Point defects, dislocations and grain boundaries (I)

Lattice vacancies:

Missing atoms or ions

- ➔ ***Schottky* defect**: transferring an atom from a lattice site in the interior to a lattice site on the surface of the crystal

For N atoms in lattice, the equilibrium number n of vacancies is given by Boltzman factor

$$\frac{n}{N-n} = \exp(-\frac{E_V}{k_B T})$$

If $E_V = 1\ eV$ and T~1000 K, then $\frac{n}{N} \approx e^{-12} \approx 10^{-5}$

If T decreases → the equilibrium concentration of the vacancies decreases

- ➔ ***Frenkel* defect** : an atom is transferred from a lattice site to the interstitial position, a position not normally occupied by an atom.

The number n of interstitial atoms in equilibrium with n lattice vacancies in a crystal having N lattice points and N' possible interstitial position is given by :

$$E_I = k_B T \ln[\frac{(N-n)(\acute{N}-n)}{n^2}]$$

If the number n of Frenkel defects is much smaller than the number of lattice sites N and the number of interstitial sites N', the results is

$$n \cong (NN')^{\frac{1}{2}} \exp(-E_{I/2k_BT})$$

Where E_I is the energy necessary to remove an atom from a lattice site to an interstitial position

Diffusion

When there is concentration gradient of impurity atoms or vacancies →a flux of these through the solid→ in equilibrium the impurities or vacancies will be distributed uniformly

The net flux J_N of atoms is related to the gradient of the concentration N → Fick's law:

$$J_N = -D\ grad\ N$$

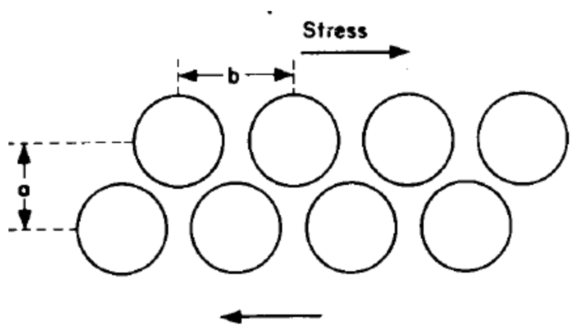
Here J_N is number of atoms crossing unit area in unit time, D is diffusion constant or diffusivity with unite of cm^2/s or m^2/s. the minus sign → diffusion occurs away from regions of high concentration.

The diffusion constant varies with temperature: $D = D_0 \exp\left(-\frac{E}{k_B T}\right)$

E: activation energy for the process.

Shear strength of single crystals

***Frenkel* method** of estimating the theoretical shear strength of a perfect crystal.



As a first approximation we represent the **stress-displacement** relation by

$\tau = (\mu b/2\pi a)\sin(2\pi x/b)$

where *a* is interplanar spacing, *b* is interatomic spacing in the direction of shear, μ denots the appropriate shear modulus.

Where. If $x/b \ll 1$ (for small elastic strains) → $\tau = \mu x/a$

The **critical shear stress** τ_c at which the lattice becomes unstable is given by the maximum value of τ

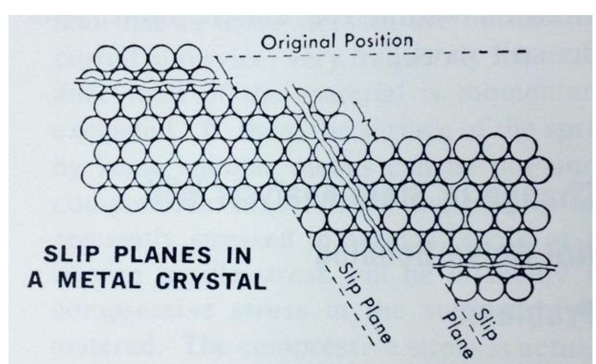
$$\tau_c = \mu b/2\pi a$$

Slip:

Plastic deformation in crystal occurs by slip. In slip, one part of the crystal slides as a unit across an adjacent part.

The surface on which slip takes place → slip plane

The direction of motion → slip direction



The property of slip is the ***Schmid* law** of the critical shear stress: slip takes place along a given slip plane and direction when the corresponding component of shear stress reaches the critical value.

Slip Systems : A slip system is a crystallographic plane, and, within that plane, a direction along which dislocation motion (or slip) occurs

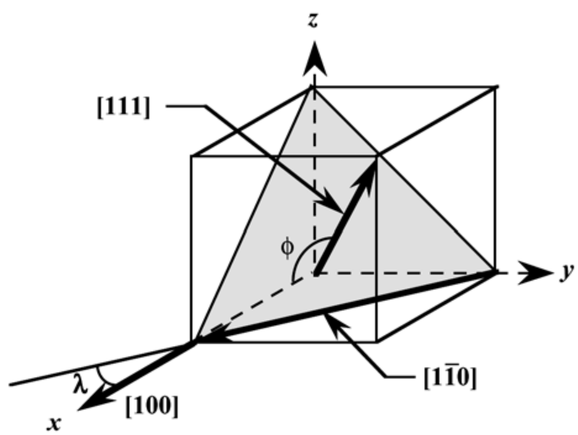
Schmid's Law

Schmid's Law states that the critically resolved shear stress (τ) is equal to the stress applied to the material (σ) multiplied by the cosine of the angle with the glide plane (ϕ) and the cosine of the angle with the glide direction (λ), which can be expressed as:

$$\tau = \sigma \times m$$

$$m = cos\phi \cos \lambda$$

where m is known as the *Schmid* factor



The angle between the [100] and directions $[1\bar{1}0]$, λ, may be determined:

$$\cos\lambda = \frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2+v_1^2 + w_1^2)(u_2^2+v_2^2 + w_2^2)}}$$

$$\cos\lambda = \frac{1 \times 1 + 0 \times (-1) + 0 \times 0}{\sqrt{(1^2 + 0^2 + 0^2)(1^2 + (-1)^2 + 0^2)}}$$

$$\lambda = 45°$$

The angle between the [100] and directions $[111]$ (normal to (111) plane),ϕ, may be determined→ $\phi = 54.7°$

$$m = cos45° \cos 54.7° = 0.408$$