3.2.3 Diffusion of Impurity Atoms

Diffusion of Impurity Atoms via Vacancies or Self-Interstitials

- In this case it is especially important not to confuse the *vehicle* (a point defect except in the case of the direct interstitial diffusion) with the *diffusing impurity atom*.
  - What we want to have are the diffusion data for the impurity atom, not for the vehicle! We will not go into details at this point, but it will come up later again.

Direct diffusion

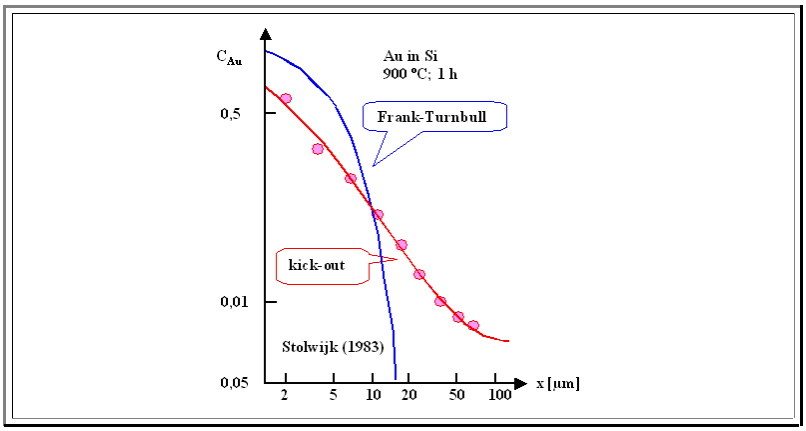
- This is the simplest mechanism, it does not need point defects. It only works for *interstitial impurity atoms*. The diffusion coefficient D_{dir} is simply given by

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

  - With H_m, S_m being the enthalpy and entropy of the jumping impurity atom.
- This is in most cases a sufficiently good approximation. The host lattice only enters in the form of the lattice factor ***g*** (and to some extent in the migration entropy), but plays no other role. This is of course a source of possible aberrations, because the ideal lattice implied in this case does normally not exist. Good examples for directly diffusing impurities are **O** in **Si**, but there are many other elements.
  - The following table (taken from K. **Graff**, Metal Impurities in **Si**-Device Fabrication; Springer Series in Mat. Science **24**) gives a few more examples.

Interstitial Impurity Atom Diffusion in **Si**					
Metal	H_{Sol} [eV]	S_{Sol}[k]	H_m [eV]	D^*[m^2/s]	T-regime [^0C]
Ti	3,05	4,22	1,79	$1{,}45 \times 10^{-2}$	950 - 1200
Cr	2,79	4,7	0,99	$1{,}0 \times 10^{-2}$	900 - 1250
Mn	2,80	7,11	0,6	$5{,}7 \times 10^{-4}$	900 - 1200
Fe	2,94	8,2	0,68	$1{,}3 \times 10^{-3}$	30 - 1200
Co	2,83	7,6	0,53	$4{,}2 \times 10^{-3}$	900 - 1100
Ni	1,68	3,2	0,47	$2{,}0 \times 10^{-3}$	800 - 1300
Cu	1,49	2,4	0,43	$4{,}7 \times 10^{-3}$	400 - 900

  - H_{Sol} and S_{Sol} denote the **solubility enthalpies** and -**entropies**. This is the extrinsic point defect quivalent of the formation enthalpy and entropy of intrinsic point defects.
- Here are some links illustrating impurity diffusion:
  - From a review of U. **Gösele**, we take the Arrhenius plot for many impurity atoms in **Si**.
  - In this link we have a somewhat unusual way of showing impurity diffusion in **Si**.
- Here some specialities: Frank-Turnbull and Kick-out Mechanism in **Si**
  - **U. Gösele** essentially "invented" the kick-out mechanism around **1985** and demonstrated that it not only provided an alternative to the already known Frank-Turnbull Mechanism, but does most likely control the diffusion of ***Au***, ***Pt***, and possibly ***Zn*** in **Si**.
  - The two mechanisms, although similar in many ways, lead under certain circumstances to very different diffusion profiles, as shown in the graph below taken from a *review article* (*Fast Diffusion in Semiconductors*) accessible through the link.



- Often it is quite difficult to decide from the data what kind of mechanism is operative. During the last few years, some research groups studying diffusion in **GaAs** came to the conclusion that the diffusion mechanisms in **GaAs** might be very different from what was accepted before (invoking, e.g., a kick-out mechanism).
- There is no evidence so far that impurity diffusion in crystals of any kind of crystal involves a **direct mechanism**. Direct mechanisms, however, are periodically suggested in the literature and should not be ruled out per se.

So, what is the *Message* of this sub-chapter?

- Many diffusion phenomena, especially in semiconductors or more complicated crystals, are still not very well understood. Precise modeling of diffusion, however, depends sooner or later on using the correct mechanisms.
- Data from diffusion measurements are always (sometimes "encrypted") data on point defects.