REPORT

POSTECH
POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

제목 : Homework #6

수강과목 : 상변태론

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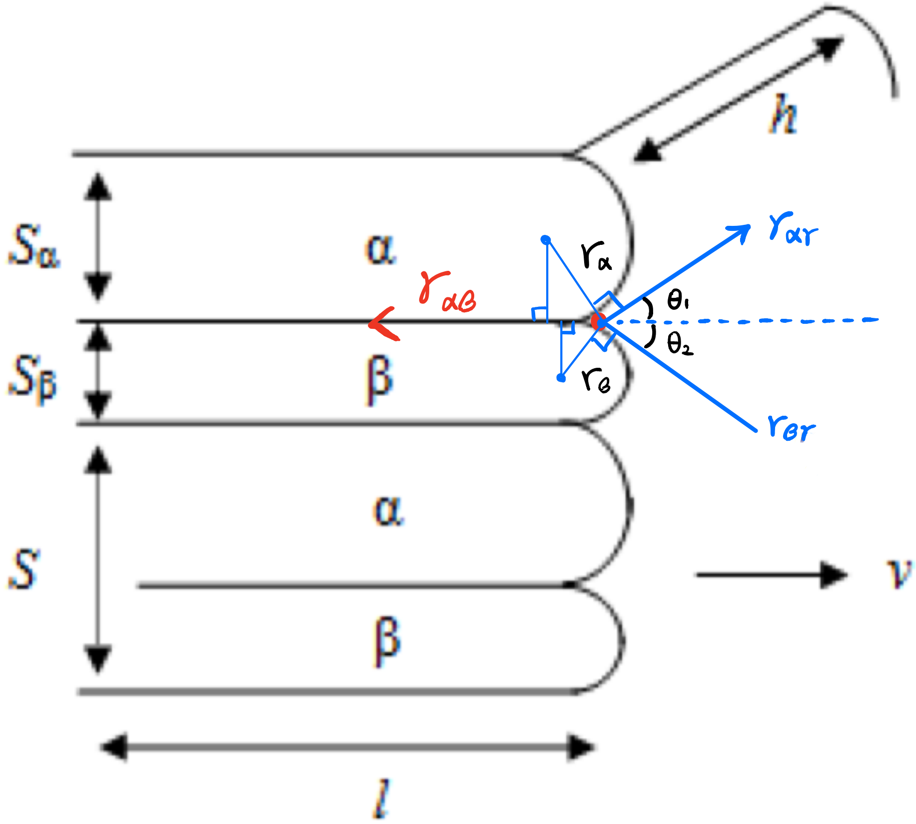


1. (a)

α - phase 와 β-phase 사이의 interface energy $\gamma_{\alpha\beta}$ 가 두 평형식을 만족

$$\begin{cases} \gamma_{\alpha\beta} = \gamma_{\alpha\gamma}\cos\theta_1 + \gamma_{\beta\gamma}\cos\theta_2 & — ① \\ \gamma_{\alpha\gamma}\sin\theta_1 = \gamma_{\beta\gamma}\sin\theta_2 & — ② \end{cases}$$

Tip이 curvature를 가지지 않는다면, $\theta_1 = \theta_2 = 90°$ 이고
$\gamma_{\alpha\beta} = 0$ 인데, surface energy 가 0인 interface가 존재할 수 없다.
따라서, 가정이 틀렸음을 알 수 있고 tip은 curvature를 가져야 한다.

1. (b) ② 식을 통해 θ_2를 θ_1 에 대해 나타내면

$$\gamma_{\alpha\gamma}^2\sin^2\theta_1 = \gamma_{\alpha\gamma}(1-\cos^2\theta_1) = \gamma_{\beta\gamma}^2(1-\cos^2\theta_2)$$

$$\cos\theta_2 = \left(\frac{\gamma_{\beta\gamma}^2 - \gamma_{\alpha\gamma}^2 + \gamma_{\alpha\gamma}^2\cos^2\theta_1}{\gamma_{\beta\gamma}^2}\right)^{\frac{1}{2}}$$ 로 나타낼 수 있고

① 식은 $\gamma_{\alpha\beta} = \gamma_{\alpha r}\cos\theta_1 + \cancel{\gamma_{\beta r}}\left(\frac{\gamma_{\beta r}^2 - \gamma_{\alpha r}^2 + \gamma_{\alpha r}^2\cos^2\theta_1}{\cancel{\gamma_{\beta r}^2}}\right)^{\frac{1}{2}}$ — ③

Curvature radius r_α 와 r_β 에 대해,

$S_\alpha = 2r_\alpha\cos\theta_1$, $S_\beta = 2r_\beta\cos\theta_2$ 를 만족한다. 이를 식 ③에 적용

$$\gamma_{\alpha\beta} = \gamma_{\alpha r}\frac{S_\alpha}{2r_\alpha} + \sqrt{\gamma_{\beta r}^2 - \gamma_{\alpha r}^2 + \gamma_{\alpha r}^2\frac{S_\alpha^2}{4r_\alpha^2}}$$

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

$$\gamma_{\alpha\beta}^2 - \frac{\gamma_{\alpha\beta}\cdot\gamma_{\alpha r}\cdot S_\alpha}{r_\alpha} + \cancel{\frac{\gamma_{\alpha r}^2 S_\alpha^2}{4r_\alpha^2}} = \gamma_{\beta r}^2 + \gamma_{\alpha r}^2 + \cancel{\gamma_{\alpha r}^2\frac{S_\alpha^2}{4r_\alpha}}$$

