

### 3.2.4 Essentials to Chapter 3.2 Diffusion Mechanisms

Considering diffusion in crystals we have exactly three basic cases

- 1. An interstitial impurity atom diffuses in the crystal=impurity diffusion.
- 2. A substitutional impurity atom diffuses in the crystal=impurity diffusion.
- 3. An atom of the crystal diffuses in the crystal=self-diffusion.

Case 2. and 3. are impossible without diffusion "vehicles", i.e. vacancies (and on occasion self-interstitials).

Diffusion mechanisms are the atomic mechanisms that are capable of moving atoms. The most important ones are:

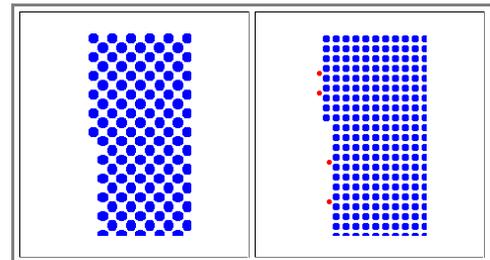
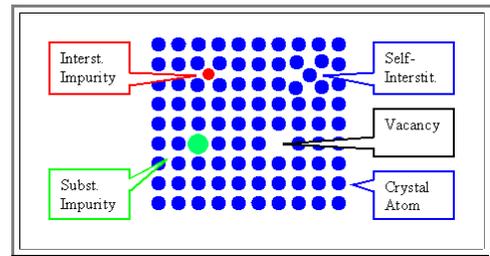
- Vacancy mechanism. Accounts for most of cases 2. and 3. from above in simple crystals,
- Direct interstitial mechanisms. Accounts for almost all of case 1.

Some more complex mechanisms exist (and are of prime importance) in **Si** (and possibly other semiconductors and somewhat more complex crystals)

- "Kick-out" mechanism, impurity and self-diffusion via self-interstitials, ...

In any case we need the migration enthalpy  $H_m$  and entropy  $S_m$  of the "jumping" entities to obtain the diffusion coefficient  $D$  of the process

- Typical values are - like always, it seems - in the **1 eV** (better: **0.5 eV - 3 eV**) and **1 k** region, respectively.
- Question to ponder: How long does it take for all atoms of crystal to be somewhere else; i.e. not at the original position? ([Exercise 3.2-1](#))



**Wait and see!**  
And keep an open mind

$$D_{dir} = g \cdot a^2 \cdot \nu_0 \cdot \exp \frac{S}{k} \cdot \exp - \frac{H_m}{kT}$$

$$D_{SD} = c_V \cdot D_V$$

$$= D^* \cdot \exp - \frac{H_m + H_f}{kT}$$