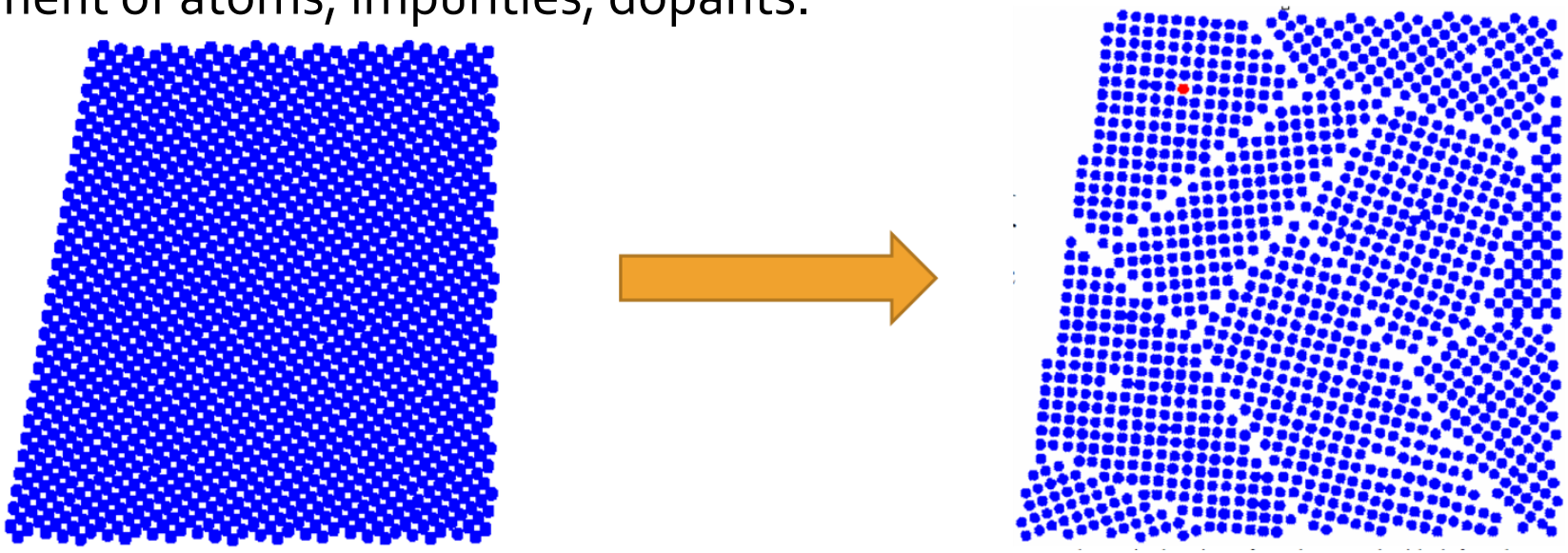
# CHAPTER 4

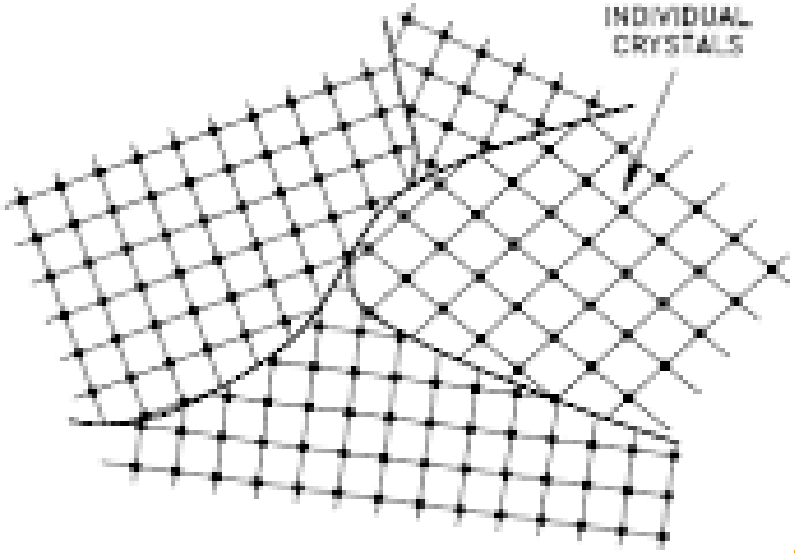
Imperfections in atomic and ionic arrangements

"Crystals are like people; it is the defects in them which tend to make them interesting!" – Colin Humphreys.

