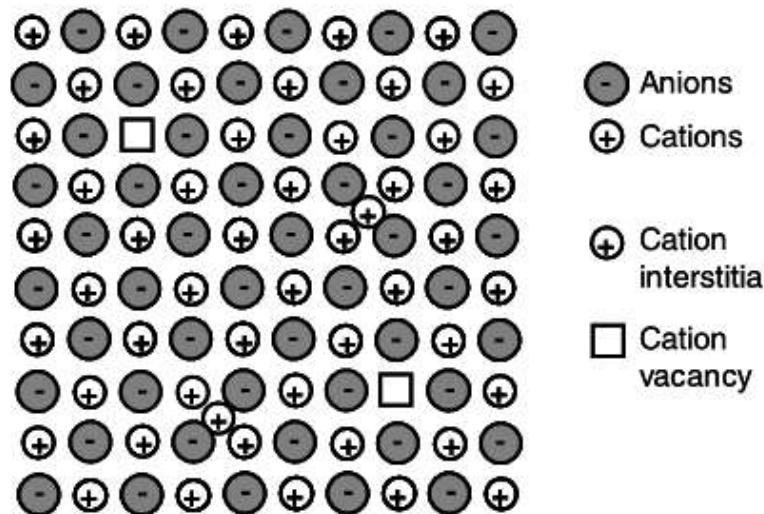
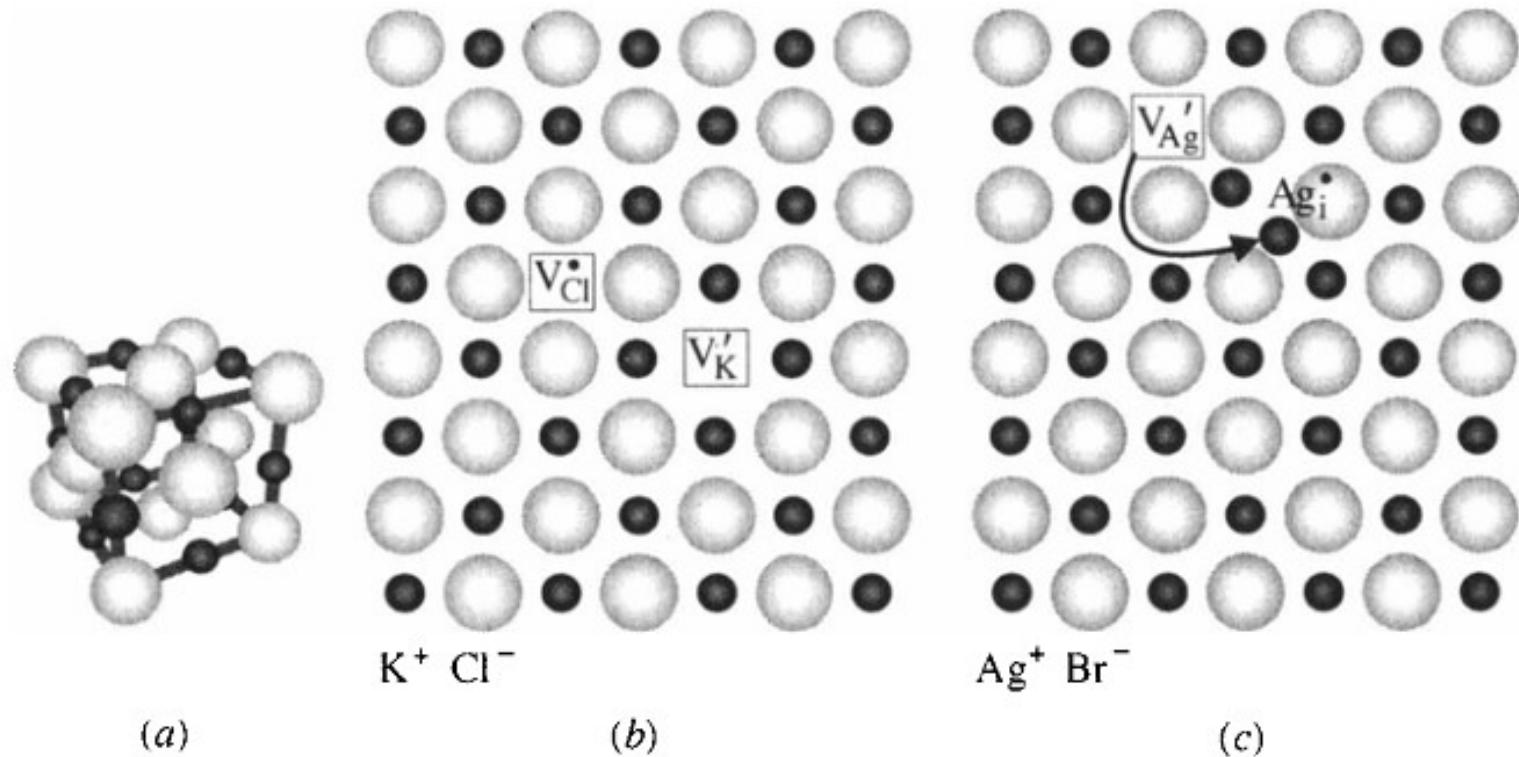


Fig. 5.8. Frenkel disorder in the cation sublattice of a CA ionic crystal





**Figure 8.11:** (a) Rocksalt structure of KCl and AgBr with (100) planes delineated. (b) Schottky defect on a (100) plane in KCl composed of anion vacancy and cation vacancy. (c) Frenkel defect on a (100) plane in AgBr composed of cation self-interstitial and cation vacancy.

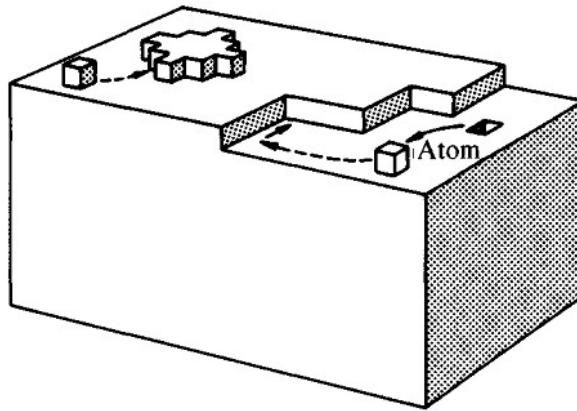


## ➤ Schottky defects

- Ions near the surface diffusing onto the surface leaving behind vacant-sites that ultimately diffuse into the bulk
- missing cation and anion from the bulk have moved to the surface
- Vacant sites in the bulk and creating new lattice sites at the surface.
- Defects form in multiple of Formula-unit
- Defects formed corresponding to each formula unit leads to increase in number of total lattice sites by one formula unit



- For Schottky defects corresponding to one formula unit in  $\text{Al}_2\text{O}_3$
- 2 vacancies on  $\text{Al}^{3+}$  sites, 3 vacancies on  $\text{O}^{2-}$  sites
- Total 5 lattice sites will be created at the surface



Atom near the surface moving onto the existing surface to become a part of the new surface and also leaving behind a vacancy which can diffuse into the bulk.

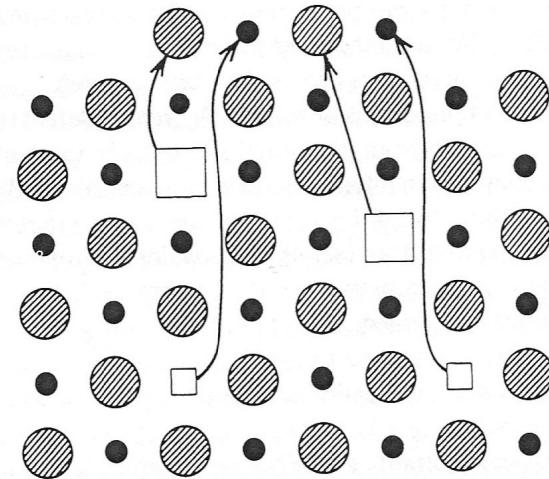


Fig. 2.2 Schottky disorder. Displacement of anion and cation to surface leaves a pair of vacancies.

***Preservation of regular site ratio and charge neutrality***

## Equilibrium concentration

- Two different sub-lattice in a solid
- Consider separate contribution due to each of the sub-lattice towards the total configurational entropy of the system.

### For Frenkel Defects

$$\frac{V_{cat}^{eq} n_i^{eq}}{N_T N^*} = \exp\left(-\frac{\Delta H_F}{kT}\right)$$

Here,  $N_T$  is total number of lattice sites on cation sub-lattice.

&  $N^*$  is total number of **those types of** interstitial sites that are being occupied by the interstitial ion.

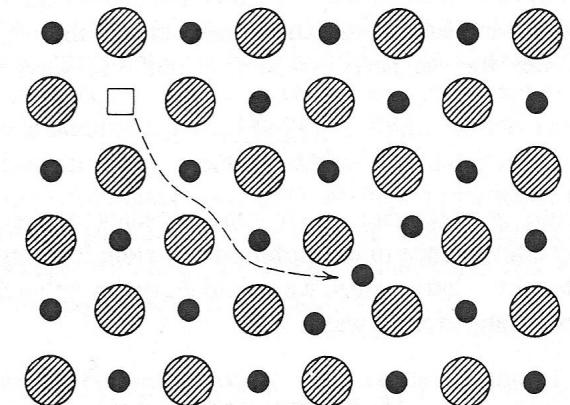
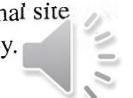
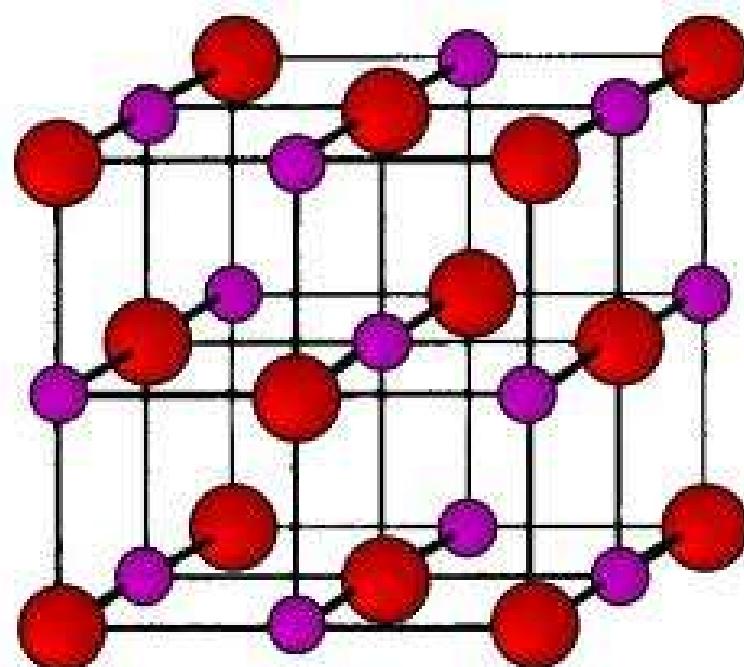


Fig. 2.1 Frenkel disorder. Ion leaving normal site forms an interstitial ion and leaves a vacancy.



