Problem 6

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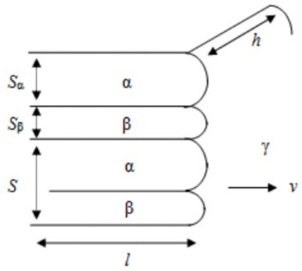
1. Consider the increase of free energy during the formation of lamellar eutectic/eutectoid. It is thought that the free energy increase comes from the creation of the α/β interfaces, and the amount of free energy increase per mole of the lamellar eutectic/eutectoid is often expressed as follows :



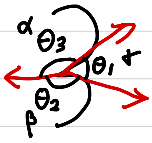
$$\Delta G_{IF}(S) = \frac{2\gamma_{\alpha\beta}}{S} \cdot V_m^L$$

where $\gamma_{\alpha\beta}$ is the α/β interfacial energy and V_m^L is the molar volume of the lamellar structure.

However, it can also be thought that the free energy increase comes from the capillarity effects due to the curvature at the growing tip of each (α/β) layer. (20point)

a) Why the tip of each layer has a curvature?
b) Estimate the radius of curvature for each layer as a function of layer thickness.
c) Show that the free energy increase due to the capillarity effects is exactly the same as that obtained by considering the α/β interfacial energy.

(a)



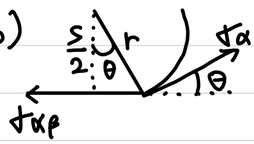
$$\frac{\gamma_{\alpha\beta}}{\sin\theta_1} = \frac{\gamma_\beta}{\sin\theta_3} = \frac{\gamma_\alpha}{\sin\theta_2}$$

$\gamma_{\alpha\beta} \neq 0$

$\theta_1 = 0$ only if $\gamma_{\alpha\beta} = 0 \rightarrow \theta_1 \neq 0$

$\boxed{\therefore \text{Curvature must exist for force balance}}$

(b)



$r_\alpha \cos\theta_\alpha = \frac{S_\alpha}{2}$, $\gamma_{\alpha\beta} = \cos\theta_\alpha \gamma_\alpha + \cos\theta_\beta \gamma_\beta$

$r_\beta \cos\theta_\beta = \frac{S_\beta}{2}$, $\sin\theta_\alpha \gamma_\alpha = \sin\theta_\beta \gamma_\beta$

$r_\alpha = \frac{S_\alpha \gamma_\alpha \gamma_{\alpha\beta}}{\gamma_{\alpha\beta}^2 + \gamma_\alpha^2 - \gamma_\beta^2}$, $r_\beta = \frac{S_\beta \gamma_\beta \gamma_{\alpha\beta}}{\gamma_{\alpha\beta}^2 + \gamma_\beta^2 - \gamma_\alpha^2}$

(c) $\Delta G = \Delta(PV) = \gamma\left(\frac{1}{r_1} + \frac{1}{r_2}\right)V_m = \frac{\gamma V_m}{r}$

$$\Delta G = \Delta G_\alpha + \Delta G_\beta = \frac{\gamma_\alpha V_m^\alpha}{r_\alpha} \cdot \frac{S_\alpha}{S} + \frac{\gamma_\beta V_m^\beta}{r_\beta} \cdot \frac{S_\beta}{S}$$

$$\Delta G = \frac{V_m^\alpha(\gamma_{\alpha\beta}^2 + \gamma_\alpha^2 - \gamma_\beta^2)}{S\gamma_{\alpha\beta}} + \frac{V_m^\beta(\gamma_{\alpha\beta}^2 - \gamma_\alpha^2 + \gamma_\beta^2)}{S\gamma_{\alpha\beta}} = \frac{2\gamma_{\alpha\beta} V_m^L}{S}$$

$(\because V_m^\alpha = V_m^\beta = V_m^L)$

$$\boxed{\therefore \Delta G = \frac{2\gamma_{\alpha\beta} V_m^L}{S}}$$

Problem 6 20232994 최찬욱

2. Use the attached Monte Carlo simulation code (KISSGG.exe) to answer to the followings:
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 (5)
b) Find the temperature dependence of grain growth and the activation energy (5)

※ The code provides the average grain size.

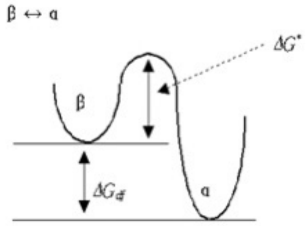
(a) average grain size : $\overline{R} = kt^n$

$$\ln(\overline{R}) = \ln k + n\ln t$$

temp	n	k
1	0.1169	5.1103
3	0.1936	3.316
5	0.2003	3.1995
7	0.2745	2.0698
10	0.3129	1.6695
15	0.3608	1.2758
20	0.3924	1.0815

$\therefore n \simeq 0.264486$

(b)



$$\text{Growth rate} = \frac{dR}{dt} = nkt^{n-1} = \lambda v$$

$$V = V_0 e^{-\frac{\Delta G^*}{RT}}\left(1 - e^{-\frac{\Delta G_{ds}}{RT}}\right) \simeq V_0 e^{-\frac{\Delta G^*}{RT}} \frac{\Delta G_{ds}}{RT}$$

$$nkt^{n-1} = \lambda V_0 e^{-\frac{\Delta G^*}{RT}} \frac{\Delta G_{ds}}{RT} \quad \left(a = \frac{\lambda V_0 \Delta G_{ds}}{R}\right)$$

$$\therefore \ln(Tnkt^{n-1}) = \ln a - \frac{\Delta G^*}{RT}$$