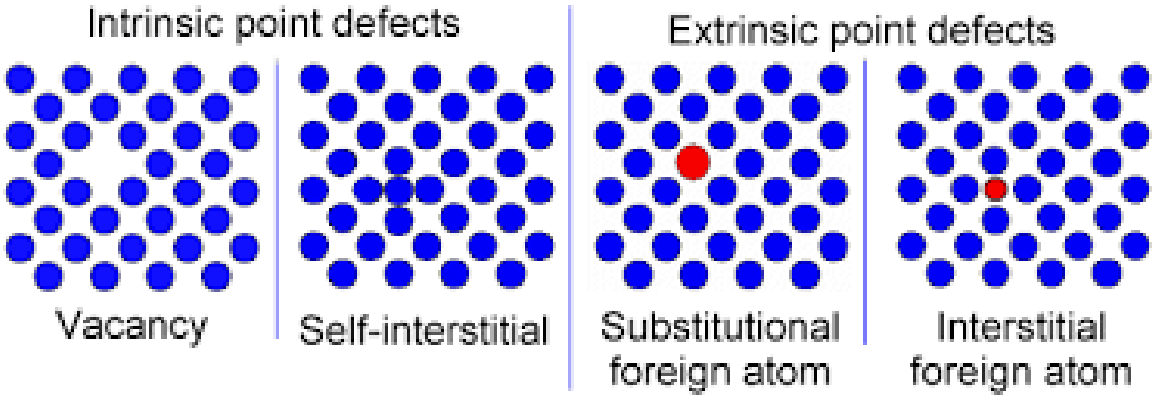
- Properties= crystal structure + bonding + DEFECTS
- Physical properties like color and texture (cost)
- Processing without changing the composition
- Movement of atoms, impurities, dopants.

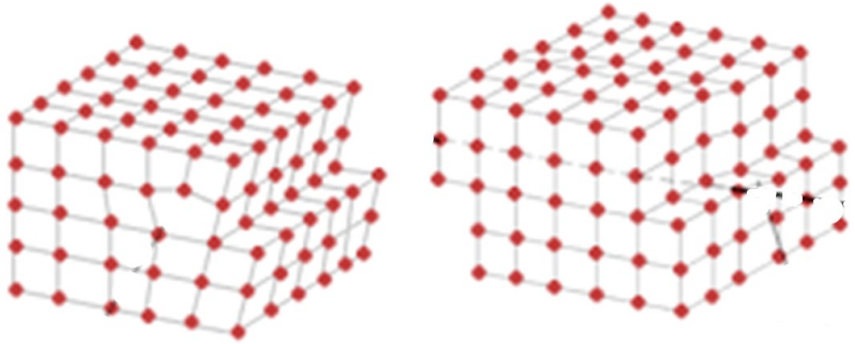


# Types of Defects



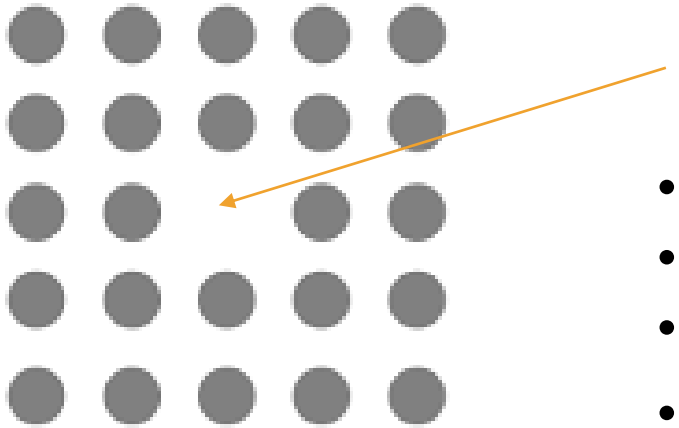

- Point defects (**0D**): atoms missing or in irregular places in the lattice.
- Linear defects (**1D**): groups of atoms in irregular positions
- Planar defects (**2D**): the interfaces between homogeneous regions of the material



# Point defects: Vacancy

Absence of an atom or ion from its normal location in a perfect crystal structure.