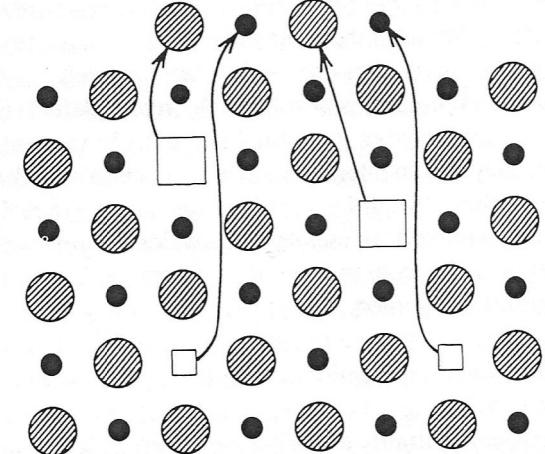
- In an unit cell of NaCl, for Chlorine sub-lattice, there are 8 tetrahedral sites for every 4 Chlorine ions.
- Same for sodium sub-lattice, therefore  $N^* = 2 \times$  total number of sites on Chlorine sub-lattice.



## For Schottky Defects

For the constraint:  $\frac{(N_{cat} + V_{cat}^{eq})}{(N_{an} + V_{an}^{eq})} = 1$

$$\frac{V_{cat}^{eq} V_{an}^{eq}}{(N_{an} + V_{an}^{eq})(N_{cat} + V_{cat}^{eq})} \approx \frac{V_{cat}^{eq} V_{an}^{eq}}{(N_{an})(N_{cat})} = \exp\left(-\frac{\Delta H_S}{kT}\right)$$



**Fig. 2.2** Schottky disorder. Displacement of anion and cation to surface leaves a pair of vacancies.

$$\frac{V_{cat}^{eq}}{N_T}, \quad , \quad \frac{n_i^{eq}}{N^*}, \quad , \quad \frac{V_{an}^{eq}}{(N_{an} + V_{an}^{eq})} \quad \& \quad \frac{V_{cat}^{eq}}{(N_{cat} + V_{cat}^{eq})}$$

Represent the concentration of point-defects in terms of site-fraction or mole-fraction

## Formation enthalpies

**Table 5.2.** Formation enthalpies of Schottky- and Frenkel pairs of ionic crystals

Ionic compound	$(H_{SP}$ or $H_{FP})/\text{eV}$	$(S_{SP}$ or $S_{FP})/k_B$	Type of disorder
NaCl	2.44	9.8	Schottky
KCl	2.54	7.6	Schottky
NaI	2.00	7.6	Schottky
KBr	2.53	10.3	Schottky
LiF	2.68		Schottky
LiCl	2.12		Schottky
LiBr	1.80		Schottky
LiI	1.34		Schottky
AgCl	1.45–1.55	5.4–12.2	Frenkel
AgBr	1.13–1.28	6.6–12.2	Frenkel

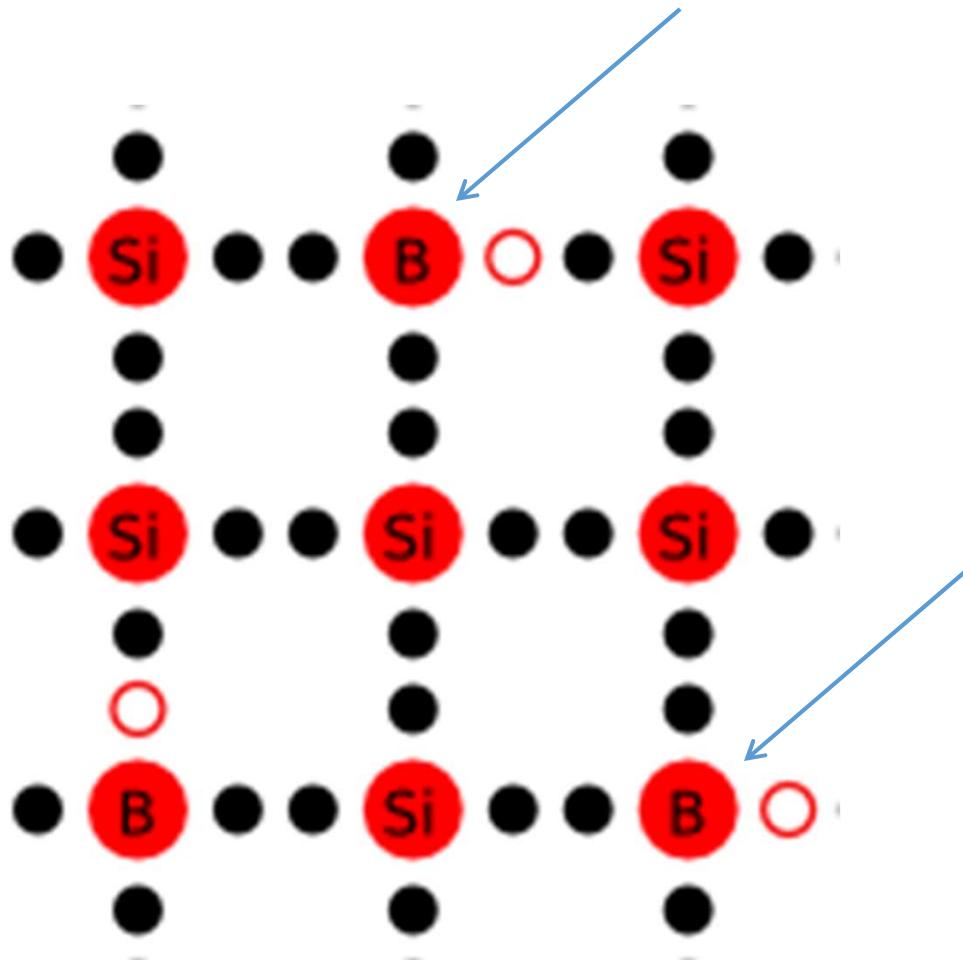


## Extrinsic point defects

- Defects introduced in a substance through reaction with an external agent, which may be another substance, or the environment (e.g. irradiation or a mechanical force) are known as **Extrinsic point defects**
- Concentration of point-defects is not governed by the criteria of Gibbs Free Energy minimization
- Examples
  - Rapid quenching
  - Irradiation
  - Plastic deformation
  - Doping: chemical addition



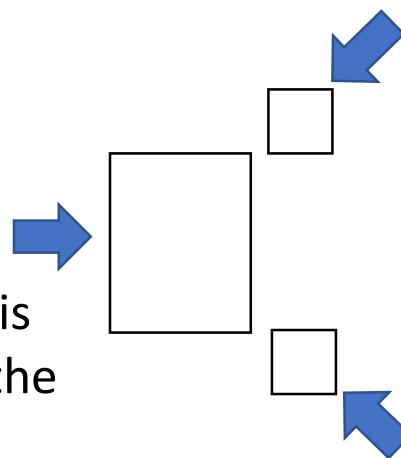
# Doping in semiconductors



# Kroger-Vink notation

## Main-Symbol:

It represents what is the entity, ion or vacancy, that is occupying this location on the host lattice



## Superscript:

Tells us about the **relative charge** on this ion or Vacancy.

Symbol • represents positive charge

Symbol ' represents negative charge

## Subscript:

Tells us about the **location** of this ion or vacancy in the host-crystal.



## ➤ Calcium on sodium site in NaCl

$\text{Ca}_{\text{Na}}^{\bullet}$  Defect free NaCl is charge neutral. Replacement of monovalent sodium cation with divalent calcium cation leads to an extra positive charge

## ➤ Sodium on calcium site in CaCl<sub>2</sub>

$\text{Na}'_{\text{Ca}}$  Defect free CaCl<sub>2</sub> is charge neutral. Replacement of divalent calcium cation with monovalent sodium cation leads to absence of a positive charge

## ➤ Vacancy on chlorine site in NaCl



Defect free NaCl is charge neutral. A vacant anion site means there is a extra positive charge.

## ➤ Vacancy on sodium site in NaCl



A vacant cation site means there is a extra negative charge.



## Effective charge and actual charge

+ and – vis a vis  $\bullet$  and ‘



Symbol *i* is used to represent an interstitial site in a crystal.

Aluminum ion located at interstitial site     $Al_{Al}^x$

Sometimes x is used to denote neutral entity

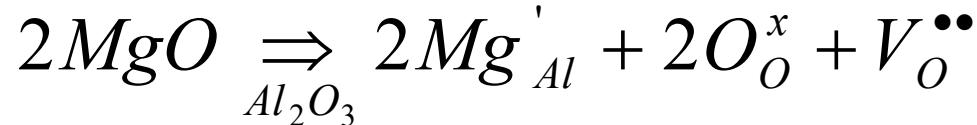


## Doping in Ionic solids

➤ Incorporation of (Nickel Oxide) in MgO (Magnesium oxide):



➤ Incorporation of MgO in Al<sub>2</sub>O<sub>3</sub>:



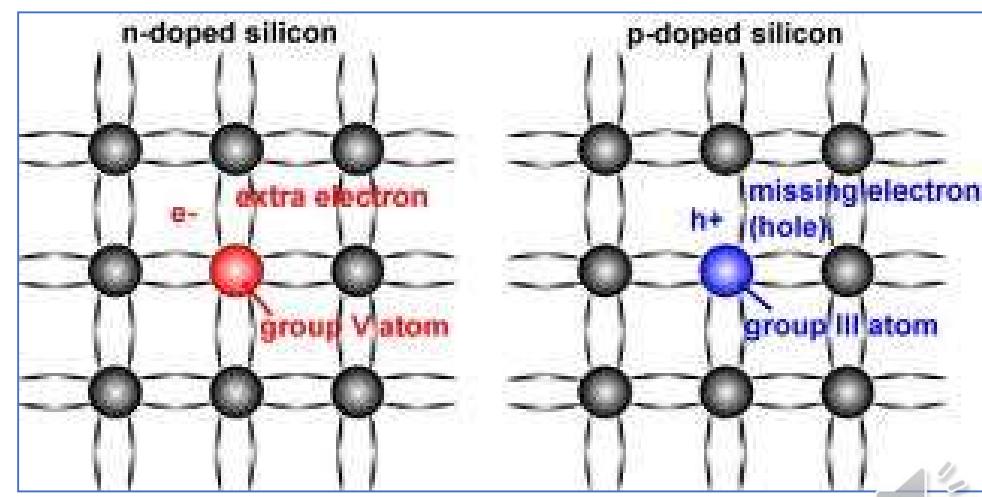
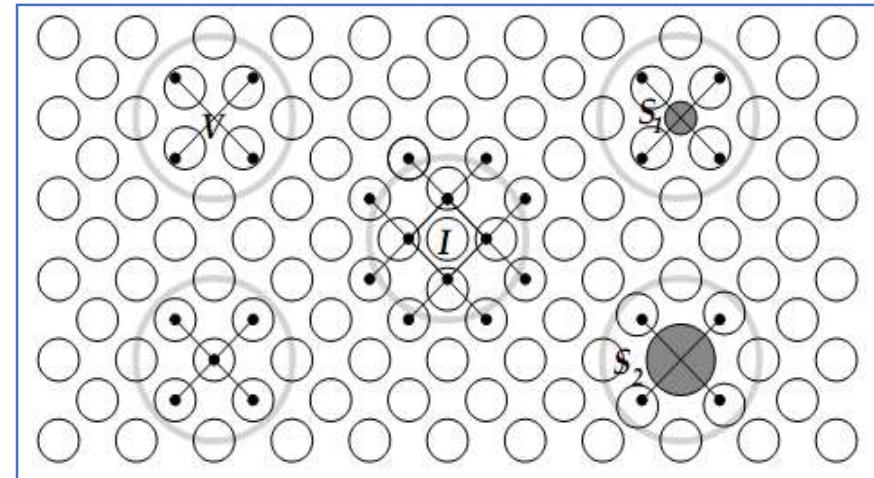
➤ Incorporation of Al<sub>2</sub>O<sub>3</sub> in MgO :



