Radiation damage in materials (SH2605) – VT 2017
Written Exam

8.00 – 13.00, March 20, 2017, Reactor Physics, AlbaNova, KTH, Stockholm

Allowed aids: pocket calculator, BETA (maths handbook) or similar, ruler, pencil/pen, eraser, snacks

To pass the exam you need at least **6 points out of 16.**

Grading is determined by the total number of points:
F: 0–5.0; Fx: 5.5; E: 6–8; D: 8.5–10.5; C: 11–12.5; B: 13–14; A: 14.5+

Half-points can be rewarded for partially correct answers.

Write clearly. Motivate your answers by calculations, text and figures if pertinent.

Make your own, reasonable assumptions, when necessary. Make sure to explicitly state what assumptions you make in the text.

Good luck and have fun!

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 Au at 1000°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]

Problem 2 [3p]

a) Gamma decay in spent fuel can potentially damage the structural material that surrounds it. Gamma-photons normally Compton-scatter electrons in the metal lattice, and these electrons can in turn scatter ions. Assume the electrons scatter ions like hard-spheres and derive an expression for the maximal total energy transfer from the gamma-photon to a lattice ion. [2p]
b) What is the energy threshold for a gamma-photon from the spent fuel to create displacement damage in a surrounding iron lattice? [1p]

Problem 3 [3p]

The threshold displacement energy of a crystal can be very roughly estimated by assuming i) that only the pair interaction of the surrounding atoms determine the barrier energy, ii) that the barrier atoms do not relax, and iii) no thermal energy losses occur.
Estimate the displacement energy in fcc Au along the ⟨100⟩, ⟨110⟩ and ⟨111⟩ directions. Base your calculation on the pair interaction and cohesive energy from figure 1 below. [3p]

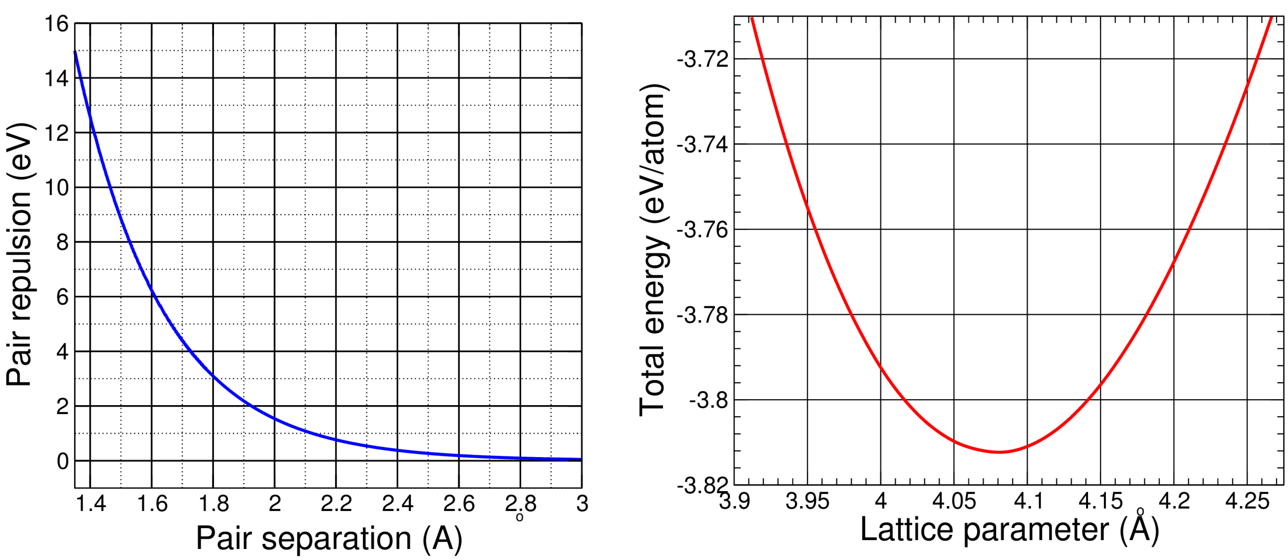

Figure 1. fcc Au: Left – pair energy as function of separation distance; Right – total energy as function of lattice parameter close to the equilibrium

Problem 4 [3p]

a) For elastic scattering of hard spheres, such as for neutrons scattering on lattice atoms we call E_i the energy of the incident neutron and T 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 MeV neutrons, assuming the total scattering cross section is 4 barns? [1p]

Problem 5 [2p]

Assume that the steady state concentration of vacancies in bcc iron, in a 2 MeV neutron flux of $5 \cdot 10^{14}$ $cm^{-2}s^{-1}$ is given by $C_v = \frac{K_0}{K_{vV} C_V}$ and that the average void radius is 4 nm, the void density is 10^{17} m^{-3} and the total scattering cross section is 3 barns.

a) 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]

Problem 6 [3p]

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

Data sheet:

Various properties of selected metals:

	a_0	A	Z	E_d	H_f^v	S_f^v	H_m^v	E_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)

Models:

Compton scattering: $E_e = \dfrac{E_\gamma^2(1-\cos\theta)}{E_\gamma(1-\cos\theta)+m_e c^2}$ (θ = photon scattering angle)

Hard-sphere scattering cross section: $\sigma_s(E_i, T) = \dfrac{\sigma_s(E_i)}{\gamma E_i}$

The Kinchin-Pease model: $$n(T) = \begin{cases} 0\ , & T < E_d \\ 1\ , & E_d < T < 2E_d \\ \dfrac{T}{2E_d}\ , & 2E_d < T < E_c \\ \dfrac{E_c}{2E_d}\ , & T > E_c \end{cases}$$

Rate theory defect generation term: $K_0 = \xi n(T) \sigma_s N \phi$

Neutral void-vacancy reaction rate: $K_{vV} = 4\pi R_V D_v$

Thermal atomic diffusion: $D_a^v = f \alpha a_0^2 \nu e^{G_a^v / k_B T}$

Constants:

Boltzmann's constant $k_B = 1.38 \cdot 10^{-23}\, J/K$

Elementary charge $e = 1.602 \cdot 10^{-19}\, C$

Electron rest mass $m_e = 9.11 \cdot 10^{-31}\, kg = 511\, keV/c^2$

Atomic mass unit $1u = 1.66 \cdot 10^{-27}\, kg = 931\, MeV/c^2$

Speed of light $c = 3 \cdot 10^8\, m/s$