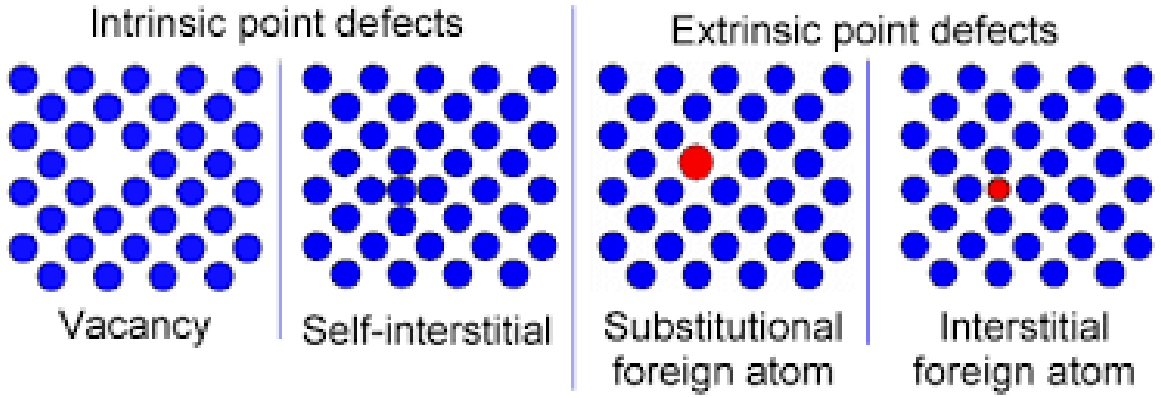
Number of vacancies:

$$n_v = ne^{(-\frac{Qv}{RT})}$$

- $n_v$: $\#\ of\ vacancies\ per\ cm^3$
- $n$: $of\ atoms\ per\ cm^3$
- $Q_v$: $Energy\ required\ to\ produce\ 1\ mole\ of\ vacancies$
- $R$: $8.314\ \frac{J}{molK}$
- $T$: $Absolute\ temperature\ (K)$

# Recap

- Properties= crystal structure + bonding + DEFECTS




$$n_v = ne^{(-\frac{Qv}{RT})}$$

# Example

- The fraction of lattice points occupied by vacancies in solid aluminum at 660°C is 10-3. What is the energy required to create vacancies in aluminum?

# $Q_v$ Required to create vacancies in Al

T= 660°$C$

$\frac{n_v}{n} = 10^{-3}$

$R = 8.315 \frac{J}{molK}$

# Example

- The density of a sample of FCC palladium is 11.98 g/cm3, and its lattice parameter is 3.8902 Å. Calculate

(a) the fraction of the lattice points that contain vacancies.

(b) the total number of vacancies in a cubic centimeter of Pd.

# Fraction of the lattice points that contain vacancies of Pd

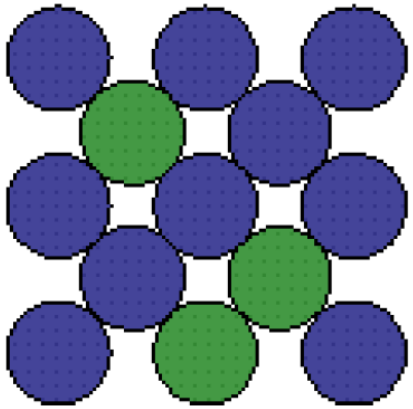
- $\rho = 11.98 \frac{g}{cm^3}$
- $a_0 = 3.8902 \times 10^{-8} cm$
- $Pd(Ar) = 106.4 \frac{g}{mol}$
- $N_{Av} = 6.023 \times 10^{23} at/mol$

# Total number of vacancies in a cubic centimeter of Pd

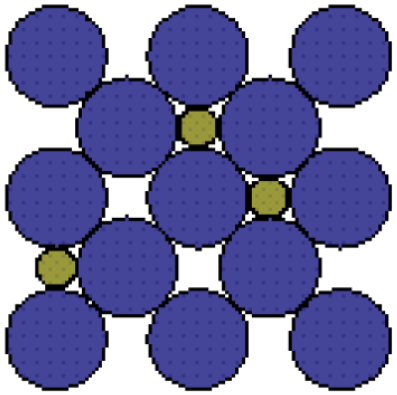
- $\rho = 11.98 \frac{g}{cm^3}$
- $a_0 = 3.8902 \times 10^{-8} cm$
- $Pd(Ar) = 106{,}4 \frac{g}{mol}$
- $N_{Av} = 6.023 \times 10^{23} \frac{at}{mol}$
- $\left(\# \frac{at}{uc}\right) = 3.9925$