➤ Unlike vacancies in covalent and metallic solids, vacancies in ionic solids are charged



- Diffusion
- Lattice distortion
- Elastic and size mismatch
- Mechanical strengthening
- Electrical conduction
- Optical Colors
- Photoluminescence

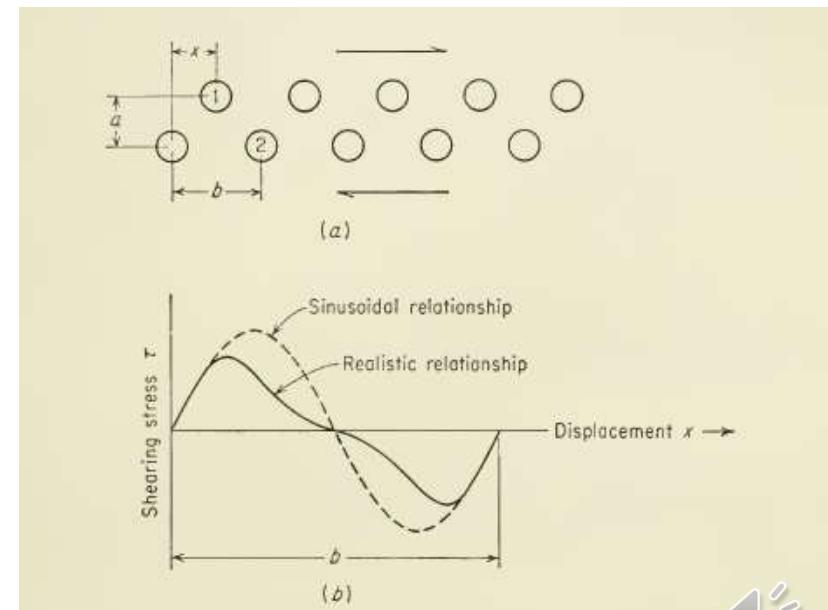
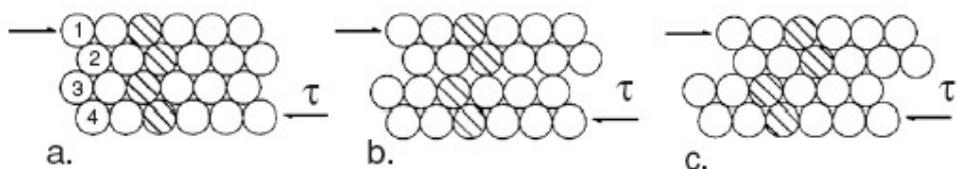


# The perfect crystal

- Perfection pursued by the Neanderthal human to the millennial
- Instagram for millennial Narcissus
- Body shaming
- FOMO
- Achieving nirvana: be content
- It is better to be a dissatisfied Socrates than a satisfied pig.
- Accept the way you are

- Crystals are also perfect
- Reversible deformation on application and release of load is elastic deformation
- Stretching of bonds
- Permanent deformation or plastic deformation is breaking of bonds and formation of new bonds
- This is what the scientists thought

- Lattice is periodic so one can consider periodic potential in a lattice
- Shearing rather than stretching
- Easy to make and break bonds

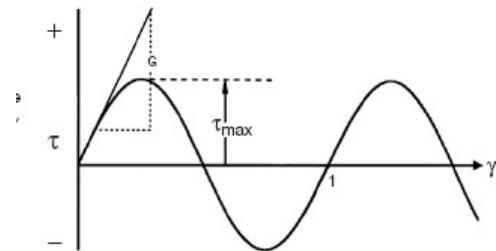
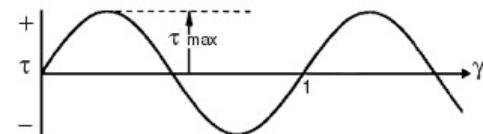
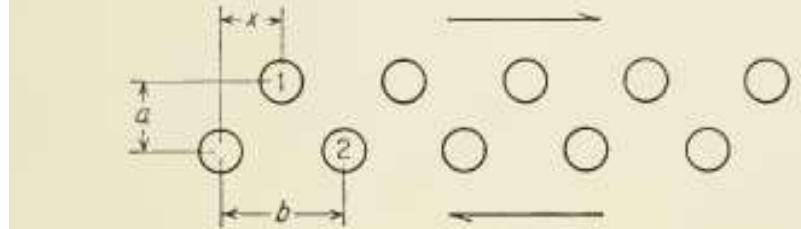


$$\tau = \tau_m \sin \frac{2\pi x}{b}$$

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

$$\tau = \tau_m \frac{2\pi x}{b}$$

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

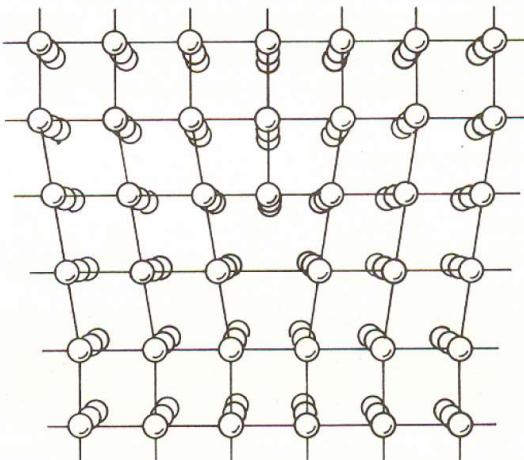


$$\tau_m \approx \frac{G}{2\pi}$$

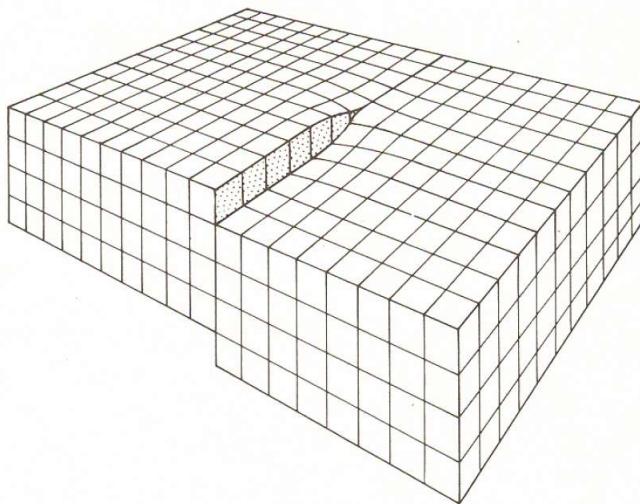
$$\tau_{\max} = G/10.$$

- Theoretical strength values predicted >>> Experimental measurements
- Difference of two to three orders of magnitude
- Something wrong with the fundamental assumption of atomic planes sliding past one another
- Taylor, Orowan, and Polanyi realized that it is not necessary for a whole plane to slip at the same time in 1934

- They postulated that crystals have preexisting defects that are boundaries between regions that are already displaced relative to one another by a unit of slip
- The line between the slipped and unslipped region are called *dislocations*. Movement of a dislocation allows slip to occur.
- The critical stress for slip is the stress required to move a dislocation. At any instant, slip need only occur at the dislocation rather than over the entire slip plane.
- Burger proposed screw dislocation in 1938

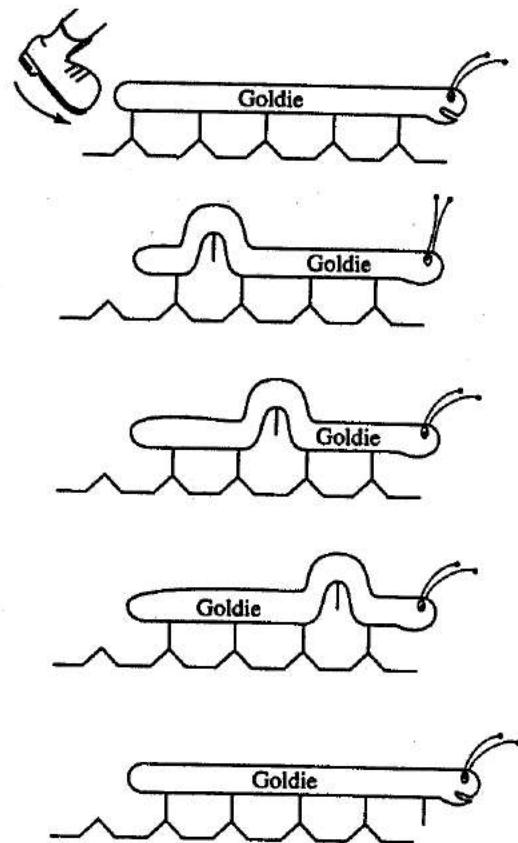


- a) E. Orowan – *Z. Phys.* **89**, 605 and 634 (1934)
- b) M. Polyani – *Z. Phys.* **89**, 660 (1934)
- c) G.I. Taylor – *Proc. Roy. Soc. A* **145**, 362 (1934)

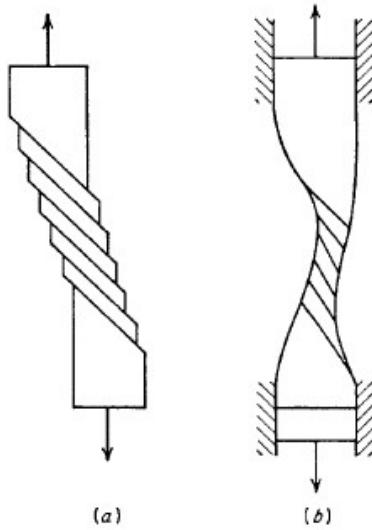


- a) J.M. Burgers – *Proc. Kon. Ned. Akad. Wetenschap* **42**, 293 and 378 (1939)

## Understanding movement of dislocation



# Shape change by slip in single crystals



**Figure 4-20** (a) Tensile deformation of single crystal without constraint; (b) rotation of slip planes due to constraint.

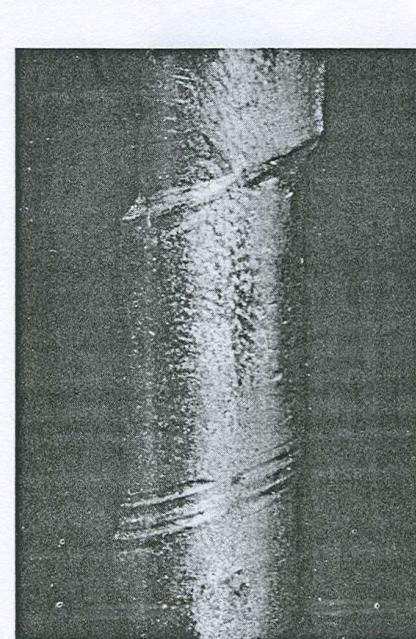
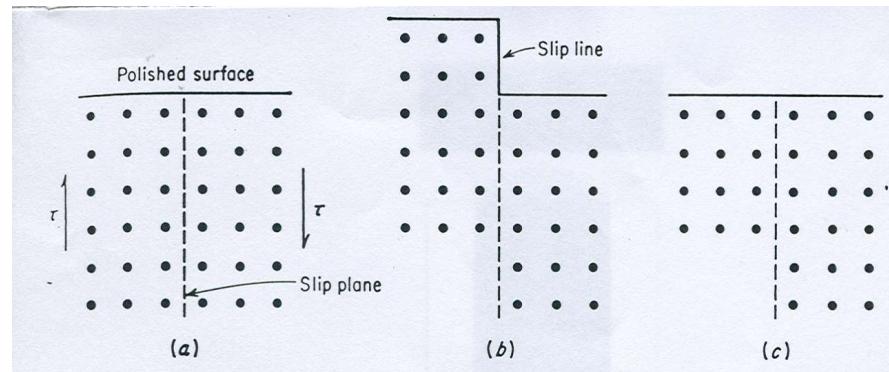
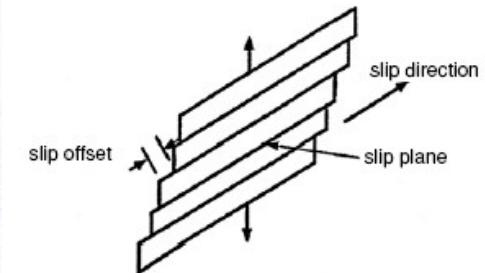


Fig. 4.31. Localized slip in a single crystal of zinc. (Courtesy of E. R. Parker.)



