Written Exam, Radiation damage in materials (SH2605) – VT 2013
08.00 – 13.00, March 8, 2013, FD41, AlbaNova, KTH, Stockholm

With solutions!

Problem 1 [2p]

In an experiment conducted at 10°C below the melting point of copper (fcc; a_0=3.61Å; T_m=1085°C), a vacancy concentration of 0.02% is found. At T = 500°C, the vacancy concentration is $5.7\cdot10^{-8}$/atom.
a) What is the vacancy formation energy in Cu? [1p]
b) How many vacancies are there per cm³ at 800°C? [0.5p]
c) Explain why there are orders of magnitude less self-interstitials than vacancies in the absence of radiation. [0.5p]

Solution:
(Firstly, I should have asked for the vacancy formation enthaply H_f to avoid ambiguity. Therefore also answers assuming that G_f is asked for are ok.)

a) Concentration is given by the Boltzmann factor: $c_{vac}=e^{-G_f/k_BT}$ where $G_f=H_f+TS_f$
We have two concentrations $c_{vac}(T_1)=2\cdot10^{-4}$ and $c_{vac}(T_2)=5.7\cdot10^{-8}$ where $T_1=1348\text{K}$ and $T_1=773\text{K}$ and we have two unknowns, H_f and S_f, giving us a system of equations:

$$c(T_1)=e^{-(H_f-T_1S_f)/k_BT_1}$$
$$c(T_2)=e^{-(H_f-T_2S_f)/k_BT_2}$$

from which we can get $H_f=\frac{\ln\frac{c(T_1)}{c(T_2)}}{1/k_BT_2-1/k_BT_1}$ and $S_f=\ln c(T_1)+\frac{H}{k_BT_1}$

Inserting numbers gives us: $H_f=1.27\ eV$ and $S_f=2.46k_B$

b) The number density of vacancies is obtained from the Boltzmann factor, as above:

$$c_{vac}=e^{-G_f/k_BT}=e^{S_f/k_B}\cdot e^{-H_f/k_BT}=e^{2.46}\cdot e^{-1.27/(8.61\cdot10^{-5}\cdot1073)}=1.2\cdot10^{-5}$$

The number of Cu atoms per cm³ is given by the lattice parameter and the fact that 4 atoms make up one unit cell: $N_{Cu}=\frac{1}{V}=\frac{4\cdot10^{24}}{a_0^3}cm^{-3}=8.5\cdot10^{22}\,cm^{-3}$

The number of vacancies is then $N_{vac}=N_{Cu}c_{vac}=1.02\cdot10^{18}cm^{-3}$

c) The concentration is an exponential of the formation energy and the formation energy of self-interstitials is typically 2-3 times higher than that of vacancies.

Problem 2 [3p]

a) Derive the expression for the maximal energy transfer from an elastic collision, as a function of the kinetic energy of the incoming particle (T_{inc}). [2p]
b) What is the maximal kinetic energy that a Zr atom in the cladding receives from 1.0 MeV neutrons coming from the fission reactions in the fuel? [1p]

Solution:
a) Conserve momentum and kinetic energy, assuming that the knocked-on particle (mass M) is at rest

and that the incoming particle (mass m) is perfectly back-scattered.

$$\begin{matrix} p_b = p_a \\ T_b = T_a \end{matrix} \rightarrow \begin{matrix} p_b^m + p_b^M = p_a^m + p_a^M \\ T_b^m + T_b^M = T_a^m + T_a^M \end{matrix} \rightarrow \begin{matrix} mv_b + Mu_b = mv_a + Mu_a \\ \frac{1}{2}(mv_b^2 + Mu_b^2) = \frac{1}{2}(mv_a^2 + Mu_a^2) \end{matrix} \rightarrow \begin{matrix} mv_b = mv_a + Mu_a \\ mv_b^2 = mv_a^2 + Mu_a^2 \end{matrix} \rightarrow$$

$$v_a = v_b - \frac{M}{m}u_a \rightarrow mv_b^2 = m\left(v_b - u_a\frac{M}{m}\right)^2 + Mu_a^2 = mv_b^2 - 2v_b u_a M + u_a^2\frac{M^2}{m} + M u_a^2 ,$$

strike out mv_b^2 from both sides and divide by M, then we get $u_a = 2\frac{mv_b}{M+m}$, thus rendering

$$T_a^M = \frac{1}{2}Mu_a^2 = \frac{1}{2}mv_b^2\frac{4\mathrm{mM}}{(M+m)^2} = \frac{4\mathrm{mM}}{(M+m)^2}T_{\mathrm{inc}} = \gamma T_{\mathrm{inc}}$$

b) m=1, M=91, T_{inc}=1MeV → $T_a^M = \frac{4\mathrm{mM}}{(M+m)^2}T_{\mathrm{inc}} = 43\,keV$, i.e. γ=0.043