# Point defects: Interstitial and impurities

- **Self-interstitial**: An atom of the same species enter an unoccupied spot in the lattice
- **Impurities**: Atoms which are different from the host

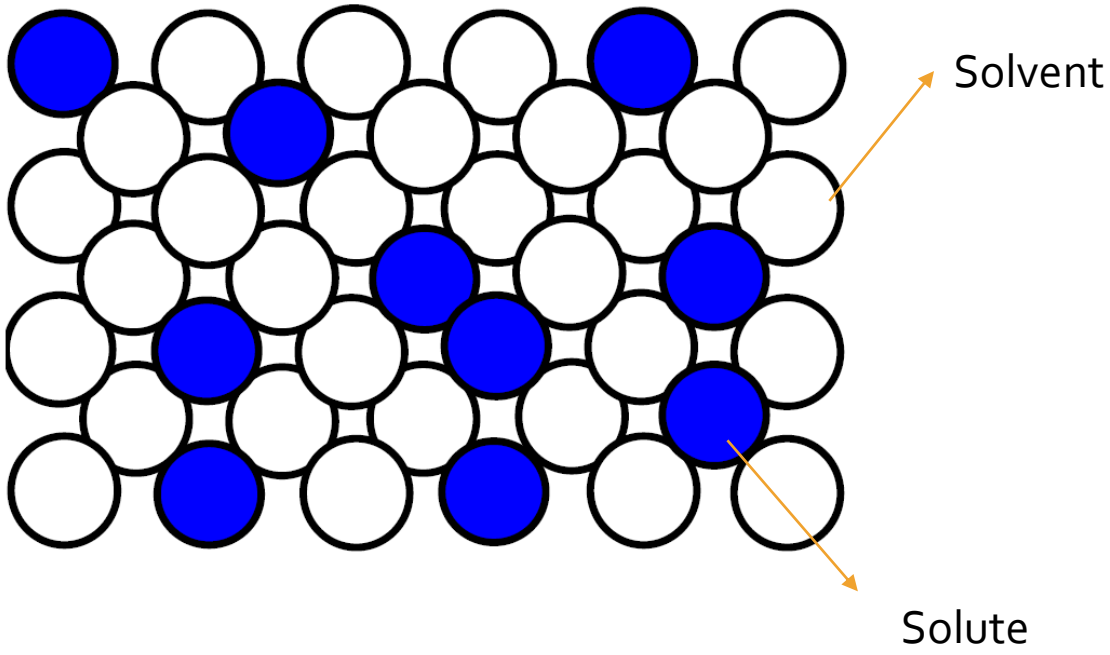


substitutional impurity



interstitial impurities

# Solids + impurities=Solid solutions




- Atomic size factor ⇒ solute and solvent atomic radii should be within ~ 15%
- Same Crystal structures
- Electronegativities of solute and solvent should be comparable

# Composition/concentration

$$C_1^{Wt\ \%} = \frac{m_1}{m_1 + m_2} \times 100$$

$$C_1^{at\ \%} = \frac{n_1}{n_1 + n_2} \times 100$$

$$n_1 = \mathrm{m}_1/\mathrm{Ar}_1$$

# Example

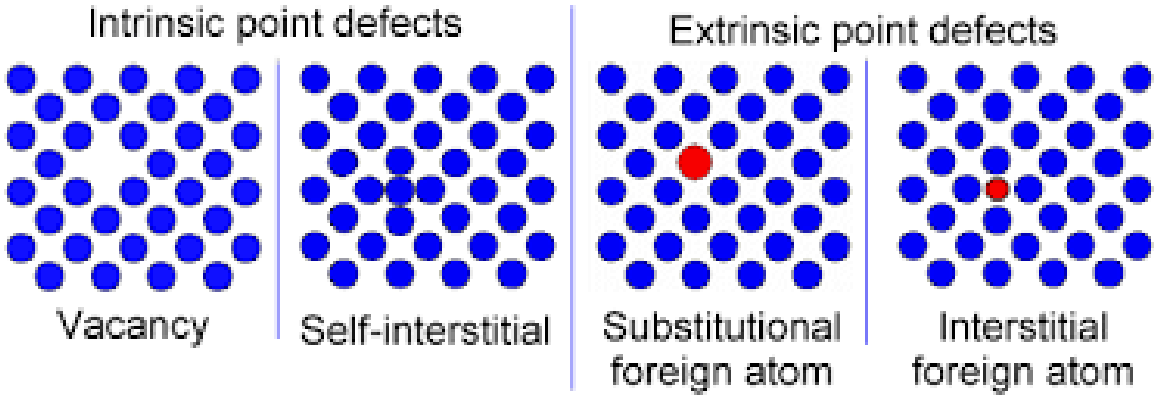
- We replace 7.5 at % of the chromium atoms in its BCC crystal with tantalum. X-ray diffraction shows that the lattice parameter is 0.29158 nm. Calculate the density of the alloy

