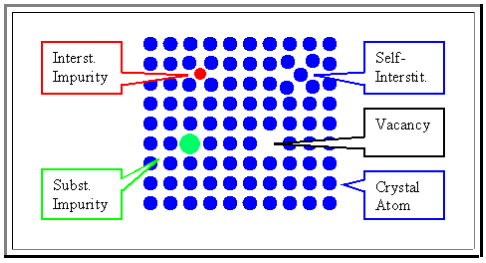
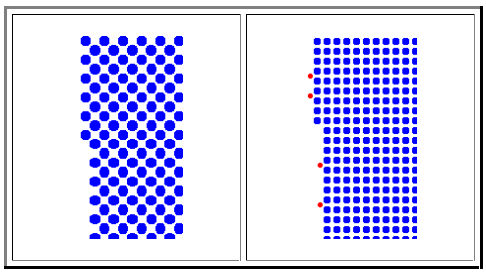
3.2.4 Essentials to Chapter 3.2 Diffusion Mechanisms

- 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, ...

Wait and see!
And keep an open mind

- 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)

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

$$D_{SD} = c_V \cdot D_V = D^* \cdot \exp -\frac{H_m + H_F}{kT}$$