**Figure 8.1.** Slip by shear between parallel planes of atoms.

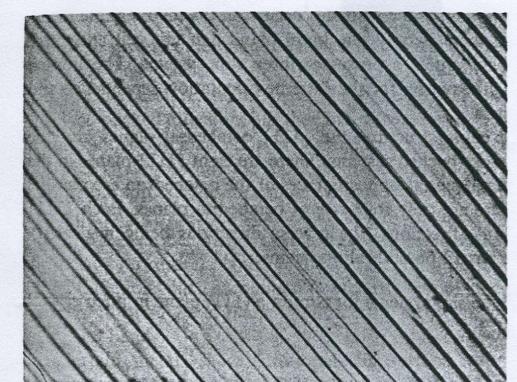
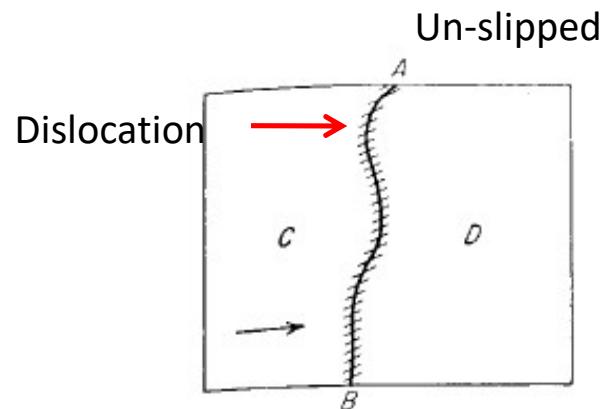


Figure 4-12 Straight slip lines in copper (500  $\times$ ). (Courtesy W. L. Phot.

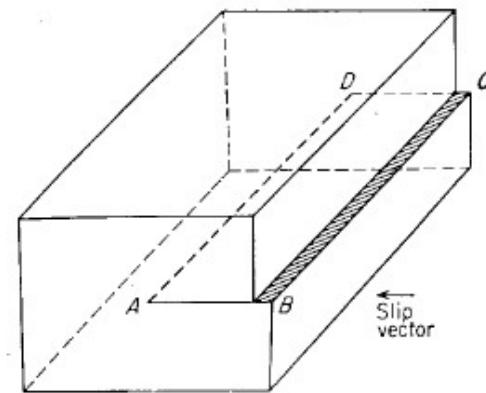


# Plastic deformation and slip

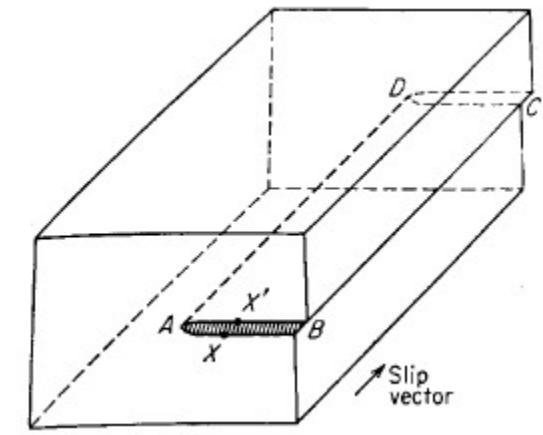
- Slip → sliding of atomic planes in crystalline materials
- The planes on which slip occurs are called *slip planes* and the directions of the shear are the *slip directions*.



Slipped region



Edge dislocation



Screw  
dislocation



- Slip occurs on closely packed but widely spaced planes in densely packed direction
- The magnitude of the shear displacement → integral number of interatomic distances
- Lattice is left unaltered

- If slip occurs on only part of a plane, there remains a boundary between the slipped and unslipped portions of the plane, which is called a dislocation
- Slip occurs by movement of dislocations through the lattice.
- It is the accumulation of the dislocations left by slip that is responsible for work hardening

➤ Slip to strain

$$d\gamma = \frac{1}{2}(b \otimes n + n \otimes b)$$

$$d\omega = \frac{1}{2}(b \otimes n - n \otimes b)$$



# Crystal structure and Slip

Structure	Slip direction	Slip planes
fcc	$<110>$	$\{111\}$
bcc	$<111>$	$\{110\}, \{112\}, \{123\}$ , pencil glide <sup>a</sup>
hcp	$<11\bar{2}0>$ $<11\bar{2}3>$ <sup>b</sup>	$(0001), \{1\bar{1}00\}, \{1\bar{1}01\}$ $\{1\bar{1}01\}$
dia. cub.	$<110>$	$\{111\}$
NaCl	$<110>$	$\{110\}$
CsCl	$<001>$	$\{100\}$

<sup>a</sup> With pencil glide, slip is possible on all planes containing the slip direction.

Almost without exception  
the slip directions are the crystallographic directions with  
the shortest distance between like atoms or ions and  
the slip planes are usually densely packed planes.



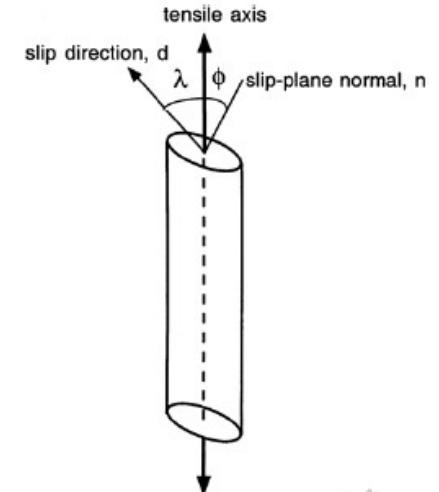
## Schmid's law: Concept of Critical resolved shear stress

- Slip begins when the shear stress on a slip system reaches a critical value,  $\tau_c$ , often called the critical resolved shear stress"
- In most crystals, equal slip in forward and backward direction

$$\tau_{nd} = \pm \tau_c$$

Schmid Law

where n and d represent slip plane normal and slip direction respectively



For uni-axial tension along x direction

$$\tau_c = \pm \sigma_x \cos \lambda \cos \phi$$

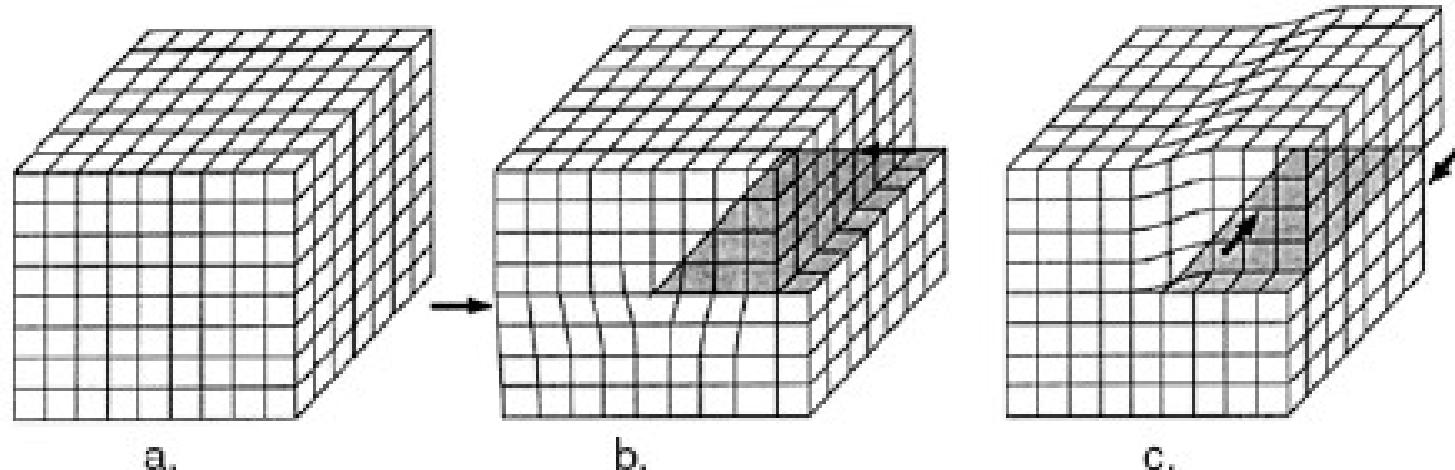
$$\tau_{nd} = l_{nx} l_{dx} \sigma_{xx}$$

where  $\lambda$  is the angle between the slip direction and the tensile axis, and  $\phi$  is the angle between the tensile axis and the slip-plane normal, so  $l_{dx} = \cos \lambda$  and  $l_{nx} = \cos \phi$

Generalized yielding criterion

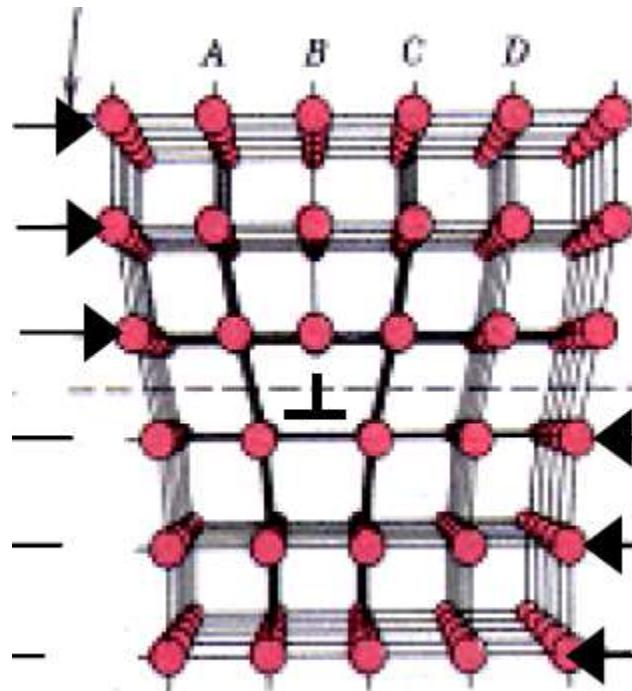
$$\tau_c = \pm l_{nx} l_{dx} \sigma_{xx} + l_{ny} l_{dy} \sigma_{yy} + \dots + (l_{nx} l_{dy} + l_{ny} l_{dx}) \sigma_{xy}$$

