NUMERICAL ANALYSIS

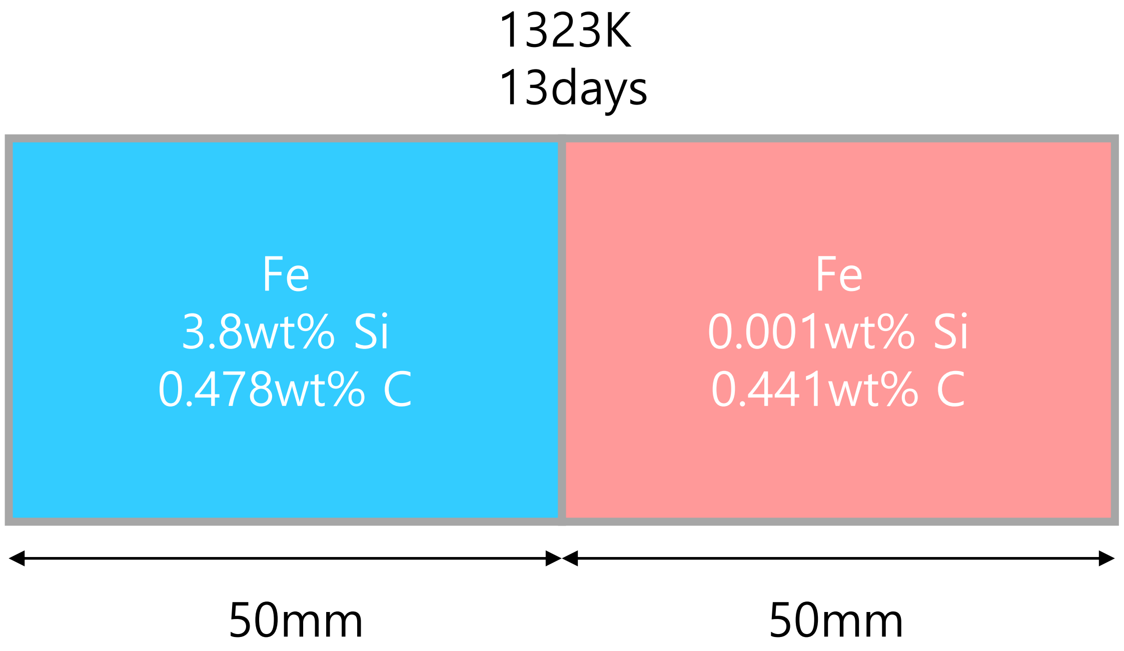
FINAL

조 혜 성

1. Darken’ s Uphill Diffusion by FDM

Simulation of Darken’s Uphill Diffusion

- 다음의 Mobility 정보와 initial condition 을 이용하여 Darken 의 uphill diffusion 실험을 FDM 으로 simulation 하시오. (SI unit)



FDM Method

$$y_{C,i}^{j+1} = y_{C,i}^{j} + \frac{\Delta t}{(\Delta x)^2}\left[\sqrt{D_{CC,i+1}\cdot D_{CC,i}}\,(y_{C,i+1}^{j} - y_{C,i}^{j}) - \sqrt{D_{CC,i-1}\cdot D_{CC,i}}\,(y_{C,i}^{j} - y_{C,i-1}^{j})\right]$$
$$+ \frac{\Delta t}{(\Delta x)^2}\left[\sqrt{D_{CM,i+1}\cdot D_{CM,i}}\,(y_{M,i+1}^{j} - y_{M,i}^{j}) - \sqrt{D_{CM,i-1}\cdot D_{CM,i}}\,(y_{M,i}^{j} - y_{M,i-1}^{j})\right]$$

1. Darken’ s Uphill Diffusion by FDM

Given Info

$$^oG_{Fe:Va} = {^oG_{Fe}^{fcc}}$$

0

$$^oG_{Si:Va} = {^oG_{Si}^{Diamond}} + 51000 - 21.8 \cdot T$$

$$^oG_{Fe:C} = {^oG_{Fe}^{fcc}} + {^oG_{C}^{graphite}} + 77207 - 15.877 \cdot T$$

$$^oG_{Si:C} = {^oG_{Si}^{Diamond}} + {^oG_{C}^{graphite}} - 20510 + 38.7 \cdot T$$

$$L_{Fe,Si:Va} = -125248 + 41.116 \cdot T - 142708(y_{Fe} - y_{Si}) + 89907(y_{Fe} - y_{Si})^2$$

$$L_{Fe,Si:C} = +143219.9 + 39.31 \cdot T - 216320.5(y_{Fe} - y_{Si})$$

$$L_{Fe:C,Va} = -34671$$

$$D_{MC} = y_{Fe} y_M \Omega_M \frac{d\mu_M}{dy_C} - y_M y_{Fe} \Omega_{Fe} \frac{d\mu_{Fe}}{dy_C}$$

$$D_{MM} = y_{Fe} y_M \Omega_M \frac{d\mu_M}{dy_M} - y_M y_{Fe} \Omega_{Fe} \frac{d\mu_{Fe}}{dy_M}$$

Fe-M-C 의 몰당 Gibbs Free E

$$G_m = y_{Fe} y_{Va} {^oG_{Fe:Va}} + y_M y_{Va} {^oG_{M:Va}} + y_{Fe} y_C {^oG_{Fe:C}} + y_M y_C {^oG_{M:C}}$$
$$+ RT(y_{Fe} \ln y_{Fe} + y_M \ln y_M) + RT(y_{Va} \ln y_{Va} + y_C \ln y_C)$$
$$+ y_{Fe} y_M y_{Va} L_{Fe,M:Va} + y_{Fe} y_M y_C L_{Fe,M:C}$$
$$+ y_{Fe} y_C y_{Va} L_{Fe:C,Va} + y_M y_C y_{Va} L_{M:C,Va}$$