# Density of Cr+Ta in 1 g

- $7.5at\%$ to be replaced
- BCC=2 at/uc
- $a_0 = 2.916 \times 10^{-8} cm$
- $Cr(Ar) = 51.99 \frac{g}{mol}$
- $Ta(Ar) = 180.95 \frac{g}{mol}$
- $N_{Av} = 6.023 \times 10^{23} \frac{at}{mol}$

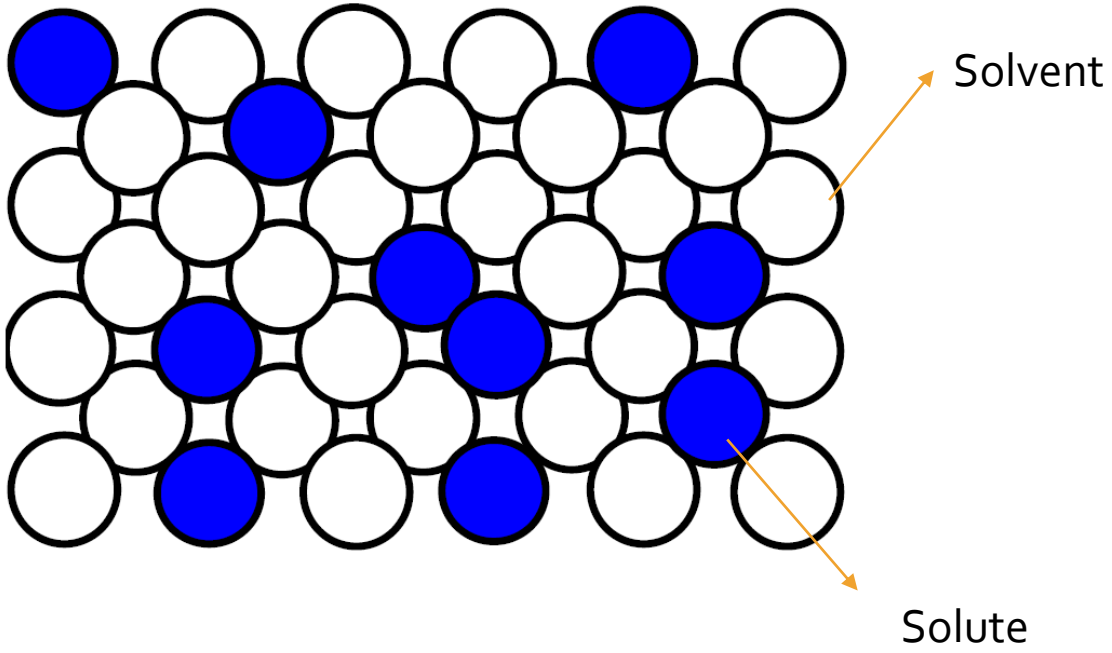
# Recap

- Properties= crystal structure + bonding + DEFECTS



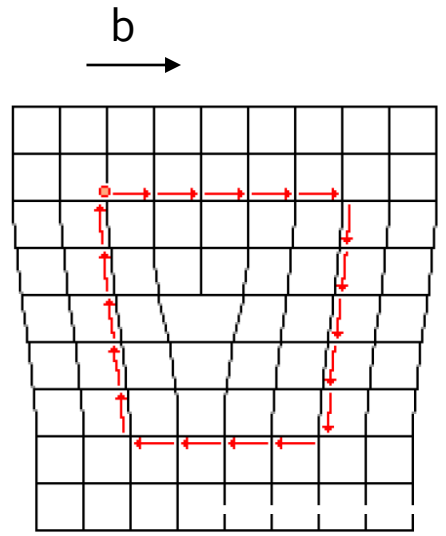

$$n_v = ne^{(-\frac{Qv}{RT})}$$