## Visualization of Dislocation



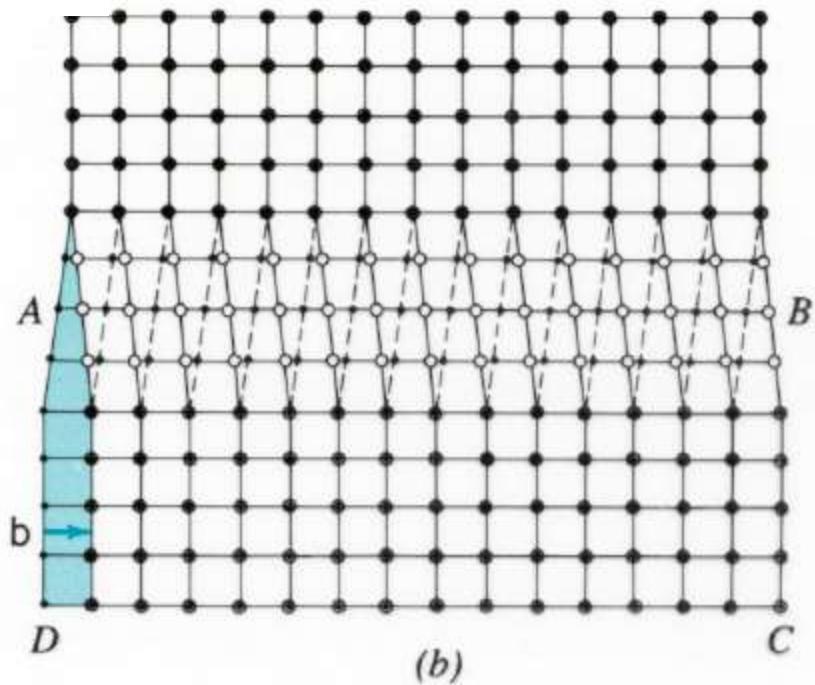
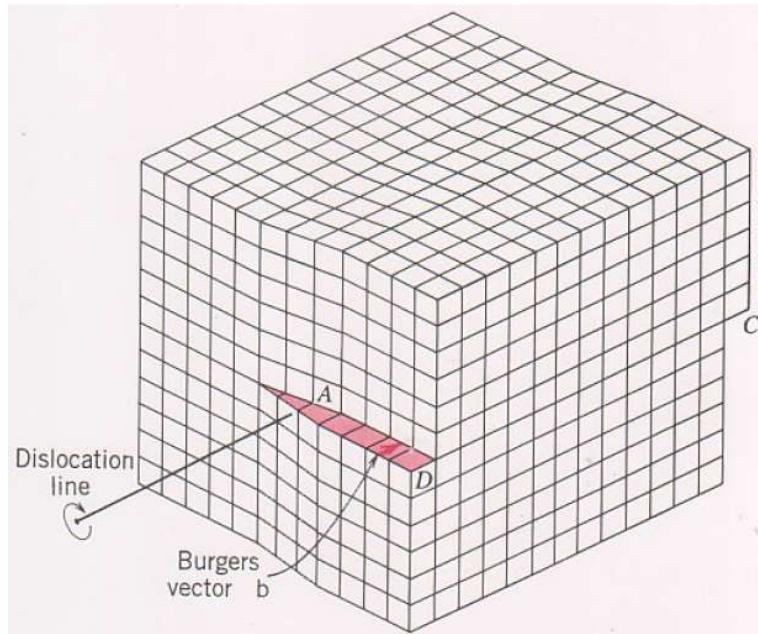
- An edge dislocation is created by shearing the top half of the crystal by one atomic distance perpendicular to the end of the cut (Figure b). This produces an extra half plane of atoms, the edge of which is the center of the dislocation.
- A screw dislocation is generated by cutting into a perfect crystal and then shearing half of it by one atomic distance in a direction parallel to the end of the cut (Figure c). The end of the cut is the dislocation.
- In both cases the dislocation is a boundary between regions that have and have not slipped.

## Edge Dislocation



Positive  and Negative  edge dislocation

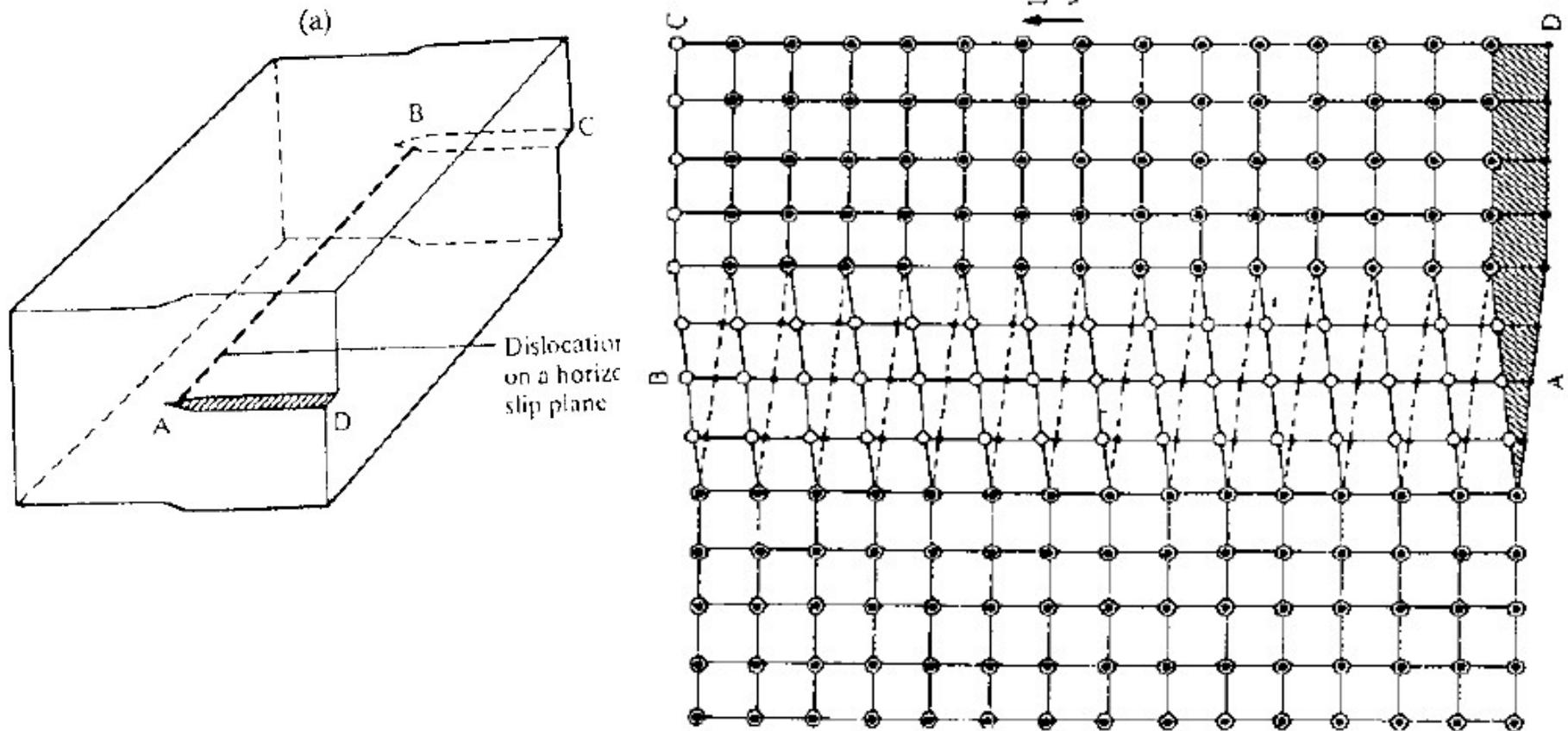
# Screw Dislocation



Positive → anti-clockwise and Negative → clockwise rotation

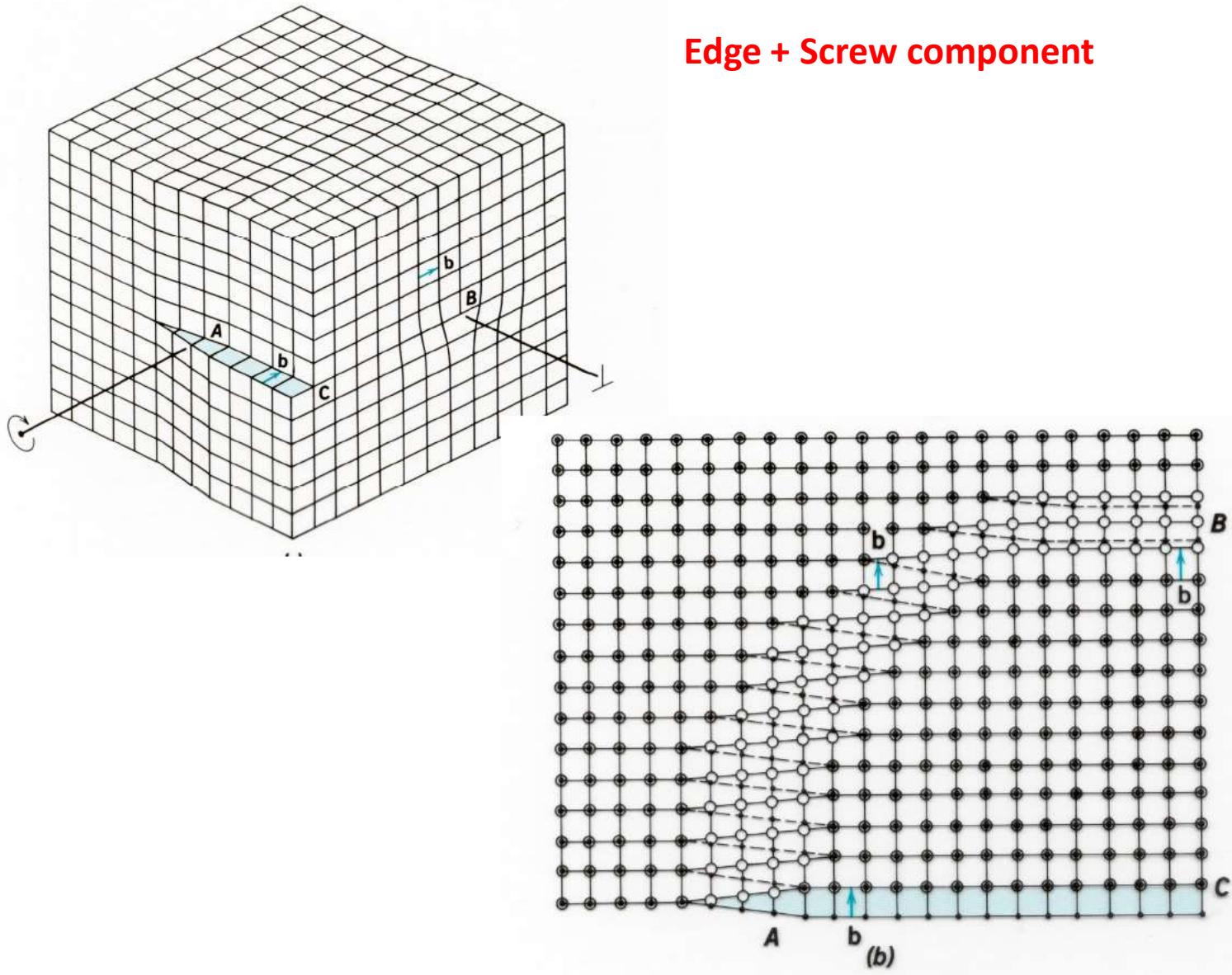


# Screw dislocation



**FIGURE 6.5** Structure of a screw dislocation: (a) displacement of upper half of crystal over lower half; (b) spiral path along the dislocation line. (From Read, 1953. Reprinted with permission from McGraw-Hill.)

