

## Fundamentals of Materials Science Homework 20

Name: Xiao, LiyangDate: 05/10/2017Student #: 15090215Homework Problems:

今天上课讲了很多造园的基础理论知识，  
我留一题以巩固知识并为下次课程做准备。

我们在上节课讲过，在平衡的开放系统中，  
假设晶胚的开放为球状，则在过冷的液体中  
出现一个半径为  $r$  的球状晶胚，所引起的自由能  
变化为：
$$\Delta G = \frac{4}{3}\pi r^3 \Delta G_v + 4\pi r^2 \gamma$$

① 试求临界晶核半径  $r^*$  和形核功  $\Delta G^*$  的  
表达式；即  $r^*$  和  $\Delta G^*$  怎样用单位体积自由能  
 $\Delta G_v$  和单位表面自由能  $\gamma$  来表示。

② 如果晶核为边长为  $a$  的立方体，试求其临界  
晶核边长  $a^*$  和形核功  $\Delta G^*$  的表达式。

这些基本公式的推导还是很重要的！

Solution:

$$1. \because \Delta G = \frac{4}{3}\pi r^3 \Delta G_v + 4\pi r^2 \gamma$$

$$\therefore \frac{d(\Delta G)}{dr} = \frac{4}{3}\pi \Delta G_v (3r^2) + 4\pi \gamma (2r) = 0$$

$$\therefore r^* = -\frac{2\gamma}{\Delta G_v} \quad \Delta G^* = \frac{16\pi\gamma^3}{3(\Delta G_v)^2}$$

2. ∴ 立方体

$$\therefore \Delta G = a^3 \Delta G_v + 6a^2 \gamma$$

$$\therefore \frac{d(\Delta G)}{da} = 3a^2 \Delta G_v + 12a\gamma = 0$$

$$\therefore a^* = -\frac{4\gamma}{\Delta G_v} \quad \Delta G^* = \frac{32\gamma^3}{\Delta G_v^2}$$

**One More Problem:**

**Calculation of Critical Radius for the Solidification of Copper**

Calculate the size of the critical radius and the number of atoms in the critical nucleus when solid copper forms by homogeneous nucleation. Comment on the size of the nucleus and assumptions we made while deriving the equation for the radius of the nucleus. The elemental data of Cu can be found in your textbook.

**Solution:**

$$\therefore T_{m(Cu)} = 1085^\circ\text{C}; \quad \Delta H_{f(Cu)} = -1628 \text{ J/cm}^3; \gamma = 1.77 \times 10^{-9} \text{ J/cm}^2; \Delta T = 236^\circ\text{C}$$

$$\begin{aligned} \therefore r^* &= \left( -\frac{2\gamma T_m}{\Delta H_f} \right) \left( \frac{1}{T_m - T} \right) \\ &= \left[ -\frac{2 \times 1.77 \times 10^{-9} \text{ J/cm}^2 \times 1358.15 \text{ K}}{-1628 \text{ J/cm}^3} \right] \left( \frac{1}{236 \text{ K}} \right) \\ &= 1.25 \text{ nm} \end{aligned}$$

$$\therefore a_{Cu} = 2\sqrt{2}r_{Cu} = 2\sqrt{2} \times 0.128 \text{ nm} = 0.362 \text{ nm}$$

$$\therefore n = \frac{V_1}{V} = \frac{\frac{4}{3}\pi r^{*3}}{a^3} = \frac{\frac{4}{3}\pi \times (1.25 \text{ nm})^3}{(0.362 \text{ nm})^3} = 172 \text{ unit cells}$$

$$\therefore N = 4 \times n = 4 \times 172 = 690 \text{ atoms/unit cells}$$