Department of Materials Science and Engineering Pohang University of Science and Technology

AMSE502 Phase Transformations

due Date: Jun. 01, 2021		Prof. Byeong-Joo Lee
	Problem Set #7	calphad@postech.ac.kr
		Room 1- 311

1. A Ag-38at%Au alloy at 510K is a single-phase solid solution at equilibrium. A multilayer thinfilm Ag-Au diffusion couple is prepared by evaporation. The initial composition of the film varies sinusoidally with distance in one dimension according to:

 $C(x,0) = (38 \text{ at\% Au}) + (12 \text{ at\% Au}) \cos \beta x$

where the wave number $\beta = 2\pi/\lambda$ and the wavelength λ is 2×10^{-9} m.

Estimate the time that it will take to homogenize the diffusion couple to the extent that the maximum composition difference in the sample is 2 at% Au. Assume a solution to the diffusion equation having the form:

 $C(x,t) = (38 \text{ at\% Au}) + (12 \text{ at\% Au}) \exp[R(\beta)t] \cos \beta x$

Perform two calculations:

(a) Use Fick's second law as the diffusion equation: (5)

$$\frac{\partial c}{\partial t} = \widetilde{D} \ \frac{\partial^2 c}{\partial x^2}$$

(b) Use Cahn's modified diffusion equation: (5)

$$\frac{\partial c}{\partial t} = \widetilde{D} \quad \frac{\partial^2 c}{\partial x^2} - \frac{2K\widetilde{D}}{f''} \frac{\partial^4 c}{\partial x^4}$$

(c) Comment on the difference between your answers to parts (a) and (b). (10)

[Note that the Ag-Au system favors bonds between unlike atoms

(ordering), and has a negative gradient energy coefficient.]

Data:

$$\widetilde{D} = 10^{-23} \text{ m}^2 \text{ s}^{-1}$$

$$f'' = 5 \times 10^9 \text{ J m}^{-3}$$

$$K = -2.6 \times 10^{-11} \text{ J m}^{-1}$$

$$\lambda = 2 \times 10^{-9} \text{ m}$$

2. Use the Monte Carlo simulation code (KISSGG.exe) to answer to the followings: (20) The average grain size can be represented by $\overline{R} = kt^n$.

Perform grain growth simulation at various time duration and temperature using the code and

- a) Find the time dependence of the average grain size (40%)
- b) Find the temperature dependence of grain growth and the activation energy (60%).
- * The code provides the average grain size.