Problem 3 [2p]

In a typical light water reactor, the flux of fast neutrons (with 1 MeV energy) in the Zr-cladding is about $3\cdot10^{13}$ $cm^{-2}s^{-1}$. The n-Zr scattering cross section is 6.5 barns. Use the Kinchin-Pease damage model, disregarding electronic stopping, to estimate the damage in units of dpa per year. [2p]

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

Solution:

The rate of damage, in unit of dpa/time is given by $\frac{R}{N} = \sigma\phi\, n(T) = \sigma\phi\gamma\frac{T_{\mathrm{inc}}}{4E_d}$ where the extra factor ½ comes from the approximation that the average kinetic energy is half the maximum and we estimate $E_d = 40\,eV$ for Zr. With the data inserted we get $\frac{R}{N} = \sigma\phi\gamma\frac{T_{\mathrm{inc}}}{4E_d} = 5.24\cdot10^{-8}\,\mathrm{dpa}/s = 1.65\,\mathrm{dpa}/y$

Problem 4 [2p]

Consider a cylindrical region of material of radius *r* around a screw dislocation with Burgers vector *b*.
a) Provided that we are outside the core, in the elastic region, show that the shear strain is $b/2\pi r$. [1p]

b) From elasticity theory, Hooke's law tells us that $u = \frac{1}{2}\left(\frac{x}{d}\right)^2\mu$, where *u* is the elastic energy, *x/d* is the shear strain and μ is the shear modulus. Show that the total elastic energy per unit length of the

screw dislocation is

$$E = \mu \frac{b^2}{4\pi} \ln \frac{R}{r_0}$$

where r_0 is an inner cut-off radius and R is an outer cut-off radius. [1p]

Solution:

a) The cylinder circumference is $2\pi r$ and the mismatch along the cylinder is b. The angle is small and thus the simple ratio of these gives us the shear strain $b/2\pi r$:

b) The total elastic energy is given by $E = \int_0^{2\pi} \int_{r_0}^{R} u \, dV = \frac{b^2 \mu}{8\pi^2} 2\pi \int_{r_0}^{R} \frac{r}{r^2} dr = \frac{b^2 \mu}{4\pi} \ln \frac{R}{r_0}$

Problem 5 [4p]

In figure 1 below is plotted the pair energy as a function of separation distance (blue) and the equation of state (red) for a model of bcc Fe. The total energy for atom j is defined in this model as

$$E_j = \sum_{i \neq j} V(r_{ij}) + \phi(a_0) \quad (1)$$

where i runs over all neighbours of a given atom, r_{ij} is the distance between atoms i and j, $V(r_{ij})$ is the pair energy and $\phi(a_0)$ is the embedding energy for a given lattice parameter.

The bulk modulus of a crystal can be defined as

$$B = -V_0 \frac{d^2 E}{dV^2} \quad (2)$$

where V_0 is the equilibrium volume, E is the total energy and V is the volume.

Calculate

a) the bulk modulus of bcc Fe [2p]

b) the equilibrium embedding energy of bcc Fe [2p]