For substitutional M,

$$\mu_M = G_m + (1 - y_M)\left(\frac{\partial G_m}{\partial y_M} - \frac{\partial G_m}{\partial y_{Fe}}\right) = G_m + (1 - y_M)\frac{dG_m}{dy_M}$$

For interstitial C

$$\mu_C = \left(\frac{\partial G_m}{\partial y_C} - \frac{\partial G_m}{\partial y_{Va}}\right) = \frac{dG_m}{dy_C}$$

2. Getting μ_C Related Derivatives

$y_{Va} = 1 - y_c$, $y_{Fe} = 1 - y_{Si}$ 로 표기 $dy_{Fe} = -dy_{Si}$ $dy_{Va} = -dy_c$

$$G_m = (1-y_{Si})(1-y_c)\,{}^\circ G_{Fe:Va} + y_{Si}(1-y_c)\,{}^\circ G_{Si:Va} + (1-y_{Si})y_c\,{}^\circ G_{Fe:C} + y_{Si}y_c\,{}^\circ G_{Si:C}$$
$$+ RT\{(1-y_{Si})\ln(1-y_{Si}) + y_{Si}\ln y_{Si}\} + RT\{(1-y_c)\ln(1-y_c) + y_c \ln y_c\}$$
$$+ (1-y_{Si})y_{Si}(1-y_c)L_{Fe,Si:Va} + (1-y_{Si})y_{Si}y_c L_{Fe,Si:C} + (1-y_{Si})y_c(1-y_c)L_{Fe:C,Va}$$
$$+ y_{Si}y_c(1-y_c)L_{Si:C,Va}$$

- for substitutional M : $\mu_M = G_m + (1-y_M)\dfrac{dG_m}{dy_M}$
- for interstitial C : $\mu_C = \dfrac{dG_m}{dy_C}$

y_c 와 y_{Si} 조성에 따른 chemical potential

$$\frac{\partial \mu_c}{\partial y_c} = \frac{\partial}{\partial y_c}\left(\frac{\partial G_m}{\partial y_c}\right)$$

$$\frac{\partial \mu_c}{\partial y_{Si}} = \frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$

$$\frac{\partial \mu_{Fe}}{\partial y_c} = \frac{\partial}{\partial y_c}\left\{G_m + (1-y_{Fe})\frac{\partial G_m}{\partial y_{Fe}}\right\} = \frac{\partial G_m}{\partial y_c} + y_{Si}\frac{\partial}{\partial y_c}\left(\frac{\partial G_m}{-\partial y_{Si}}\right)$$
$$= \frac{\partial G_m}{\partial y_c} - y_{Si}\frac{\partial}{\partial y_c}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$

$$\frac{\partial \mu_{Fe}}{\partial y_{Si}} = \frac{\partial}{\partial y_{Si}}\left\{G_m - y_{Si}\frac{\partial G_m}{\partial y_{Si}}\right\} = \frac{\partial G_m}{\partial y_{Si}} - 1\cdot\left(\frac{\partial G_m}{\partial y_{Si}}\right) - y_{Si}\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$
$$= -y_{Si}\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$

$$\frac{\partial \mu_{Si}}{\partial y_c} = \frac{\partial}{\partial y_c}\left\{G_m + (1-y_{Si})\frac{\partial G_m}{\partial y_{Si}}\right\} = \frac{\partial G_m}{\partial y_c} + (1-y_{Si})\frac{\partial}{\partial y_c}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$

$$\frac{\partial \mu_{Si}}{\partial y_{Si}} = \frac{\partial}{\partial y_{Si}}\left(G_m + (1-y_{Si})\frac{\partial G_m}{\partial y_{Si}}\right) = \frac{\partial G_m}{\partial y_{Si}} - \frac{\partial G_m}{\partial y_{Si}} + (1-y_{Si})\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$
$$= (1-y_{Si})\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)$$

2. Getting μ_C Related Derivatives

$$\frac{\partial G_m}{\partial y_C} = -(1-y_{Si})\,{}^{\circ}G_{Fe:Va} - y_{Si}\,{}^{\circ}G_{Si:Va} + (1-y_{Si})\,{}^{\circ}G_{Fe:C} + y_{Si}\,{}^{\circ}G_{Si:C}$$
$$+ RT(\ln y_C - \ln(1-y_C)) - (1-y_{Si})y_{Si}\cdot L_{Fe,Si:Va} + y_{Si}(1-y_{Si})L_{Fe,Si:C}$$
$$+ (1-y_{Si})(1-2y_C)L_{Fe:C,Va} + y_{Si}(1-2y_C)L_{Si:C,Va}$$

$$\frac{\partial}{\partial y_C}\left(\frac{\partial G_m}{\partial y_C}\right) = \frac{RT}{y_C} + \frac{RT}{1-y_C} - 2(1-y_{Si})L_{Fe:C,Va} - 2y_{Si}L_{Si:C,Va}$$

$$\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_C}\right) = +{}^{\circ}G_{Fe:Va} - {}^{\circ}G_{Si:Va} - {}^{\circ}G_{Fe:C} + {}^{\circ}G_{Si:C}$$
$$- (1-2y_{Si})L_{Fe,Si:Va} + (1-2y_{Si})L_{Fe,Si:C} - (1-2y_C)L_{Fe:C,Va} + (1-2y_C)L_{Si:C,Va}$$
$$- (1-y_{Si})y_{Si}\frac{\partial L_{Fe,Si:Va}}{\partial y_{Si}} + y_{Si}(1-2y_C)\frac{\partial L_{Si:C,Va}}{\partial y_{Si}}$$