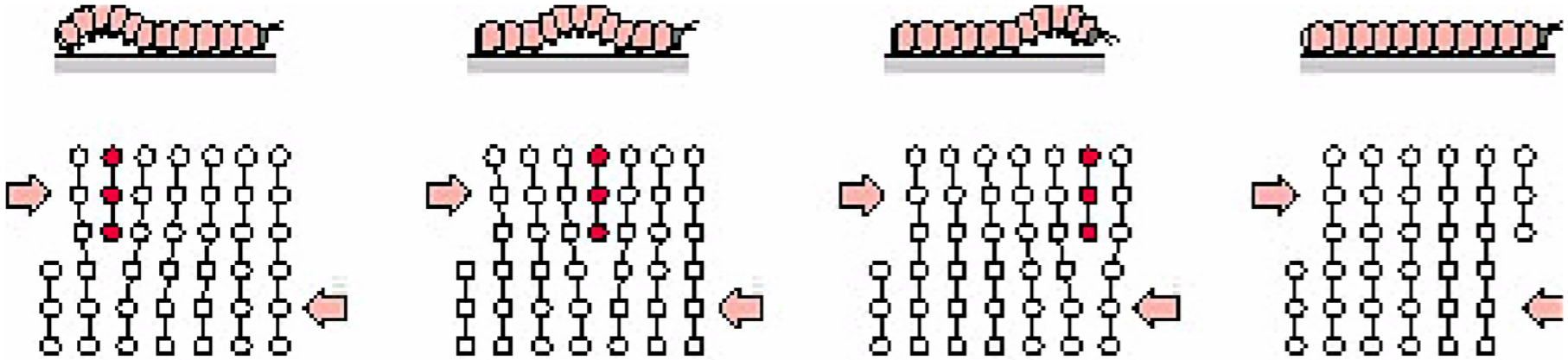
$$\rho = \frac{\Sigma\left(\left(\#\frac{at}{uc}\right)_i (Ar_i)(f_i)\right)}{V_{uc}N_{Av}}$$



# Linear Defects: Dislocation

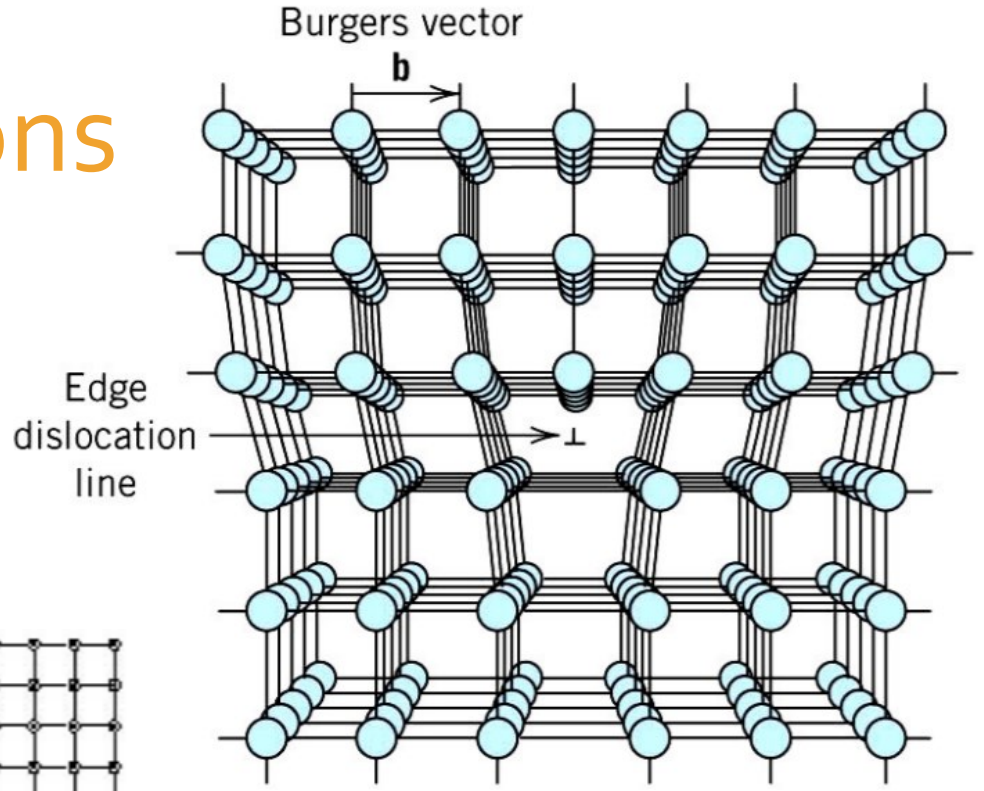
- Areas were the atoms are out of position in the crystal structure.
- **Burgers vector:** describe the size and the direction of the lattice distortion caused by a dislocation