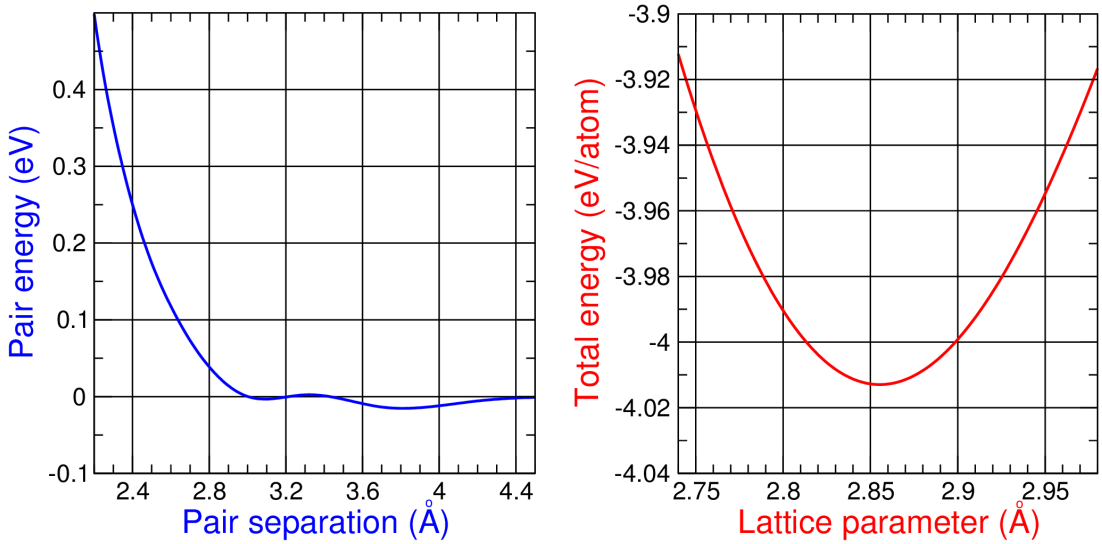

Figure 1. bcc Fe: Left – pair energy as function of separation distance; Right – total energy as function

of lattice parameter close to the equilibrium

Solution:
a) The bulk modulus is given by the second derivative of the total energy, at the equilibrium. So, either take finite difference sampling from the figure or fit a second order polynomial to it and differentiate it.

$V_0 = \frac{a_0^3}{2}$ for a bcc lattice, and $a_0 = 2.855$ from the figure.

Using finite difference sampling, the second derivative is $\frac{d^2E}{dV^2} = -\frac{E(V_0 - h) - 2E(V_0) + E(V_0 + h)}{h^2}$

where *h* is the volume interval, not lattice parameter interval. Selecting *h* and corresponding values for *E* from the figure, one obtains $\frac{d^2E}{dV^2} = -0.084\,eV/\AA^6 \rightarrow B = -V_0\frac{d^2E}{dV^2} = 0.982\,eV/\AA^3 = 157\,GPa$

b) The embedding energy is the difference between the total energy and the pair interaction, the latter summed over all interacting neighbours. In bcc we have:

Neighbour shell	Coordination	Distance	V(r) (eV) from fig	Sum (eV)
1	8	$\frac{\sqrt{3}}{2}a_0$	0.185	1.48
2	6	a_0	0.03	0.18
3	12	$\sqrt{2}a_0$	-0.01	-0.12
4	24	$\frac{\sqrt{11}}{2}a_0$	0	0

Giving us a total pair energy of (sum up the sums in the table): $\sum_{i \neq j} V(r_{ij}) = 1.54\,eV$

The embedding energy is then $\phi(a_0) = E_j - \sum_i V(r_{ij}) = -4.013\,eV - 1.54\,eV = -5.55\,eV$

Problem 6 [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 bcc Fe along the ⟨100⟩, ⟨110⟩ and ⟨111⟩ directions. Base your calculation on the pair interaction from figure 1. [3p]

Solution:
Using these assumptions, the displacement energy is the difference between the saddle point energy going through the window of barrier atoms and the equilibrium energy: $E_d = E^{sp} - E_{eq}$

$E_{eq} = -4.01\,eV$ from the figure.

In order to figure out the geometry of the barrier windows, draw a bcc cell and imagine one of the atoms being displaced in the three given directions. In summary we have:

Direction	⟨100⟩	⟨110⟩	⟨111⟩
Distance(s) r_B	$\frac{a_0}{\sqrt{2}} \approx 2\ \text{Å}$	$\frac{a_0}{2} \approx 1.43\ \text{Å}$ and $\frac{a_0}{\sqrt{2}} \approx 2\ \text{Å}$	$\frac{\sqrt{6}}{3} a_0 \approx 2.33\ \text{Å}$
Pair repulsion $V(r_B)$	1 eV	8 eV and 1 eV	0.3 eV
# barrier atoms	4	2 and 2	3
E^{sp}	4 eV	18 eV	0.9 eV
$E_d = E^{sp} - E_{eq}$	**8 eV**	**22 eV**	**5 eV**

The $V(r_B)$ for $r_B < 2.2\ \text{Å}$ are estimated through extrapolation from the figure.

Note the large difference between the ⟨110⟩ direction and the two others. This difference is in very good agreement with experiments, although of course all these values are underestimated.