$$\frac{\partial G_m}{\partial y_{Si}} = -(1-y_C)\,{}^{\circ}G_{Fe:Va} + (1-y_C)\,{}^{\circ}G_{Si:Va} - y_C\,{}^{\circ}G_{Fe:C} + y_C\,{}^{\circ}G_{Si:C}$$
$$+ RT(\ln y_{Si} - \ln(1-y_{Si})) + (1-2y_{Si})(1-y_C)L_{Fe,Si:Va} + (1-y_{Si})y_{Si}(1-y_C)\frac{\partial L_{Fe,Si:Va}}{\partial y_{Si}}$$
$$+ (1-2y_{Si})y_C L_{Fe,Si:C} + (1-y_{Si})y_{Si}y_C\frac{\partial L_{Fe,Si:C}}{\partial y_{Si}} - y_C(1-y_C)L_{Fe:C,Va} + y_C(1-y_C)L_{Si:C,Va}$$

$$\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right) = \frac{RT}{y_{Si}} - \frac{RT}{1-y_{Si}} - 2(1-y_C)L_{Fe,Si:Va} + 2(1-2y_{Si})(1-y_C)\frac{\partial L_{Fe,Si:Va}}{\partial y_{Si}} + (1-y_{Si})y_{Si}(1-y_C)\frac{\partial^2 L_{Fe,Si:Va}}{\partial^2 y_{Si}}$$
$$- 2y_C L_{Fe,Si:C} + 2(1-2y_{Si})y_C\frac{\partial L_{Fe,Si:C}}{\partial y_{Si}}$$

$$\left(\because \frac{\partial^2 L_{Fe,Si:C}}{\partial y_{Si}^2} = 0\right)$$

2. Getting μ_C Related Derivatives

$$D_{CC} = y_C(1-y_C)\Omega_C \cdot \frac{\partial \mu_C}{\partial y_C} = y_C(1-y_C)\Omega_C \cdot \frac{\partial^2 G_m}{\partial y_C^2}$$

$$D_{CSi} = y_C(1-y_C)\Omega_C \frac{\partial \mu_C}{\partial \mu_{Si}} = y_C(1-y_C)\Omega_C \frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_C}\right)$$

$$D_{SiC} = y_{Fe}\, y_{Si}\, \Omega_{Si} \frac{d\mu_{Si}}{d y_C} - y_{Si}\, y_{Fe}\, \Omega_{Fe} \frac{d\mu_{Fe}}{d y_C}$$

$$= (1-y_{Si})y_{Si}\Omega_{Si}\left\{\frac{\partial G_m}{\partial y_C} + (1-y_{Si})\frac{\partial}{\partial y_C}\left(\frac{\partial G_m}{\partial y_{Si}}\right)\right\} - (1-y_{Si})y_{Si}\Omega_{Fe}\left(\frac{\partial G_m}{\partial y_C} - y_{Si}\frac{\partial}{\partial y_C}\left(\frac{\partial G_m}{\partial y_{Si}}\right)\right)$$

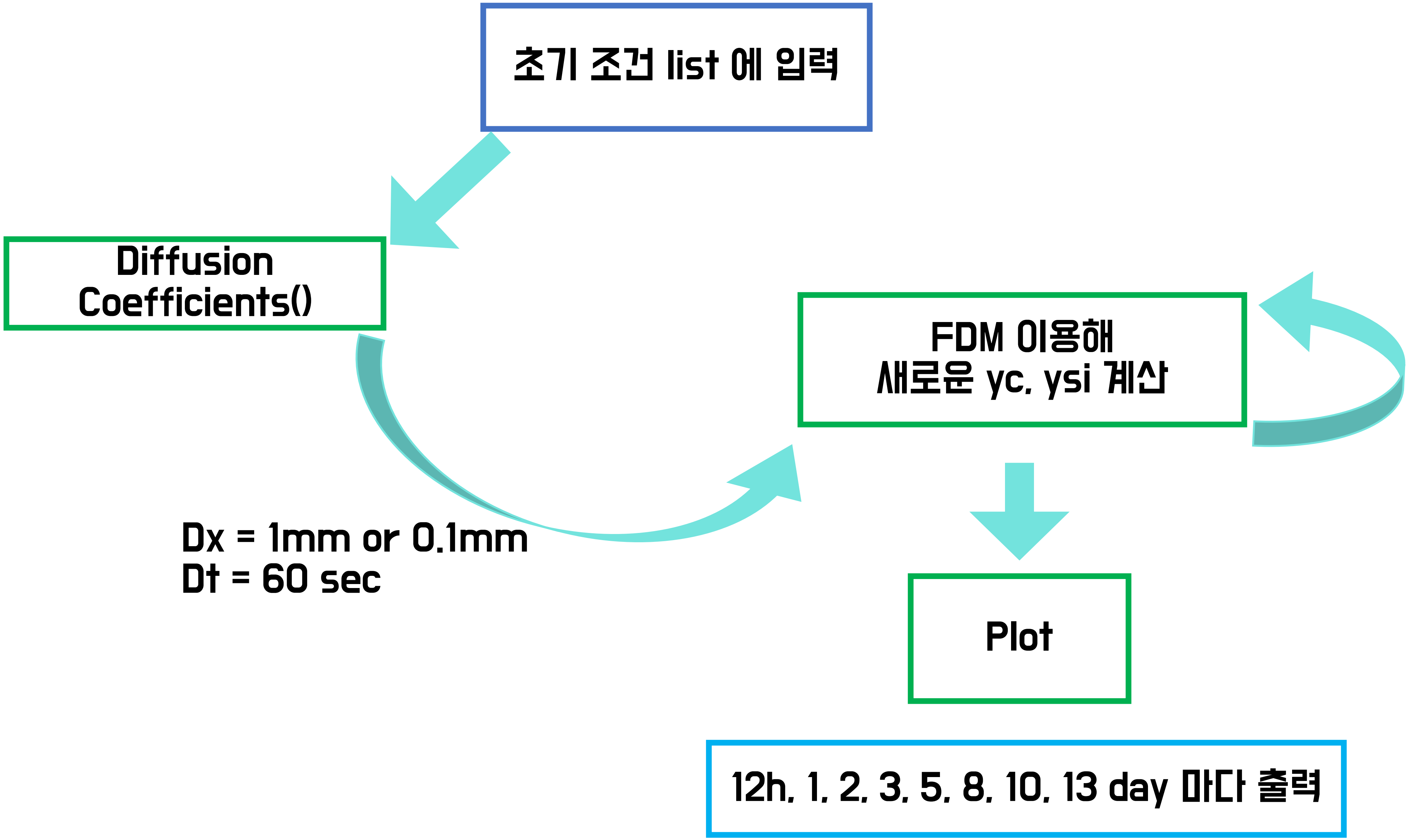
$$= (1-y_{Si})y_{Si}\left\{\frac{\partial G_m}{\partial y_C}(\Omega_{Si} - \Omega_{Fe}) + \frac{\partial}{\partial y_C}\left(\frac{\partial G_m}{\partial y_{Si}}\right)\left\{\Omega_{Si}(1-y_{Si}) + \Omega_{Fe}\, y_{Si}\right\}\right\}$$

