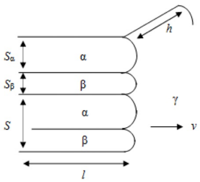
1. Consider the increase of free energy during the formation of lamellar eutectic/eutectoid. It is thought that the free energy increase comes from the creation of the α/β interfaces, and the amount of free energy increase per mole of the lamellar eutectic/eutectoid is often expressed as follows :



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

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

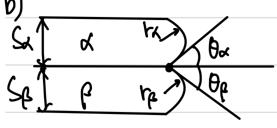
However, it can also be thought that the free energy increase comes from the capillarity effects due to the curvature at the growing tip of each (α/β) layer. (20point)

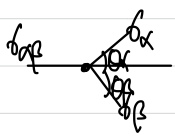
a) Why the tip of each layer has a curvature?
b) Estimate the radius of curvature for each layer as a function of layer thickness.
c) Show that the free energy increase due to the capillarity effects is exactly the same as that obtained by considering the α/β interfacial energy.

a)

자연적으로 낮은 표면에너지가 안정적이므로. lamella 구조에서도 낮은 표면에너지를 갖기 위해 곡선형의 모양을 갖게 됨.
local equilibrium에서 세 힘 ($\gamma_{\alpha\beta}$. γ_α. γ_β)가 평형.

b)





$S_\alpha = 2r_\alpha \cos\theta_\alpha \quad \cdots ①$

$S_\beta = 2r_\beta \cos\theta_\beta \quad \cdots ②$

$\gamma_{\alpha\beta} = \gamma_\alpha \cos\theta_\alpha + \gamma_\beta \cos\theta_\beta \quad \cdots ③$

$0 = \gamma_\alpha \sin\theta_\alpha - \gamma_\beta \sin\theta_\beta \quad \cdots ④$

From ④

$\gamma_\alpha^2 \sin^2\theta_\alpha = \gamma_\beta^2 \sin^2\theta_\beta$

$\gamma_\alpha^2 (1-\cos^2\theta_\alpha) = \gamma_\beta^2 (1-\cos^2\theta_\beta)$

$\therefore \cos\theta_\beta = \sqrt{\dfrac{\gamma_\beta^2 - \gamma_\alpha^2(1-\cos^2\theta_\alpha)}{\gamma_\beta^2}} \quad \cdots ⑤$

③ + ⑤

$\gamma_{\alpha\beta} = \gamma_\alpha \cos\theta_\alpha + \sqrt{\gamma_\beta^2 - \gamma_\alpha^2(1-\cos^2\theta_\alpha)} \quad \cdots ⑥$

① + ⑥

$$\gamma_{\alpha\beta} = \frac{\gamma_\alpha S_\alpha}{2r_\alpha} + \sqrt{\gamma_\beta^2 - \gamma_\alpha^2\left(1 - \frac{S_\alpha^2}{4r_\alpha^2}\right)}$$

$$\gamma_{\alpha\beta} - \frac{\gamma_\alpha S_\alpha}{2r_\alpha} = \sqrt{\gamma_\beta^2 - \gamma_\alpha^2\left(1 - \frac{S_\alpha^2}{4r_\alpha^2}\right)}$$

$$\gamma_{\alpha\beta}^2 - \frac{\gamma_{\alpha\beta}\gamma_\alpha S_\alpha}{r_\alpha} + \cancel{\frac{\gamma_\alpha^2 S_\alpha^2}{4r_\alpha^2}} = \gamma_\beta^2 - \gamma_\alpha^2\left(1 - \cancel{\frac{S_\alpha^2}{4r_\alpha^2}}\right)$$

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

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

c)

Capillary effect

$\rightarrow \Delta G = \Delta G_\alpha + \Delta G_\beta$

$= \dfrac{\gamma_\alpha}{r_\alpha} V_\alpha + \dfrac{\gamma_\beta}{r_\beta} V_\beta$

result b)