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

(c) Capillary effect에 의한 Gibbs free energy increase ΔG

$$\Delta G = \frac{\gamma_{\alpha r}}{r_\alpha}V_\alpha + \frac{\gamma_{\beta r}}{r_\beta}V_\beta$$ (cylinder 에서 Capillary effect)

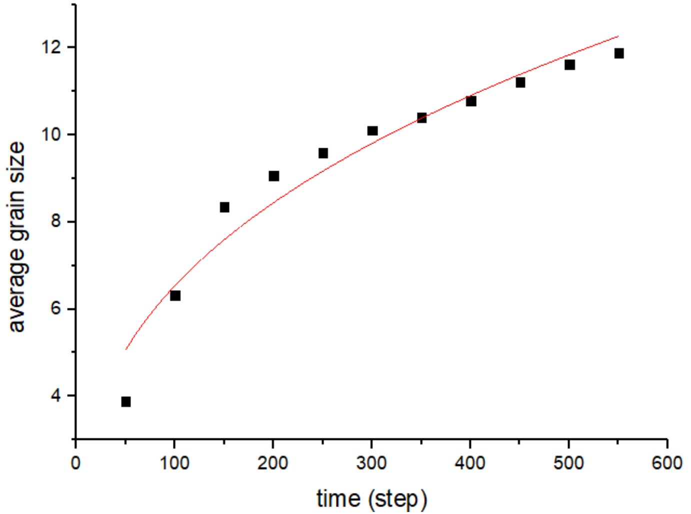
(b) 의 결과를 적용하면,

$$\Delta G = \frac{\cancel{\gamma_{\alpha r}}(\gamma_{\alpha\beta}^2 - \gamma_{\beta r}^2 + \gamma_{\alpha r}^2)}{S_\alpha\gamma_{\alpha\beta}\cancel{\gamma_{\alpha r}}}V_\alpha + \frac{\cancel{\gamma_{\alpha r}}(\gamma_{\alpha\beta}^2 - \gamma_{\alpha r}^2 + \gamma_{\beta r}^2)}{S_\alpha\gamma_{\alpha\beta}\cancel{\gamma_{\alpha r}}}V_\beta$$

$\frac{V_\alpha}{S_\alpha} = \frac{V_\beta}{S_\beta} = \frac{V_m}{S}$ 이라고 하면, $\Delta G = \frac{V_m}{S}\left(\frac{2\gamma_{\alpha\beta}^2}{\gamma_{\alpha\beta}}\right) = \frac{2\gamma_{\alpha\beta}V_m}{S}$

2(a) Set:

- Initial 64000 grain,
- 10 temperature
- 50 step as time goes on



Equation	a*x^b		
Reduced Chi-Sqr	0.32495		
Adj. R-Square	0.94491		
		Value	Standard Error
average grain size	a	1.19424	0.22987
	b	0.36919	0.03292

The average grain size can be represented

$$R = Kt^n$$

n= 0.36919, k=1.722 – (a)

2(b) Set: Initial 64000 grain,

200 step at each temperature(1~20)

$$R = kt^n$$

$$\frac{dR}{dt} = nkt^{n-1} = \lambda \nu$$

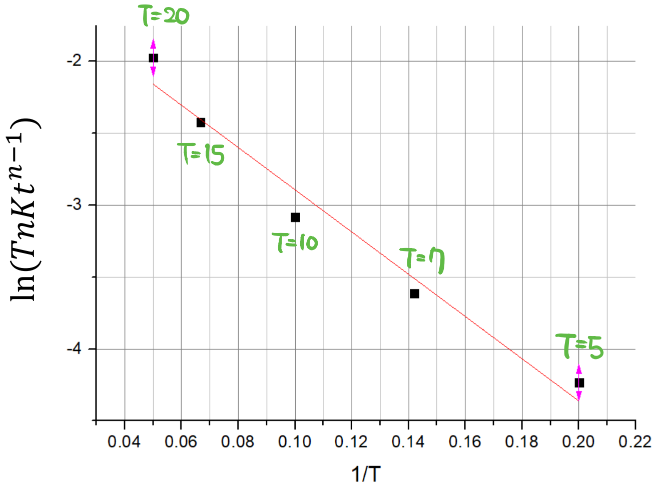
$$\nu = \nu_0 e^{-\frac{\Delta G^*}{RT}}\left(1 - e^{-\frac{\Delta G_{df}}{RT}}\right) = \nu_0 e^{-\frac{\Delta G^*}{RT}} \frac{\Delta G_{df}}{RT} \quad (\Delta G_{df} \ll RT)$$

$$nkt^{n-1} = \lambda \nu_0 e^{-\frac{\Delta G^*}{RT}} \frac{\Delta G_{df}}{RT} \quad \left(C = \frac{\lambda \nu_0 \Delta G_{df}}{R}\right)$$

$$\therefore \Rightarrow \ln(Tnkt^{n-1}) = \ln C - \frac{\Delta G^*}{RT} \qquad \text{(b)-①}$$

$$\therefore \Delta G^* = (\text{slope}) \times R = (14.69) \times (8.314)$$

$$= 122.13 \qquad \text{(b)-②}$$



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.09789		
Pearson's r	-0.98491		
Adj. R-Square	0.96005		
		Value	Standard Error
B	Intercept	-1.42448	0.1851
	Slope	-14.69068	1.49056