$$D_{SiSi} = y_{Fe}\, y_{Si}\, \Omega_{Si} \frac{d\mu_{Si}}{d y_{Si}} - y_{Si}\, y_{Fe}\, \Omega_{Fe} \frac{d\mu_{Fe}}{d y_{Si}}$$

$$= (1-y_{Si})y_{Si}\Omega_{Si}\left\{(1-y_{Si})\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)\right\} - (1-y_{Si})y_{Si}\Omega_{Fe}\left\{-y_{Si}\frac{\partial}{\partial y_{Si}}\left(\frac{\partial G_m}{\partial y_{Si}}\right)\right\}$$

$$= (1-y_{Si})y_{Si} \cdot \frac{\partial^2 G_m}{\partial y_{Si}^2}\left\{(1-y_{Si})\Omega_{Si} + y_{Si}\,\Omega_{Fe}\right\}$$

3. Algorithms

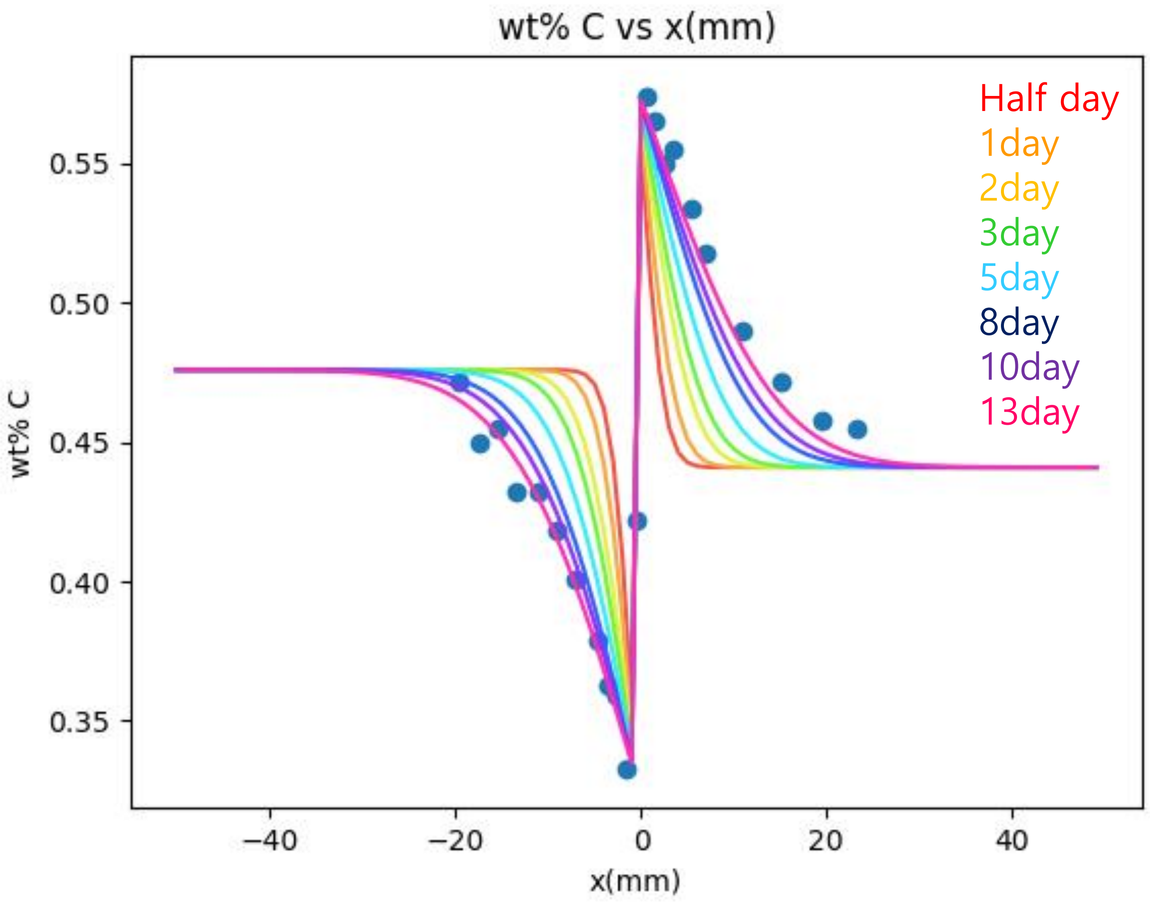


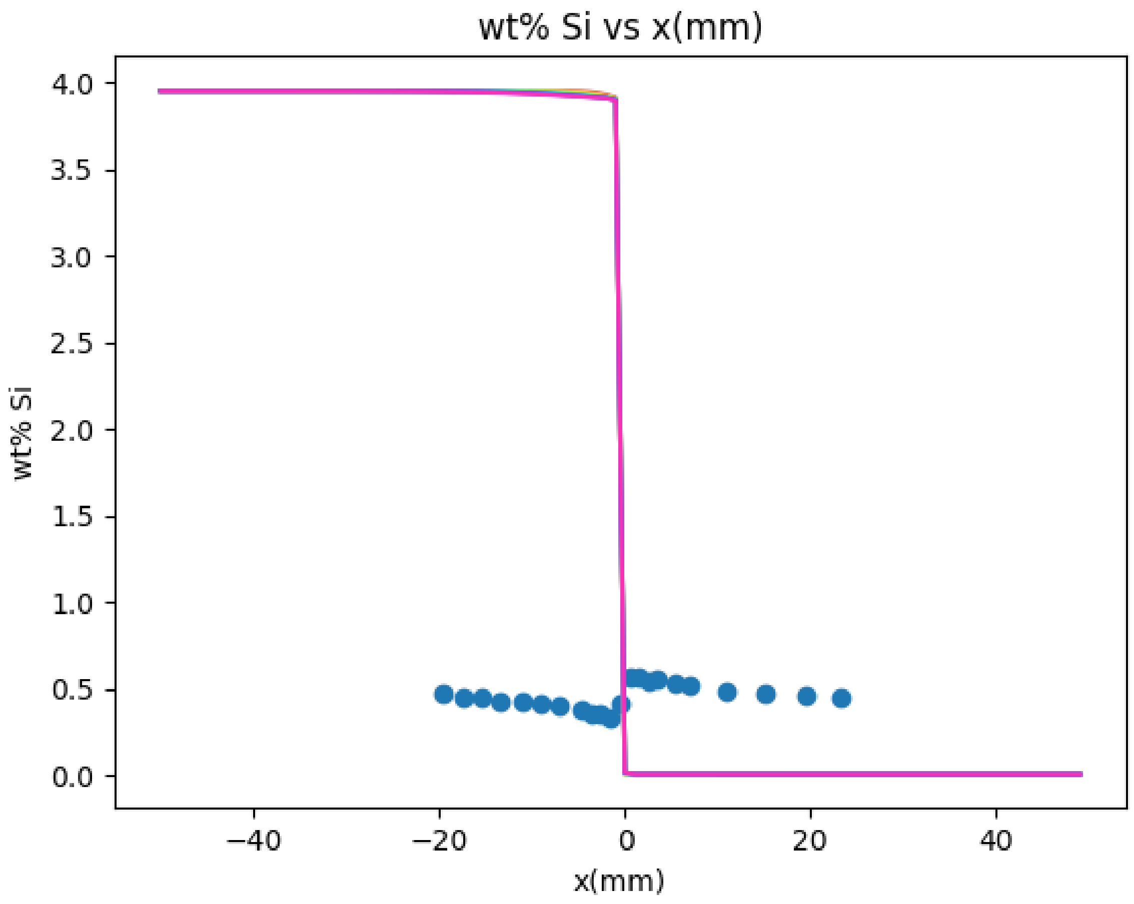
4. Code

```python
##############################Diffusion Coefficients##############################
def DiffC(si, c):
    G_FeVa = 0
    G_SiVa = 51000 - 21.8*T
    G_SiC = -20510 + 38.7*T
    G_FeC = 77207 - 15.877*T
#L values
    L_FeSiVa = -125248 + 41.116*T - 142708*(1 - 2*si) + 89907*((1- 2*si)**2)
    dL_FeSiVa= 142708*2-4*89907*(1-2*si)
    L_FeSiC= 143219.9 + 39.31*T -216320.5*(1-2*si)
    dL_FeSiC= 216320.5*2
    L_FeCVa = -34671
    ddL_FeSiVa = 8*89907
#Chemical Potentials
    dGm_dyC=-(1-si)*G_FeVa-si*G_SiVa+(1-si)*G_FeC+si*G_SiC+R*T*(np.log(c/(1-c)))-(1-si)*si*L_FeSiVa+si*(1-si)*L_FeSiC+(1-si)*(1-2*c)*L_FeCVa
    ddGm_dyC2= R*T*(1.0/c + 1/(1-c)) - 2*(1 - si)*(-34671)
