Fundamentals of Materials Science Homework 12

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Homework Problems:

Point Defects

1. Gold has 5.82×10^{8} vacancies/cm^3 at equilibrium at 300 K. What fraction of the atomic sites is vacant at 600 K?

Solution:

Atomic weight of Au is 196.97amu
Density of Au is 19.32g/cm^3

$$\because \rho=\frac{nA}{VN_A}\therefore N=\frac{\rho VN_A}{A}=\frac{19.32g/cm^3\times1cm^3\times6.02\times10^{23}atoms/mol}{196.97amu}=5.9\times10^{22}$$

$$\because N_V=N\exp\left(-\frac{Q_V}{kT}\right)$$

$$\therefore Q_V=-kT\ln\frac{N_V}{N}=-1.38\times10^{-23}J/(atom\cdot K)\times300K\times\ln\frac{5.82\times10^{8}}{5.9\times10^{22}}=1.34\times10^{-19}J$$

$$\therefore N_{V(600k)}=N\exp\left(-\frac{Q_V}{kT}\right)=5.9\times10^{22}\times\exp\left(-\frac{1.34\times10^{-19}J}{1.38\times10^{-23}J/(atom\cdot K)\times600K}\right)$$

$$=5.52\times10^{15}vacancies/cm^3$$

$$\therefore \frac{N_V}{N}=\frac{5.52\times10^{15}vacancies/cm^3}{5.9\times10^{22}vacancies/cm^3}=9.4\times10^{-8}$$

2. Calculate the number of vacancies per m^3 for gold at 900°C. The energy for vacancy formation is 0.86 eV/atom.

Solution:

Atomic weight of Au is 196.97amu
Density of Au is 19.32g/cm^3

$$\because \rho=\frac{nA}{VN_A}\therefore N=\frac{\rho VN_A}{A}=\frac{19.32g/cm^3\times10^6cm^3\times6.02\times10^{23}atoms/mol}{196.97amu}=5.9\times10^{28}$$

$$\therefore N_{V(900k)}=N\exp\left(-\frac{Q_V}{kT}\right)=5.9\times10^{28}\times\exp\left(-\frac{0.86\times1.602\times10^{-19}J}{1.38\times10^{-23}J/(atom\cdot K)\times900K}\right)$$

$= 8.98 \times 10^{23} \, vacancies / cm^3$

3. The density of a sample of FCC palladium is 1980 kg/m³, and its lattice parameter is 0.38902 nm. Calculate (a) the fraction of the lattice points that contain vacancies; and (b) the total number of vacancies in a cubic centimeter of Pd.

Solution:

(a) Atomic weight of Pd is 106.24g/mol

$$\because \rho = \frac{nA}{VN_A} = \frac{4 \times 106.24 g / cm^3}{\left(0.38902 \times 10^{-7} cm\right)^3 \times 6.02 \times 10^{23} atoms / mol} = 11.99 g / mol$$

$$\therefore N = \frac{\rho V N_A}{A} = \frac{1.98 g / cm^3 \times \left(0.38902 \times 10^{-7} cm\right)^3 \times 6.02 \times 10^{23} atoms / mol}{106.24 g / mol}$$

=0.66atoms

$$\therefore k = \frac{N_V}{N} = \frac{n - N}{n} = \frac{4 - 0.66}{4} = 0.835 ,$$

(b) $$\frac{k}{V} = \frac{0.835}{\left(0.38902 \times 10^{-7} cm\right)^3} = 1.42 \times 10^{22}$$

4. The number of vacancies in some hypothetical metal increases by a factor of five when the temperature is increased from 1000K to 1130K. Calculate the energy for vacancy formation assuming that the density of the metal remains the same over this temperature range.

Solution:

$$N_V = N \exp(-\frac{Q_V}{kT})$$

$$\frac{N_{V1}}{N_{V2}} = \frac{N \exp(-\frac{Q_V}{kT_1})}{N \exp(-\frac{Q_V}{kT_2})} = \exp\left(\frac{Q_V}{kT_1} - \frac{Q_V}{kT_2}\right) = 5$$

$$Q_V = \ln 5 \times \frac{KT_1T_2}{T_2 - T_1} = \ln 5 \times \frac{8.62 \times 10^{-5} eV\left(atom \cdot K\right) \times 1000K \times 1130K}{1130K - 1000K} = 1.206eV$$

Solid Solution

5. Cu and Ni form a substitutional solid solution. This means that the crystal structure of a Cu-Ni alloy consists of Ni atoms substituting for Cu atoms in

the regular atomic positions of the FCC structure. For a Cu–30% wt% Ni alloy, what fraction of the atomic sites does Ni occupy?

Solution:

Atomic weight of Cu is 63.55amu
Atomic weight of Ni is 58.69amu

$$C'_{Ni} = \frac{C_{Ni}A_{Cu}}{C_{Ni}A_{Cu} + C_{Cu}A_{Ni}} \times 100\% = \frac{70 \times 63.55amu}{70 \times 63.55amu + 30 \times 58.69amu} \times 100\% = 71.6wt\%$$

6. A niobium alloy is produced by introducing tungsten substitutional atoms into the BCC structure; eventually an alloy is produced that has a lattice parameter of 0.32554 nm and a density of 11950 kg/m^3. Calculate the fraction of the atoms in the alloy that are tungsten.

