Written Exam, Radiation damage in materials (SH2605) – VT 2015
14.00 – 19.00, March 16, 2015, FB51, AlbaNova, KTH, Stockholm

With some solutions!

Problem 1 [2p]

a) Determine the *atomic* diffusion coefficients D_a^v (for the vacancy mechanism) and D_a^i (for the self-interstitial mechanism) for fcc gold at 100°C? [1p]
b) Determine the *defect* diffusion coefficients D^v and D^i for the same conditions and discuss eventual differences with respect to the atomic diffusion coefficients. [1p]

Solution:
a) The atomic diffusion coefficients are given by $D_a^x = \alpha a_0^2 \nu e^{-G_a^x/k_B T}$ where α is given by the crystalline symmetry and the rest are in the table (given that $G = H - TS$). This gives us

$$D_a^v = 2.3 \cdot 10^{-33} m^2/s$$
$$D_a^i = 1.1 \cdot 10^{-43} m^2/s$$

b) The defect diffusion coefficients are similar but don't have the equilibrium concentration component. Thus, they are $D^x = \alpha a_0^2 \nu e^{-G_m^x/k_B T}$ and we get

$$D^v = 1.3 \cdot 10^{-16} m^2/s$$
$$D^i = 1.6 \cdot 10^{-8} m^2/s$$

+ comments on differences that I leave to you!

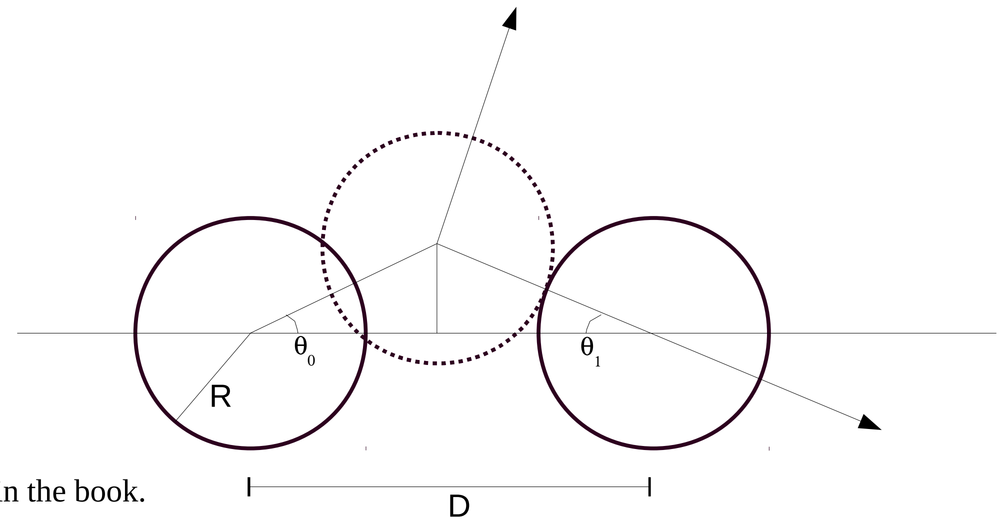
Problem 2 [2p]

In the experiment by Geiger and Marsden, 8 MeV α-particles were scattered against thin metal foils. The condition for Rutherford scattering to take place is that the projectiles are reaching close to the nucleus, compared to the size of the atom. Calculate the minimum distance in a head on collision, assuming the target is gold. Compare with the Bohr radius. [2p]

Solution: See exercise notes!

Problem 3 [3p]

Focusing means that a chain of successive collisions in a crystalline solid converges the collision angles to zero. It can occur when a PKA has a velocity vector close to a high-symmetry direction. Assume that the atoms scatter elastically as hard-spheres.
a) Using the nomenclature of the figure below, derive the criterion for focusing to occur. [2p]
b) In which direction is focusing most likely to occur, in e.g. a bcc lattice? [1p]



Solution: See chapter 2.2.4 in the book.

Problem 4 [3p]

a) Considering that for elastic scattering of hard spheres, such as for neutrons scattering on lattice atoms, the scattering cross section is $\sigma_s(E_i, T) = \frac{\sigma_s(E_i)}{\gamma E_i}$, where E_i is the energy of the incident neutron and T is the energy transferred to the lattice atom. Show that the average transferred energy, assuming isotropic scattering, is $\bar{T} \approx \frac{\gamma E_i}{2}$ [2p]

b) What is the average damage rate (in dpa/s) in gold irradiated with a flux of 10^{15} cm^{-2}s^{-1} of 2 keV neutrons, assuming the total scattering cross section is 4 barns? [1p]

Solution:

a) See lecture notes!

b) Given the data in the table we can calculate the dose rate by $R = \phi\sigma\nu(T)$ but since $\gamma = 0.02$ here, a 2 keV neutron transfers on average 20 eV to the Au atoms, thus there is **no** damage in this simple model!

Problem 5 [2p]

Assume that the steady state concentration of vacancies in bcc iron, in a 1 MeV neutron flux of $4 \cdot 10^{14}$ cm^{-2}s^{-1} is given by $C_v = \frac{K_0}{K_{vV} C_V}$ and that the average void radius is 10 nm, the void density is 10^{16} m^{-3} and the total scattering cross section is 3 barns.

Determine the temperature at which the supersaturation factor of vacancies becomes unity, i.e. the temperature at which thermal effects start to dominate over irradiation ones. [2p]

Solution:

The supersaturation factor is given by $S_v = \frac{C_v}{C_v^{eq}}$. The critical temperature can be obtained by expanding the equation $S_v = \dfrac{K_0}{C_v^{eq} K_{vV} C_V}$ in all its details. The temperature enters in the factors C_v^{eq} and $K_{vV} = 4\pi R_V D_v$

Once all the algebra has been done, we are left with

$$T_{crit} = \frac{H_f^v + H_m^v}{k_B \ln\left(4\pi S_v R_V \alpha a_0^2 \nu_0 C_V e^{S_f^v/k_B} / \xi \nu(T) \sigma N \varphi\right)}$$ (which can be slightly simplified I realize now)

and we get a critical temperature of 1000°C.

Problem 6 [4p]

a) Order the {100},{110}, {111} planes in a simple cubic crystal according to their planar density. [1p]
b) Which and how many are the slip systems in a simple cubic crystal? [1p]
c) Which slip system will activate first during plastic deformation of the crystal in the direction n_T = [1, 3, 5] ? [2p]

Solution:
a) The density ordering of the planes is {100} > {110} > {111}
b) The <100> directions have the highest linear density and thus the slip systems are the six {100}<100> combinations.
c) Make sure to normalize, then the (001)[010] system has the highest Schmid factor (0.18) and will be activated first.

Data table: Various properties of selected metals:

	a_0	A	Z	E_d	H_f^v	S_f^v	H_m^v	H_f^i	S_f^i	H_m^i	γ	ν
bcc Fe	2.86 Å	56	26	40 eV	2.1 eV	2.4 k_B	0.7 eV	4.0 eV	0.7 k_B	0.3 eV	1.8 J/m²	15 THz
fcc Au	4.08 Å	197	79	40 eV	1.3 eV	1.9 k_B	0.8 eV	2.6 eV	0.6 k_B	0.2 eV	1.0 J/m²	49 THz

(The migration entropies of both vacancies and SIAs are very close to zero)