# Mixed Dislocation

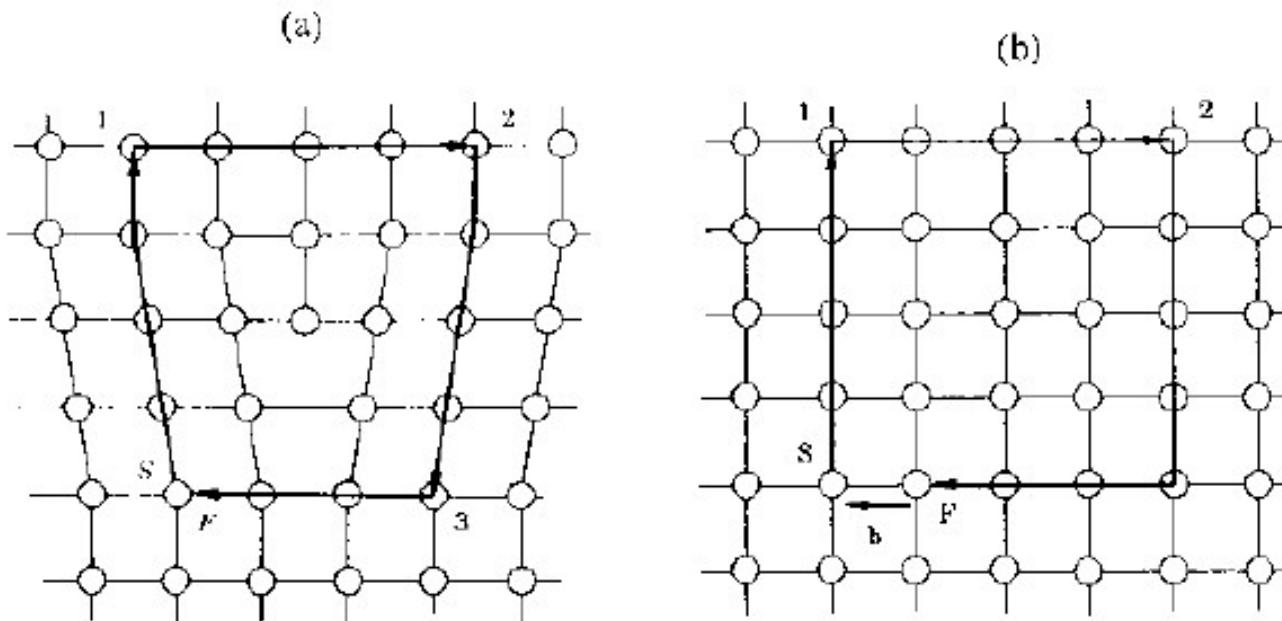


## The Burgers vector – Burgers circuit

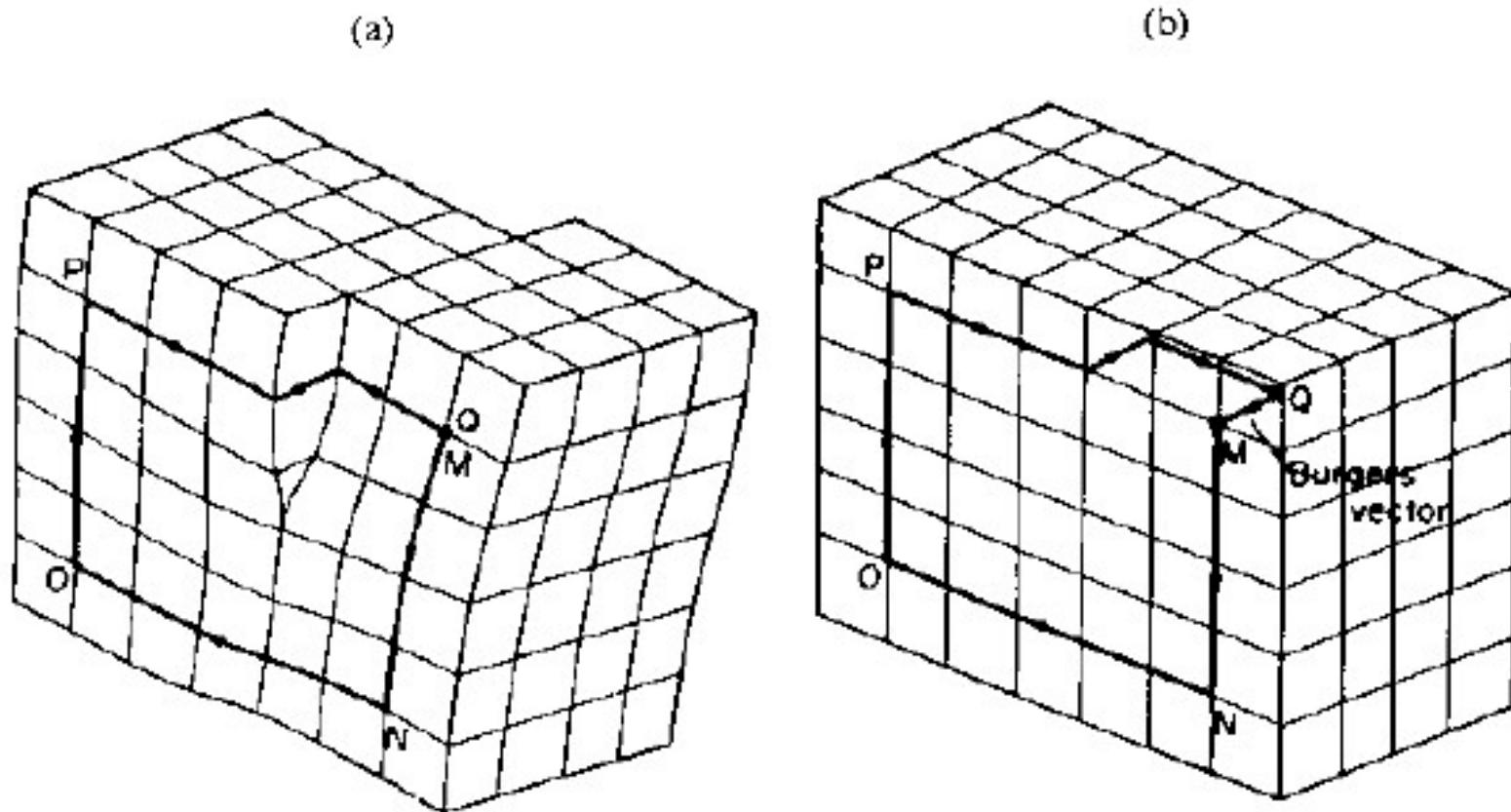
- In any deformation situation the Burgers vector is defined by constructing a Burgers circuit in the dislocated crystal
- A sequence of lattice vectors is taken to form a closed clockwise circuit around the dislocation.
- The same sequence of vectors is then taken in the perfect lattice when it is found that the circuit fails to close.
- The closure vector FS (finish-start) defines  $b$  for the dislocation
- With this FS/RH (right-hand) convention it is necessary to choose one direction along the dislocation line as positive. If this direction is reversed the vector  $b$  is also reversed

- The Burgers vector defines the atomic displacement produced as the dislocation moves across the slip plane
- Its value is governed by the crystal structure because during slip it is necessary to retain an identical lattice structure both before and after the passage of the dislocation
- This is assured if the dislocation has a Burgers vector equal to one lattice vector and, since the energy of a dislocation depends on the square of the Burgers vector, its Burgers vector is usually the shortest available lattice vector
- This vector, by definition, is parallel to the direction of closest packing in the structure, which agrees with experimental observation of the slip direction

## Burgers circuit construction



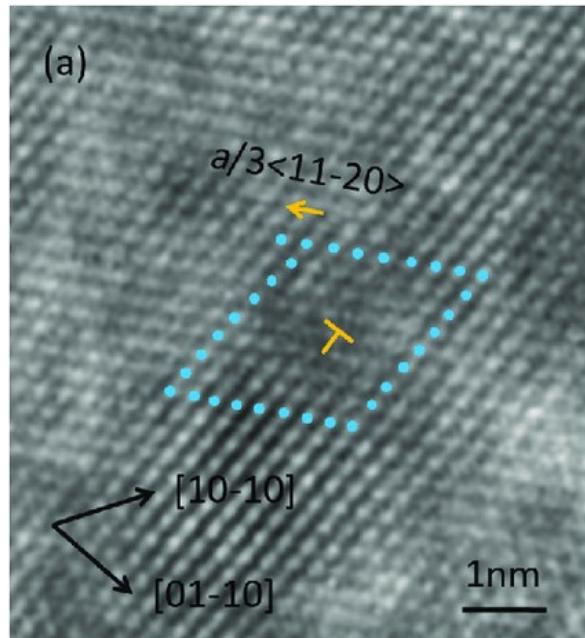
**FIGURE 6.4** Finish to start ( $F/S$ ) right-handed Burgers circuits: (a) around edge dislocation; (b) in a perfect reference crystal. (Taken from Hirthe and Lothe, 1982. Reprinted with permission from John Wiley.)



**FIGURE 6.6** Right-handed Burgers circuits: (a) around screw dislocation; (b) in perfect reference crystal. (From Hull and Bacon, 1984. Reprinted with permission from Pergamon Press.)

# Hey, we can see atoms !!!

- Not atoms but column of atoms
- High resolution transmission electron microscope
- Dislocation in HCP Ti-Al alloy



We et al. Materials and Design 2018

# Edge and Screw dislocations

**Table 5-1 Geometric properties of dislocations**

Dislocation property	Type of dislocation	
	Edge	Screw
Relationship between dislocation line and $b$	perpendicular	parallel
Slip direction	parallel to $b$	parallel to $b$
Direction of dislocation line movement relative to $b$ (slip direction)	parallel	perpendicular
Process by which dislocation may leave slip plane	climb	cross-slip

Dieter, Mechanical Metallurgy



## Energy of dislocations

- Dislocation is a line defect represented by line vector  $\vec{\xi}$  and the Burgers vector  $\vec{b}$
- Energy per unit length for screw dislocation

$U_L \approx Gb^2$ , where *G is shear modulus and b is Burgers vector*

- Energy per unit length for edge dislocation

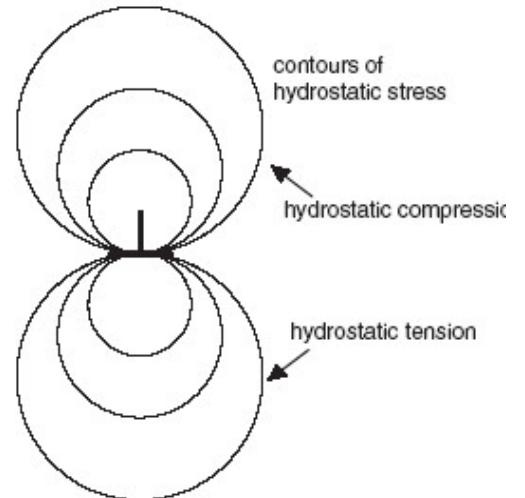
$$U_L \approx Gb^2/(1 - \nu),$$

where  $\nu$  is Poisson's ratio. Thus the energy of an edge dislocation is greater than that of a screw by a factor of  $1/(1 - \nu) \approx 1.5$ . For most metals Poissson's ratio is 0.33.