⊕

$\dfrac{V_m^l}{S} = \dfrac{V_\alpha}{S_\alpha} = \dfrac{V_\beta}{S_\beta}$

$$= \cancel{\gamma_\alpha} \cdot \frac{\gamma_{\alpha\beta}^2 - \gamma_\alpha^2 + \gamma_\beta^2}{\gamma_{\alpha\beta}\cancel{\gamma_\alpha}\cancel{S_\alpha}} \cdot \frac{\cancel{S_\alpha}V_m^l}{S} + \cancel{\gamma_\beta} \frac{\gamma_{\alpha\beta}^2 - \gamma_\beta^2 + \gamma_\alpha^2}{\gamma_{\alpha\beta}\cancel{\gamma_\beta}\cancel{S_\beta}} \cdot \frac{\cancel{S_\beta}V_m^l}{S}$$

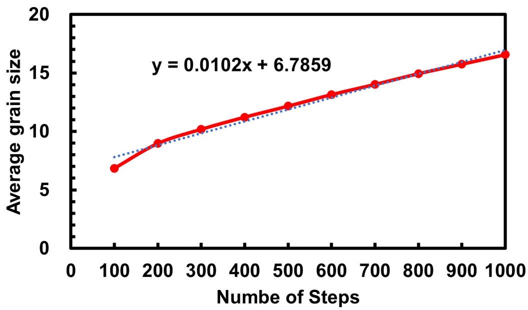
$$= 2 \cdot \gamma_{\alpha\beta} \cdot \frac{V_m^l}{S} = \Delta G_{IF}(S)$$

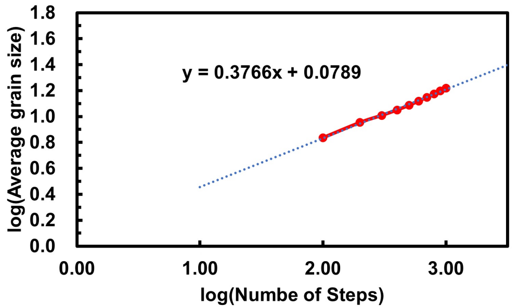
2. Use the attached Monte Carlo simulation code (KISSGG.exe) to answer to the followings:
The average grain size can be represented by $\overline{R} = kt^n$.
Perform grain growth simulation at various time duration and temperature using the code and

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)



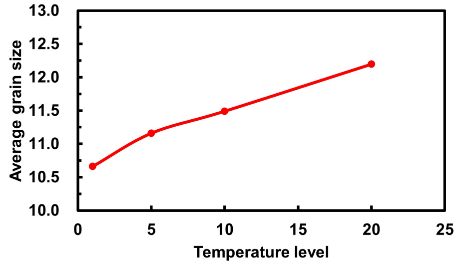


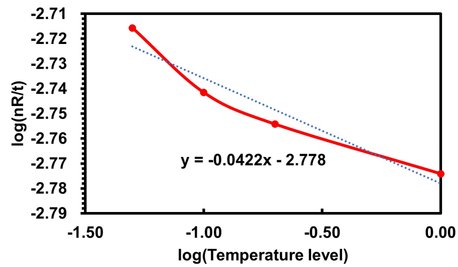
$\bar{R} = kt^n$

$\ln\bar{R} = \ln k + n\ln t$

$\therefore n = 0.0789$

b)





$\bar{R} = kt^n$

Growth Rate $= \frac{d\bar{R}}{dt} = nkt^{n-1} = \lambda v. = \frac{n\bar{R}}{t}.$

$v = v_0\exp(-\Delta G^*/RT)(1-\exp(-\Delta G^*/RT))$

$= v_0\exp(-\Delta G^*/RT)\cdot\frac{\Delta G^*}{RT}$ (if $\Delta G^* \ll RT$)

$\frac{n\bar{R}}{t} = \lambda v$

$= \lambda v_0\exp(-\Delta G^*/RT)\cdot\frac{\Delta G^*}{RT}$

$\ln\left(\frac{n\bar{R}}{t}\right) = \ln\frac{\lambda\Delta G^*}{RT}v_0 - \frac{\Delta G^*}{RT}.$

($t = 100$(steps) , $n = 0.0789$ from 2-a)

$\therefore \frac{\Delta G^*}{R} = 0.0422$