    ddGm_dySidyC=G_FeVa-G_SiVa-G_FeC+G_SiC-(1-2*si)*L_FeSiVa+(1-2*si)*L_FeSiC-(1-2*c)*L_FeCVa-(1-si)*si*dL_FeSiVa
#   dGm_dySi= (c-1)*G_FeVa+(1-c)*G_SiVa- c*G_FeC+c*G_SiC + R*T*(np.log(si)-np.log(1-si)) +(1-2*si)*(1-c)*L_FeSiVa+ (1-si)*si*(1-c)*dL_FeSiVa + (
    ddGm_dySi2=R*T*(1/si-1/(1-si)) -2*(1-c)*L_FeSiVa+2*(1-2*si)*(1-c)*dL_FeSiVa +(1-si)*si*(1-c)*ddL_FeSiVa-2*c*L_FeSiC +2*(1-2*si)*c*dL_FeSiC

    DiffusionCoeffients.append(c*(1-c)*Ohm_C(c)*ddGm_dyC2)
    DiffusionCoeffients.append(c*(1-c)*Ohm_C(c)*ddGm_dySidyC)
    DiffusionCoeffients.append(si*(1-si)*(dGm_dyC*(Ohm_Si-Ohm_Fe) + ddGm_dySidyC*(Ohm_Si*(1-si)+Ohm_Fe*si)))
    DiffusionCoeffients.append(si*(1-si)*((1-si)*Ohm_Si+si*Ohm_Fe)*ddGm_dySi2)

    return DiffusionCoeffients
```

```python
##FDM METHOD
ct[i]= c[i] + dt/(dx**2)*(np.sqrt(DCCp*DCC)*(c[i+1]-c[i])-np.sqrt(DCC*DCCm)*(c[i]-c[i-1]))
+dt/dx/dx*(np.sqrt(DCSip*DCSi)*(si[i+1]-si[i])-np.sqrt(DCSim*DCSi)*(si[i]-si[i-1]))
sit[i] = si[i] +dt/(dx**2)*(np.sqrt(DSiCp*DSiC)*(c[i+1]-c[i])-np.sqrt(DSiC*DSiCm)*(c[i]-c[i-1])
+dt/dx/dx*(np.sqrt(DSiSip*DSiSi)*(si[i+1]-si[i])-np.sqrt(DSiSim*DSiSi)*(si[i]-si[i-1]))
ct[0] = c_near0
sit[0]= si_near0
ct[n-1] = c_near100
sit[n-1]= si_near100

 for i in range(0, n):
     c[i] = ct[i]
     si[i] = sit[i]
```

