

Q1. Darken's uphill diffusion

• Fe-Si-C 의 sub-lattice model $(\text{Fe}, \text{Si})_1 (\text{C}, \text{vac})_1$ FCC 바탕

↳ Volume fixed model : $J_{\text{Fe}} + J_{\text{Si}} = 0, J_{\text{C}} + J_{\text{vac}} = 0$ / $\nabla C_{\text{Fe}} + \nabla C_{\text{Si}} = 0, \nabla C_{\text{C}} + \nabla C_{\text{vac}} = 0$

(불확) $\Rightarrow J_{\text{C}} = -D_{\text{CC}} \nabla C_{\text{C}} - D_{\text{CSi}} \nabla C_{\text{Si}}$ $\rightarrow \begin{pmatrix} J_{\text{C}} \\ J_{\text{Si}} \end{pmatrix} = \begin{pmatrix} -D_{\text{CC}} & -D_{\text{CSi}} \\ -D_{\text{SiC}} & -D_{\text{SiSi}} \end{pmatrix} \begin{pmatrix} \nabla C_{\text{C}} \\ \nabla C_{\text{Si}} \end{pmatrix}$

$J_{\text{Si}} = -D_{\text{SiC}} \nabla C_{\text{C}} - D_{\text{SiSi}} \nabla C_{\text{Si}}$

$\rightarrow D_{\text{CSi}}/D_{\text{CC}} = - (dJ_{\text{C}}/dJ_{\text{Si}})/J_{\text{C}}$

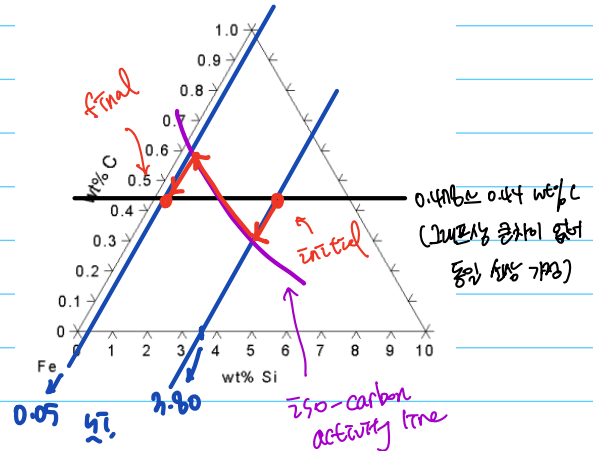
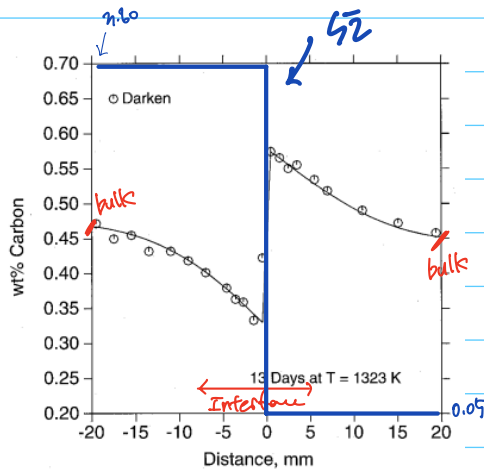
$\sim$ Limbomon $\sim$ 둘이 같은 값.

특정점에서의 activity가 거의 (같다) (상대적)

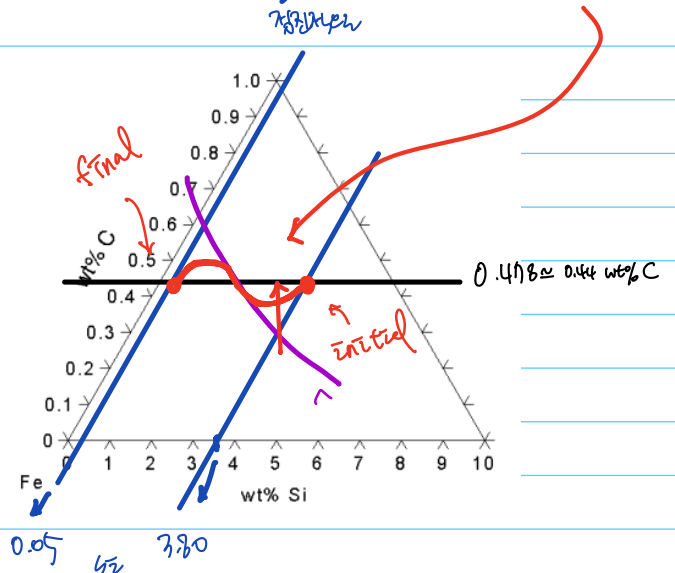
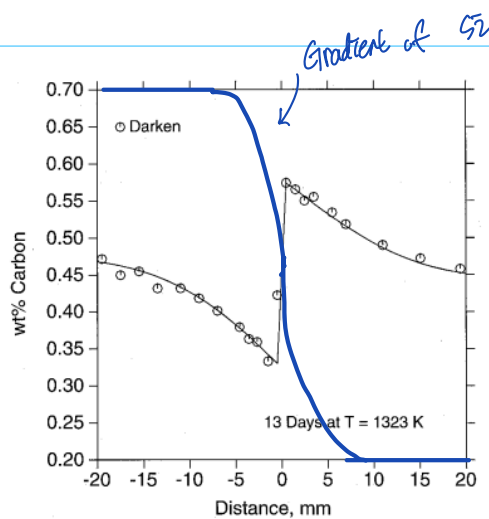
In Darken's experiment,