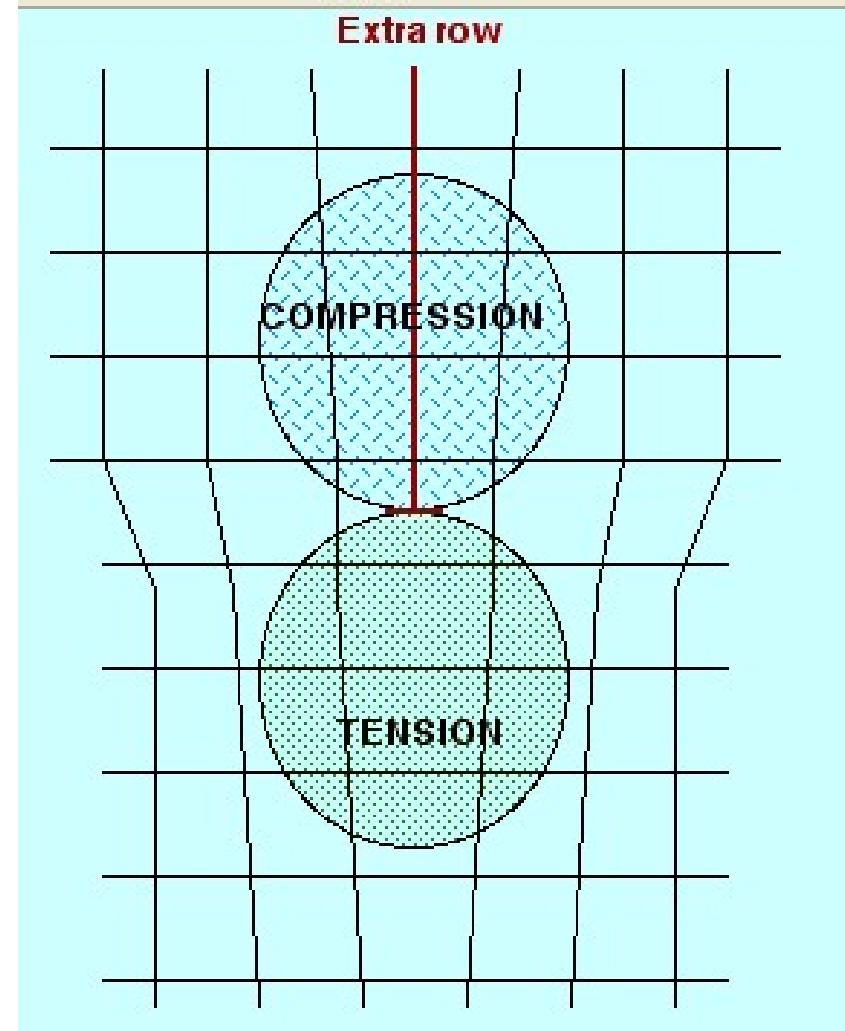
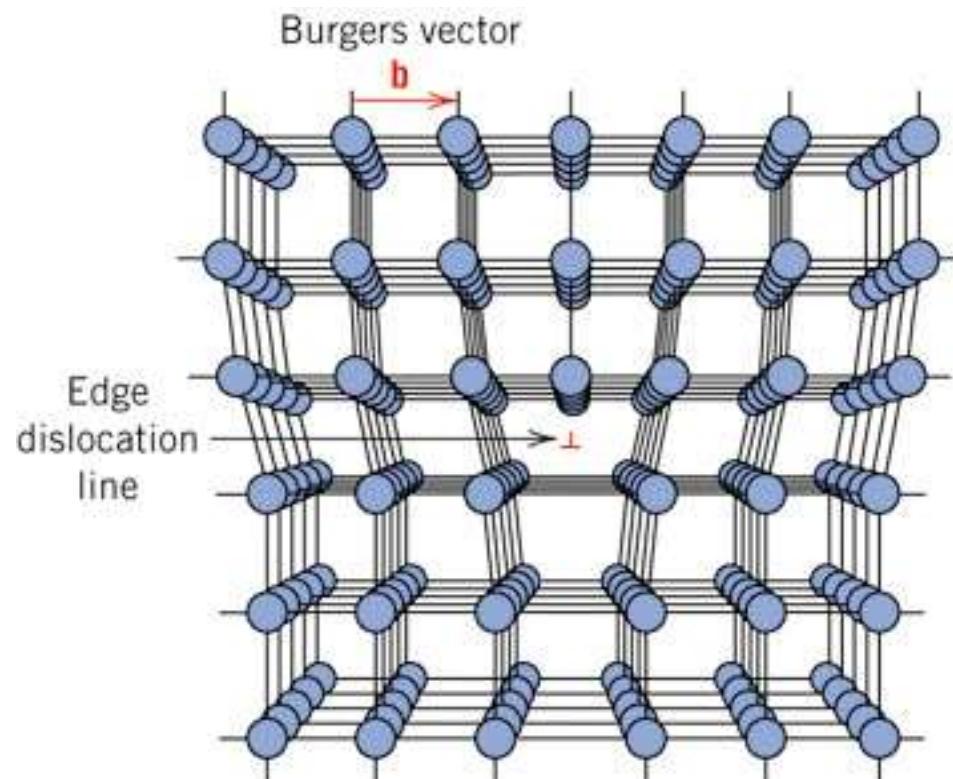
- Screw dislocation fraction higher than edge in annealed material



## Forces and stress field

- Edge dislocation like an atomistic crack
  - Compressive stress field above and tensile below
  - Shear stress field for screw dislocations
  - Interaction with other defects including dislocations
  - C in BCC iron is asymmetric defect
  - Interaction with edge and screw dislocations so higher strengthening
- 





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

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

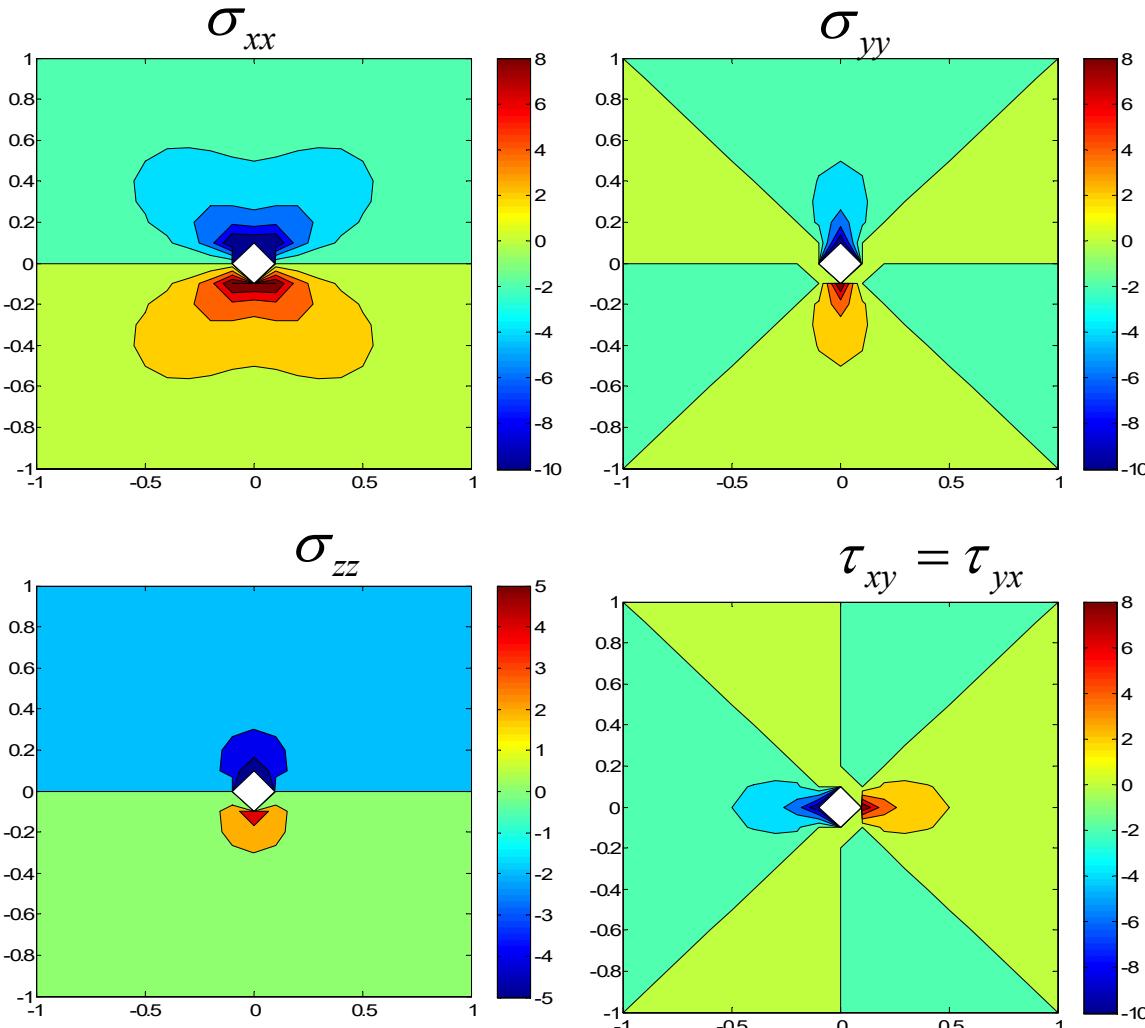
$$\tau_{xy} = \tau_{yx} = \frac{\mu bx}{2\pi(1-\nu)} \frac{(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

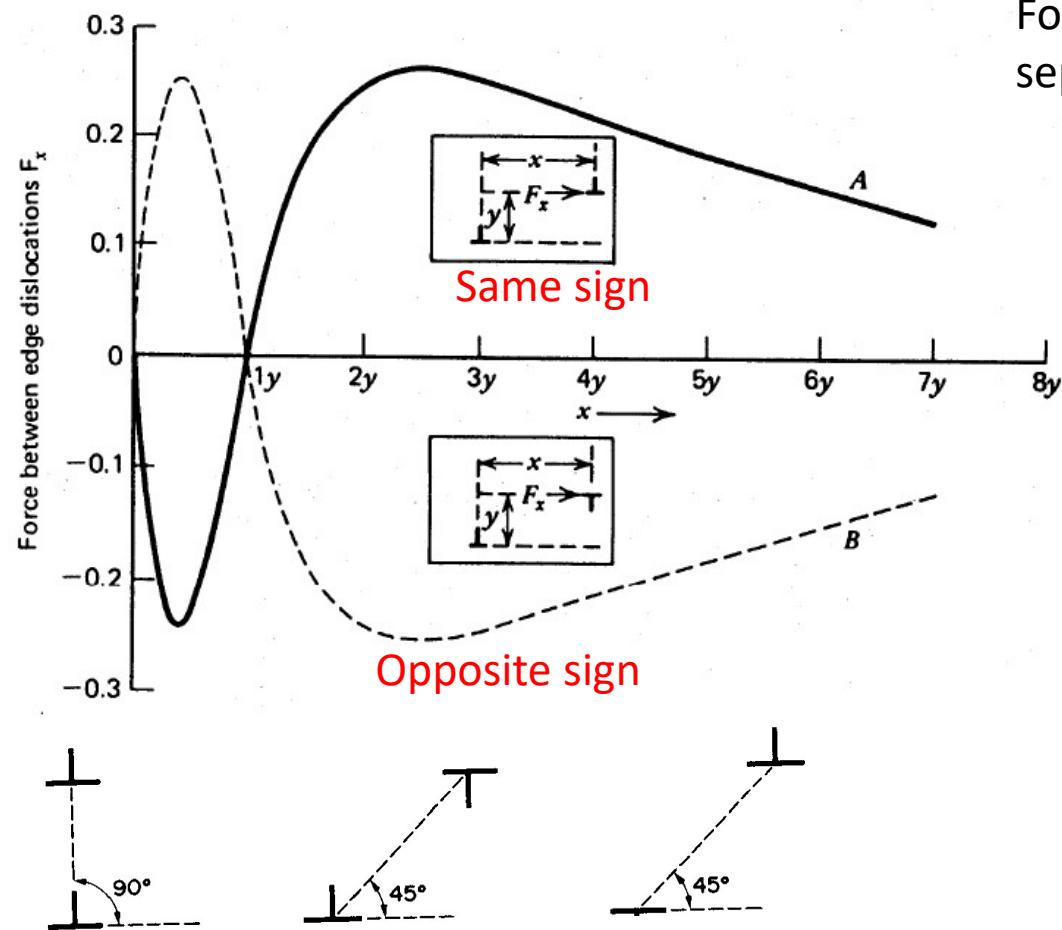
$$\tau_{xz} = \tau_{zx} = \tau_{zy} = \tau_{yz} = 0$$