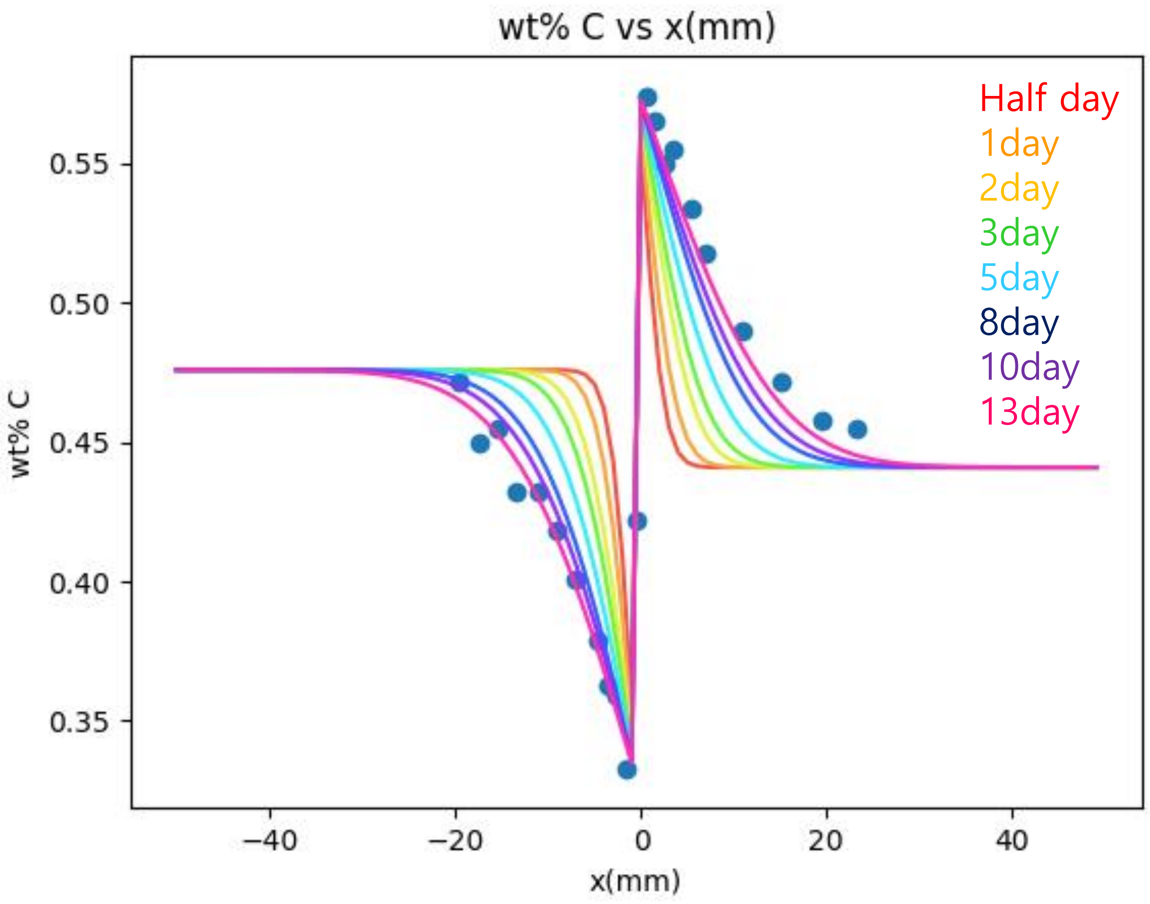
5. Results


wt% C vs x(mm)
wt% C
x(mm)
0.55
0.50
0.45
0.40
0.35
−40
−20
0
20
40
Half day
1day
2day
3day
5day
8day
10day
13day

