Numbers for Self-Diffusion

Illustration

- Here a few numbers for self diffusion
  - Numbers like this always should be taken with a grain of salt; they are often to a bit of doubt. It is not uncommon that newer measurements or new interpretations of old measurements give quite different results.
  - You may wonder a bit yourself, what self-diffusion in crystasl with two or more different atoms means, and how it relates to the prevalent defetc type, e.g. Schottky defects in **NaCl**.
- First some not-so-simple crystals:

Crystal	Diffusing Particle	Melting Point [^{o}C]	Activation enthalpy H [eV] (= $H_{M,V} + H_{F,V}$)
H_2	H_2	- 259	0,016
Ar	Ar	- 189	0,18
H_2O	H_2O	100	0,58
NaCl	Cl	801	2,3
NaCl	Na	801	0,86
Ge	Ge	940	2,94
Si	Si	1412	5,11
GaAs	Ga	1238	5,54
GaAs	As	1238	9,96
Al	Al	660	1,47
Cu	Cu	1083	2,03
Ni	Ni	1455	2,86

- Now some metals; the values are form Neumann and Toelle (1986, 1990) as compiled by Kraftmakher
  - You will find *two* pre-exponential factors D_0 and *two* activation enthalpies H in tke left part of the table.
  - That is, because according to Neumann and Toelle, the self-diffusion data taken over a large region of temperatures do *not* form a straight line in an Arrhenius plot and therefore cannot be fitted with just *one* exponential.
  - So you fit with two exponentials, and it is anyone's guess what the second set (with the higher activation energy) actually describes. A common explanation is that you see the influence of double vacancies. While the formation energy is almost twice that of a single vacancy, the mgration energy canbe substantially lower - the sum thus may weel be relavant for self-diffusion.
  - But you could also argue that you see the influence of self-interstitials, or that this is all baloney; and that any curvature of the Arrhenius plots, if there is indeed some, is due to some temperature dependence of the formation/migration entrpopies and enthalpies (which could exist on theoretical reasons).
- However - the numbers you get are quite different for fits with one or two sets.
  - This serves as another example for how difficult it is to obtain unambiguos, air-tight data in the business!

Crystal	Fitting with two sets				Fitting with one set	
	$D_0(1)$ cm^2s^{-1}	Activation enthalpy H_1 [eV]	$D_0(2)$ cm^2s^{-1}	Activation enthalpy H_1 [eV] $D_1(1)$ cm^2s^{-1}	D_0 cm^2s^{-1}	Activation enthalpy H_1 [eV]
Al						2,86
K	0.05	0.386	1	0.487		
Na	0.006	0.372	0.81	0.503		
Li	0.038	0.52	9.5	0.694		
Ag	0.055	1.77	15.1	2.35		
Au	0.025	1.70	0.83	2.20		
Cu	0.13	2.05	4.5	2.46		2,03
Ni	0.85	2.87	1350	4.15		1,47
Pt	0.034	2.64	88.6	4.05		
V	0.31	3.21	2420	4.70		
Nb	0.115	3.88	65	5.21		
Mo	0.13	4.54	140	5.70		
Ta	0.002	3.84	1.16	4.78		
W	0.13	5.62	200	7.33		