$$p = \frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

$$= -\frac{2}{3}(1+\nu) \frac{\mu b}{2\pi(1-\nu)} \frac{y}{(x^2 + y^2)}$$



# Forces on dislocations

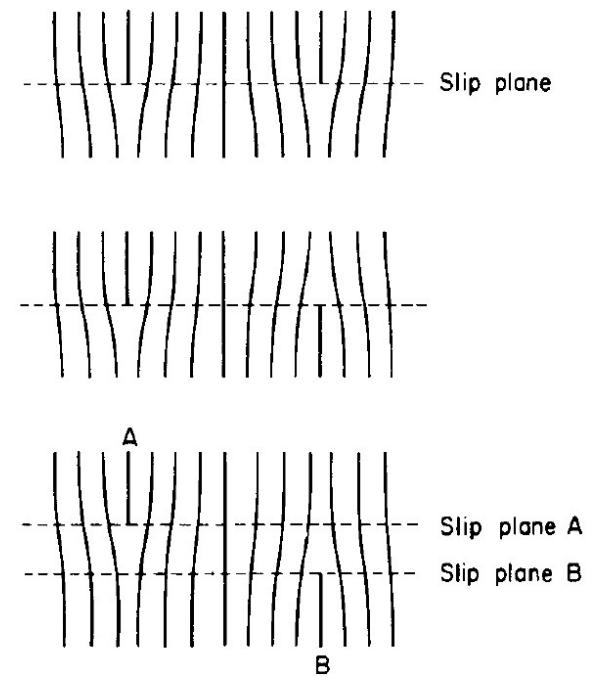


Peach-Kohler force

$$\vec{F} = -\vec{\xi}_x (\vec{b} \cdot \vec{\sigma}_{ij})$$

For dislocations on parallel planes separated by distance  $y$

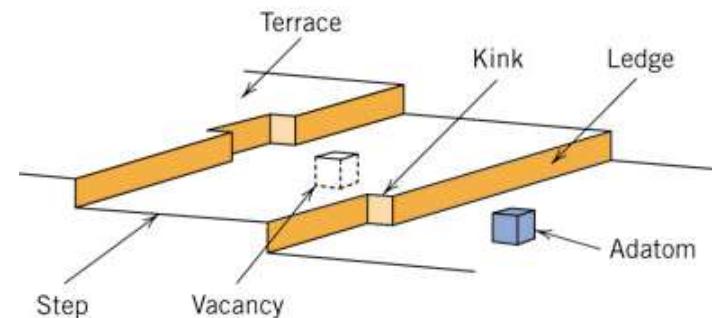
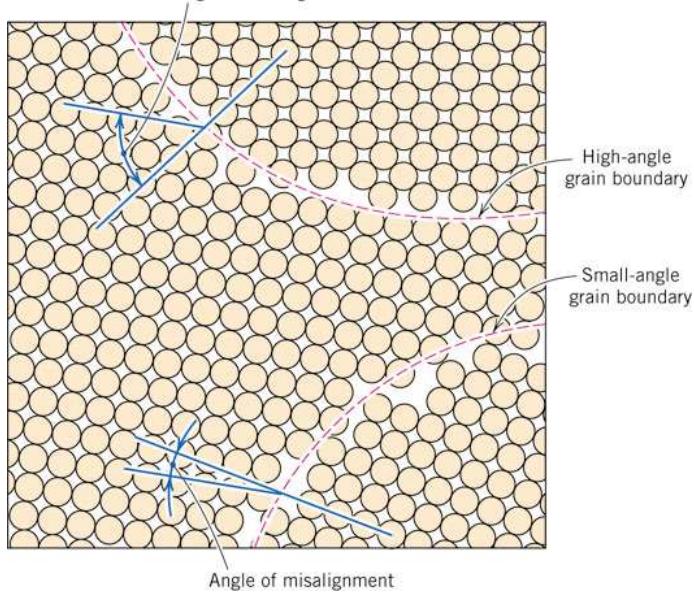
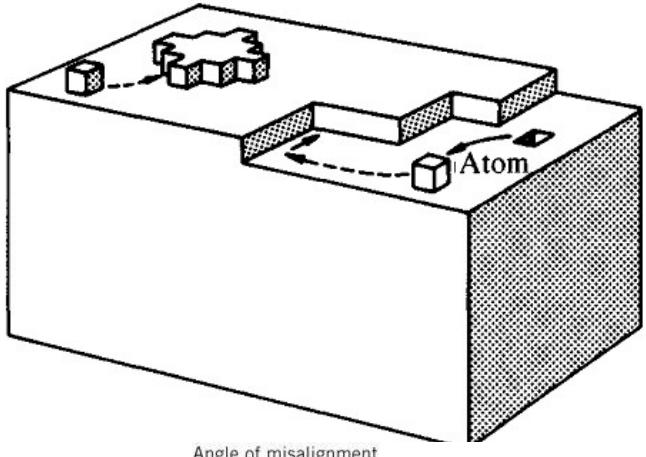
$$F_x = \frac{Gb^2 x(x^2 - y^2)}{2\pi(1-\nu)(x^2 + y^2)^2}$$



- Dislocation motion governs plasticity
- Controlling strength and ductility
- Interaction of dislocations with point defects and other 2D and 3D defects that will follow later
- Fundamental to many engineering applications
- Malleability of gold to high temperature strength of superalloys



## 2D or planar defects



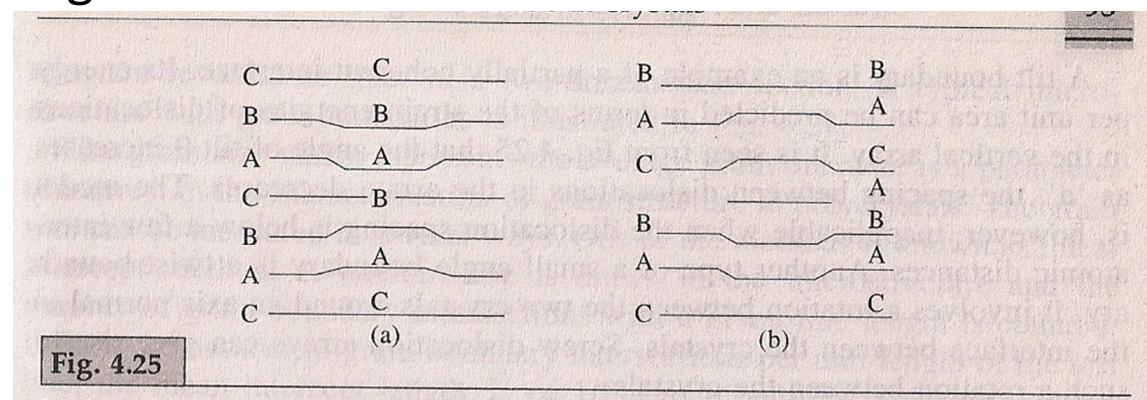
➤ Surfaces and ledges

➤ Stacking faults: HCP in FCC and vice versa

➤ Grain boundaries: high and low angle GB

➤ Tilt and Twist boundaries

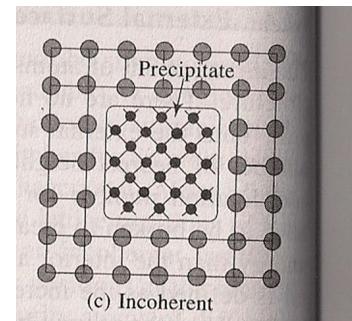
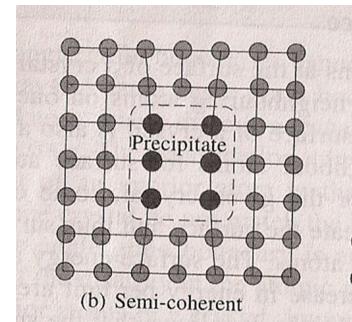
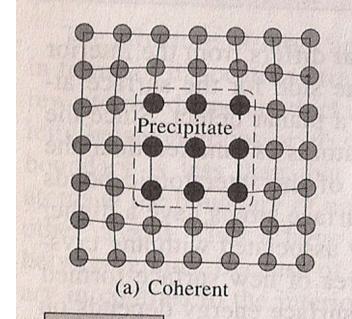
➤ GB plane, axis angle misorientation



Stacking faults in an FCC crystal (a) Missing {111} plane, and (b) Extra layer of {111} plane.

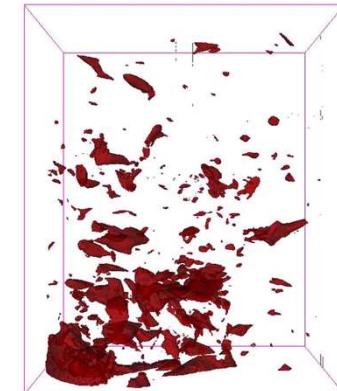


- Coincident Site lattice or special boundaries
- Twin boundaries: coherent and incoherent
- Interphase boundaries
- Coherent, semi-coherent, incoherent
- Interaction with dislocations controls deformation
- GB or microstructural engineering



## 3D or volume defects

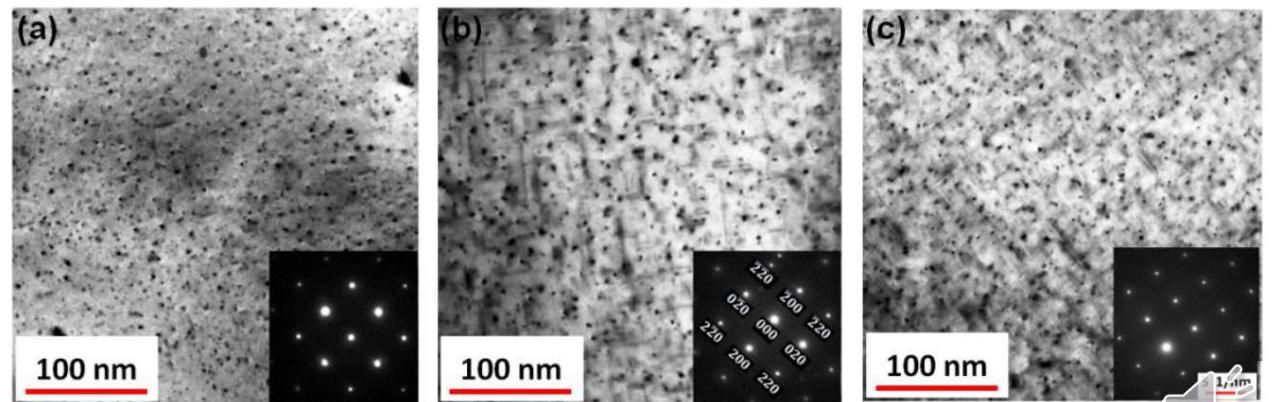
- Voids from casting or additive manufacturing



- Twins

- Precipitates: superalloys to Wright brothers using Duralumin

- Interaction with dislocations decide deformation behaviour



## Microstructure is 3D

- Most engineering materials are polycrystalline
- Vacancies and grain boundaries with triple junctions and quadruple points
- Interaction of defects with each other govern properties
- Materials engineering
- Engineering of defects in materials
- Achieve optimum properties
- Different length and time scales in materials science