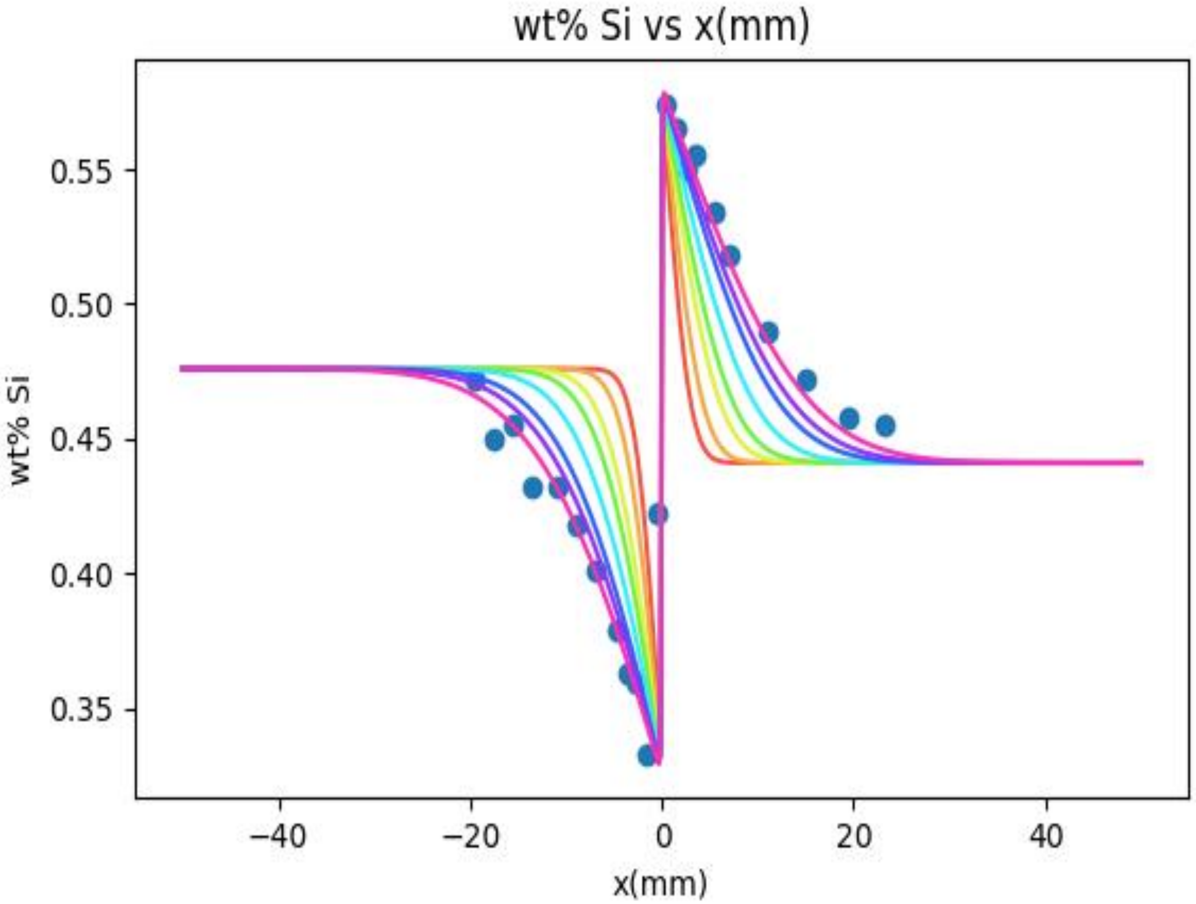

wt% Si vs x(mm)
wt% Si
x(mm)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−40
−20
0
20
40