Solution:

Atomic weight of Nb is 92.91amu
Atomic weight of W is 183.84amu
Density of Nb is 8.57g/cm^3
Density of W is 19.3g/cm^3

$$\rho_{ave} = \frac{100}{\frac{C_{Nb}}{\rho_{Nb}} + \frac{C_W}{\rho_W}} = \frac{100}{\frac{100 - C_W}{8.57\text{g/cm}^3} + \frac{C_W}{19.3\text{g/cm}^3}} = 11.95g/cm^3$$

So $C_W = 50.875$, $C_{Nb} = 49.125$

$$C'_W = \frac{C_W A_{Nb}}{C_W A_{Nb} + C_{Nb} A_W} \times 100 = \frac{50.857 \times 92.91}{50.857 \times 92.91 + 49.125 \times 183.84} \times 100 = 34.35\%$$

$\therefore C'_{Nb} = 65.65\%$

7. Suppose we introduce one carbon ato for every 100 iron atoms in an m interstitial position in BCC iron, giving a lattice parameter of 0.2867 nm. For this steel, find the density and the packing factor.

Solution:

Atomic weight of C is 12.011g/mol
Atomic weight of Fe is 55.85g/mol
Atomic radius of C is 0.071nm
Atomic radius of Fe is 0.124nm

$$\rho = \frac{nA}{V_C N_A} = \frac{2\times 55.85 + 2\times \frac{1}{100}\times 12.001}{2.357\times 10^{-23}\times 6.023\times 10^{23}} = 7.885 g/cm^3$$

$$APF = \frac{2\times \frac{4}{3}\pi\left(0.124\times 10^{-7}\right)^3 + 2\times \frac{1}{100}\times \frac{4}{3}\pi\left(0.071\times 10^{-7}\right)^3}{2.357\times 10^{-23}} = 0.66$$

Alloy Design（这题才是真正要做的）

8. 这个题是我2010年10月份留的，当时正值工大50年校庆，是在当时的情景下留的，今年我就不改题目了，你们穿越回2010年。

美国普度大学上周借一年一度的 Homecoming 之机，刚刚颁布了学校新的宣传口号，以宣扬普度精神。新的标语口号是：

"We are Purdue. Makers, all."

普度大学网站上介绍说："**'Makers, All' embraces the university's strengths -- energy, optimism, enthusiasm, curiosity and reliability -- while staying grounded in the historic Boilermaker reputation. It is uncomplicated, powerful and real. It brings to life the university's persona as a visionary institution that serves as a catalyst for transformation.**"我觉得这个新的宣传很振奋人心，每一个人都要有决心做一个 maker，用自己的实际行动去创新，去创造，去改变世界。普度大学在我校建校 50 周年之际推出新的与“不息为体，日新为道”有异曲同工之效的宣传口号，在实际行动上祝贺了我校的生日。

作为一个材料人，我们要学会 make things，要学会 make things work，不会做具有实际应用价值的材料的人不能成为是一个真正学材料懂材料的人，这也正是北工大材料人“真材实料”核心价值观的体现。那么，我们现在就亲自试着利用自己现有的知识开始设计材料吧。

In Materials Engineering, there are a lot of opportunities for us to design (or, in another word, engineer) a material. Now let's practice this. This problem calls for a unit cell edge length design in Fe-V solid solution. Iron and vanadium both have the BCC crystal structure and V forms a substitutional solid solution in Fe for concentrations up to approximately 20 wt% V at room temperature. Please determine the concentration in weight percent of V that must be added to iron to yield a unit cell edge length of 0.289 nm.

同样是这道题目，在 2013 年材料科学基础以功夫熊猫为主题的“铁之万象”的期末考试试卷里面是这样出的，见下图。

分阵二　铁之缺陷世界

难题六：这一天，探马快螳螂（Mantis）来报，得知沈王爷在冶炼的过程中，将先预制一部分铁胚，这些铁胚中会把钒（V）作为合金元素加入，V 和 Fe 在室温具有相同的晶体结构，并能够作为溶质原子与 Fe 形成置换固溶体。赶紧帮助阿宝计算一下，Fe 中加入多少 V 可以使晶胞的边长达到 0.289 nm。同样，为了让阿宝不晕，V 的单位就用重量百分比吧。 100

Solution:

Atomic weight of V is 50.94amu
Atomic weight of Fe is 55.85amu
Density of V is 6.1g/cm^3
Density of Fe is 7.87g/cm^3

$$V_c = \frac{nA}{\rho N_A} = \left(0.289\times10^{-7}\right)^3 = 2.414\times10^{-23}\,cm^3$$

$$A_{ave} = \frac{100}{\frac{C_{Fe}}{A_{Fe}}+\frac{C_V}{A_V}} = \frac{100}{\frac{1-C_V}{55.85}+\frac{C_V}{50.94}} \quad ; \quad \rho_{ave} = \frac{100}{\frac{C_{Fe}}{\rho_{Fe}}+\frac{C_V}{\rho_V}} = \frac{100}{\frac{1-C_V}{7.87}+\frac{C_V}{6.1}}$$

$$V_c = \frac{2\times\dfrac{100}{\dfrac{1-C_V}{55.85}+\dfrac{C_V}{50.94}}}{\dfrac{100}{\dfrac{1-C_V}{7.87}+\dfrac{C_V}{6.1}}\times6.022\times10^{23}} = 2.414\times10^{-23} \quad \therefore C_V = 12.9wt\%$$