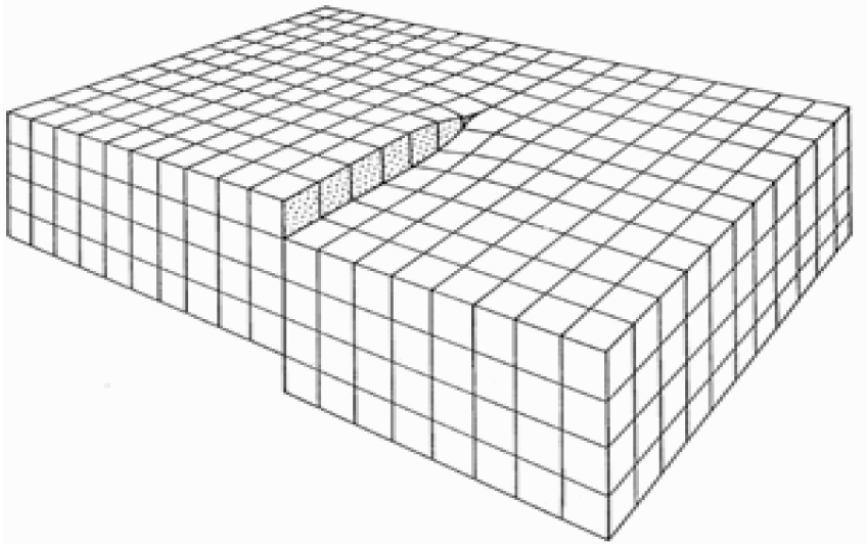


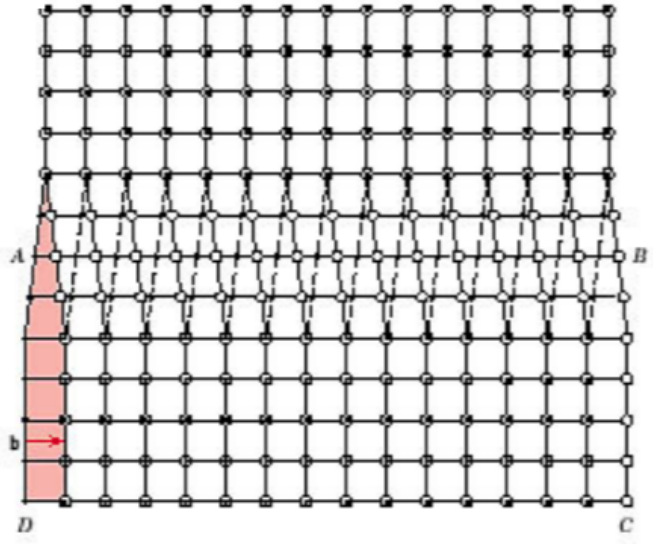



# Edge and screw dislocations

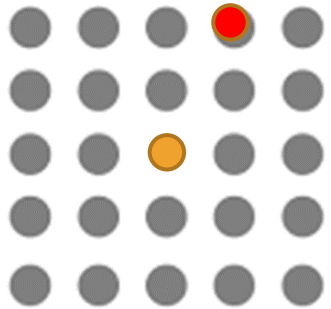
- **Edge Dislocation**: extra plane is inserted.
- **Screw dislocations:** result when displacing planes relative to each other through shear.





# Surface defects



**External Surfaces**

Surface atoms have unsatisfied atomic bonds, and higher energies than the bulk atoms
⇒ Surface energy, γ (J/m2)

Minimization of surface areas reduces the energy of the system (e.g. liquid drop).

**Grain Boundaries**

Polycrystalline material comprised of many small crystals or grains. The grains have different crystallographic orientation. There exist atomic mismatch within the regions where grains meet. These regions are called grain boundaries.