7.90 wt% Si	0.05 wt% Si
0.498 wt% C	0.44 wt% C

(Fe-base)



시간이 흐르 Si의 gradient가 생기기 되면 phase diagram 상에서 Si의 weight%가 감소하는 방향으로 쫓겨 이동할것임,

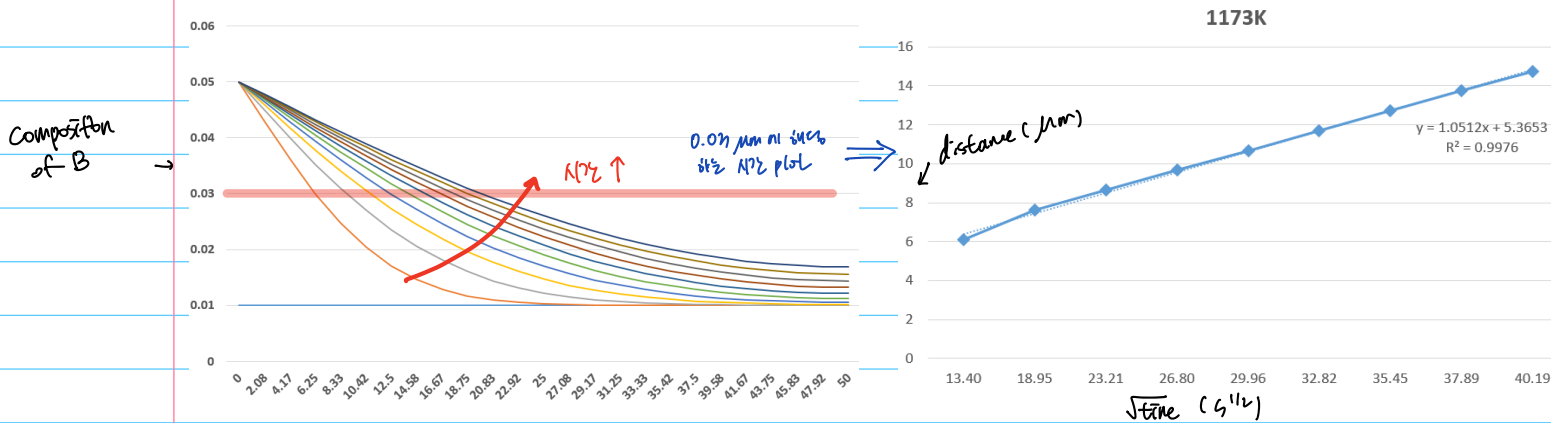


Q2.

T range = 1173 ~ 1473 K, $D = 4.529 \times 10^{-11} \times \exp[-140923/RT]$ m/s

Initial = 0.01 → 0.05 개시농도 / Inject distance = 0

(A) 1173 K에서 실험. 7600 ~ (60초)을 25 개의 grid 바꿈 개수



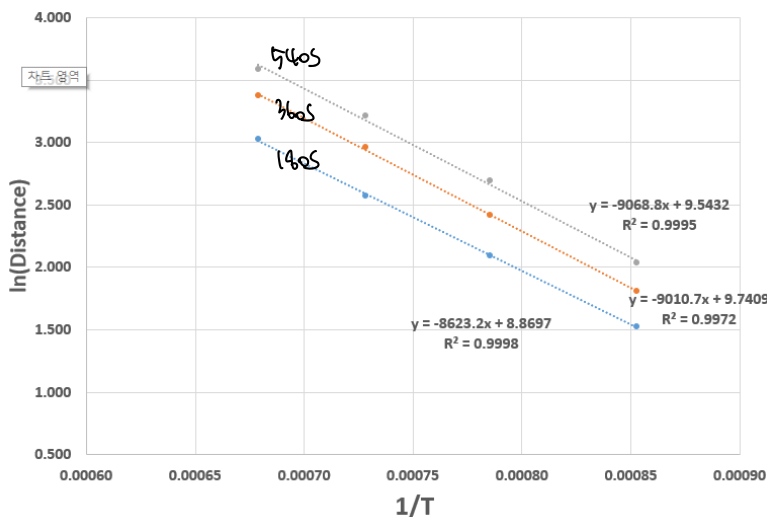
⇒ sqrt(time)과 distance가 선형하므로 fitting 실행 ($R^2 = 0.9976$)을 보아 Distance와 sqrt(time)이 "비례" 한다는 결론.

(b) Temperature dependant of injection distance.

$$x = \sqrt{Dt} = \sqrt{D_0 \cdot \exp(-Q/RT) \cdot t} \Rightarrow x^2 = D_0 \cdot \exp(-Q/RT) \cdot t$$

$$\Rightarrow 2 \ln x = -\frac{Q}{RT} + \ln D_0 + \ln t \quad \rightarrow \ln(x) \text{와 } -1/T \text{는 비례관계}$$

$$\Rightarrow \ln x = \left(+\frac{Q}{2R} \right) \left(-\frac{1}{T} \right) + \ln \sqrt{D_0 \cdot t}$$



$(\frac{1}{T})$ 과 $\ln(x)$ 가 특정 온도에서 비례관계를 가짐

(C) 온도 의존된 부분이 $1/T$ 와 $\ln(\text{distance})$ 간의 비례상수이다.

따라서, $\frac{Q}{2R} = \text{기울기(비례상수)} \rightarrow Q = \text{기울기} \times 2R$ (기울기는 그래프에서 $\ln(x)$ 의 기울기 = -8900.9)

$$\therefore Q = 2 \times 8.3144 \times (-8900.9) = -146011 \text{ J}$$