5. Results

Dx=1 mm

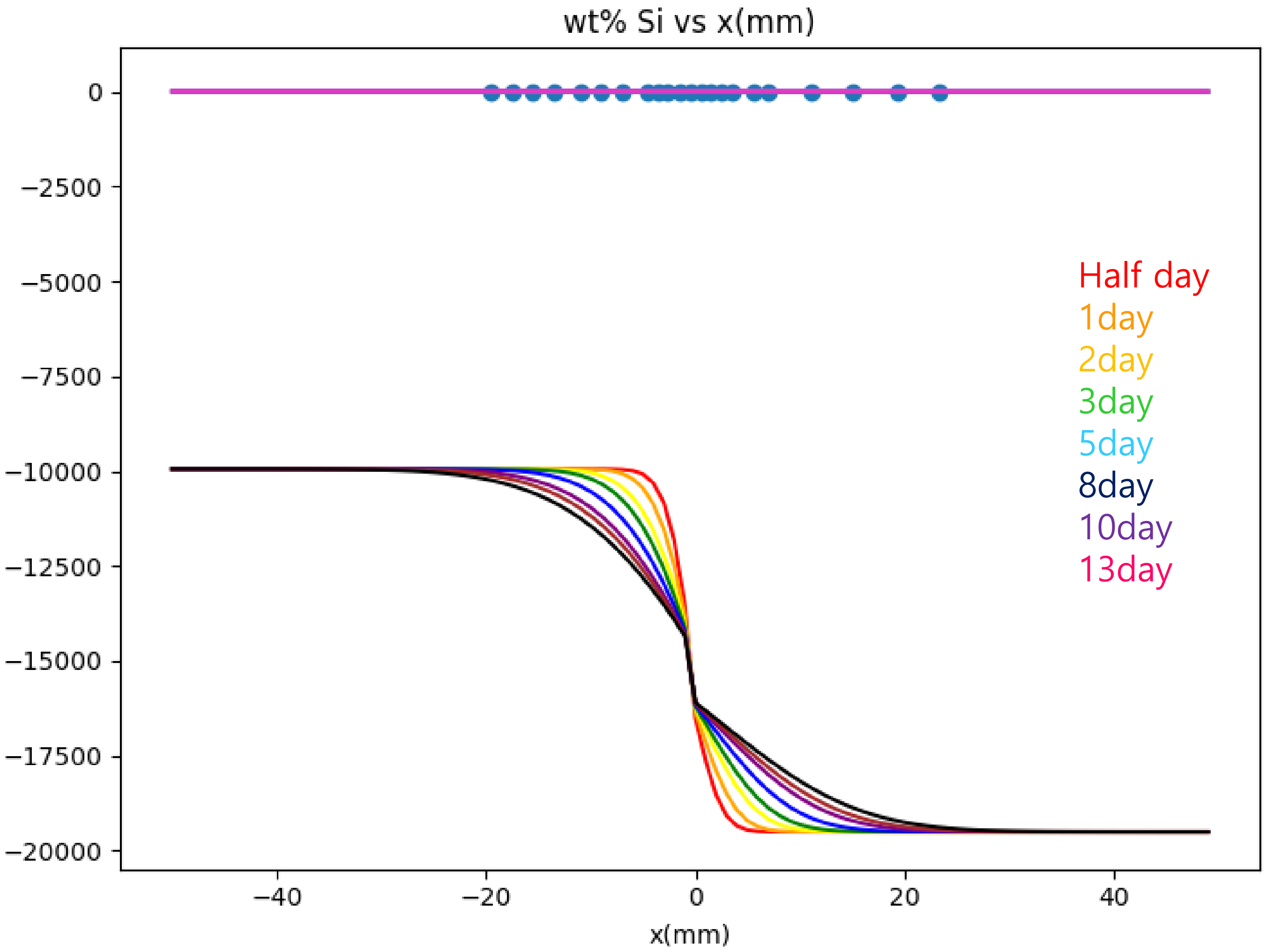


Dx=0.1 mm



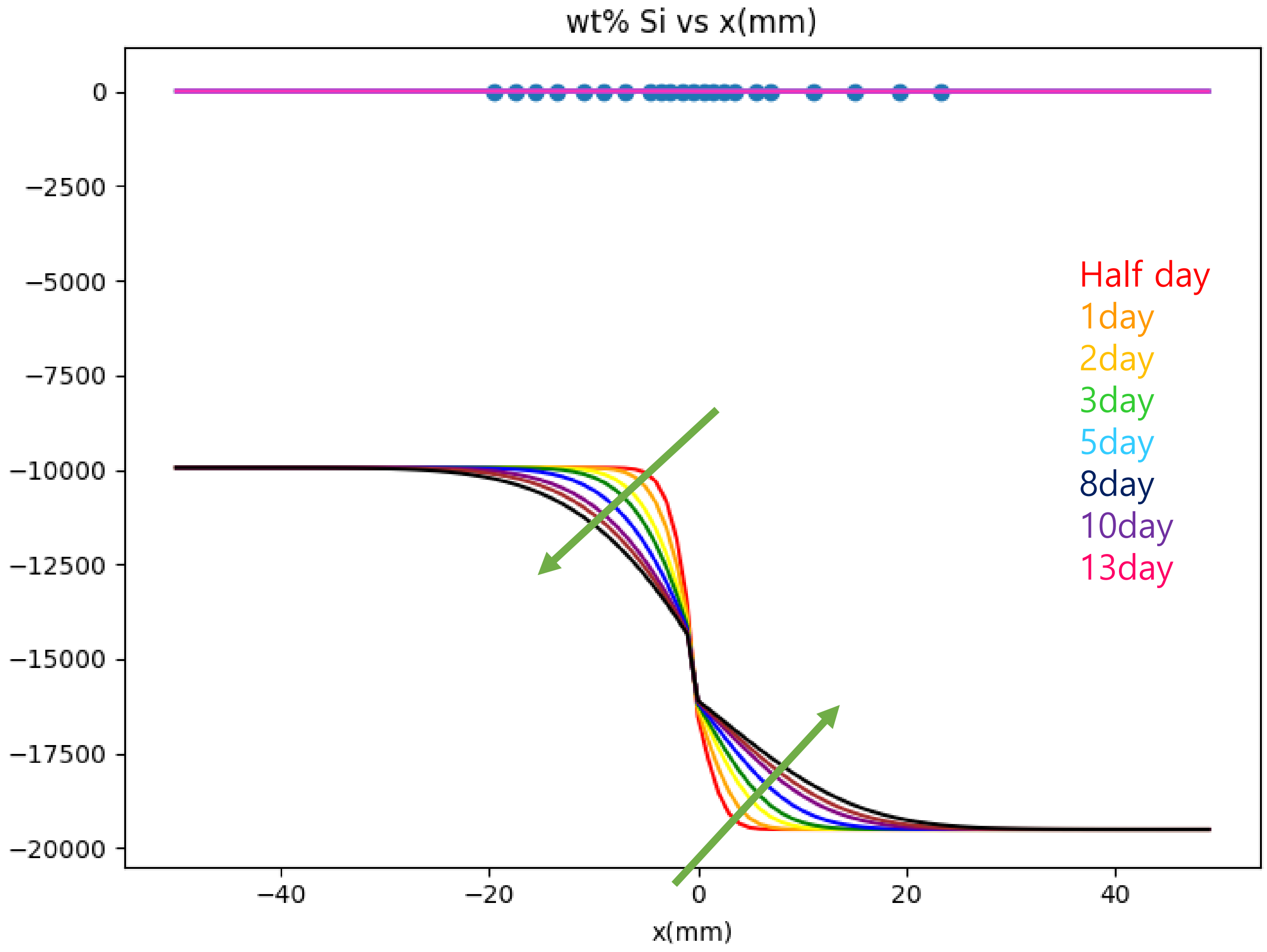
5. Results

$$\mu_C = \frac{dGm}{dy_C}$$



5. Results

$$\mu_C = \frac{dGm}{dy_C}$$



5. Results

0.py   00.py*   1.py   a.py   ex.py*   f.py

```python
    c.append(x_C/(x_Si+x_Fe))
    ct.append(x_C/(x_Si+x_Fe))
    si.append(x_Si/(x_Fe+x_Si))
    sit.append(x_Si/(x_Fe+x_Si))
################################################################################
###################################Ohm Parameters##############################
Ohm_Fe=7*10**-5*np.exp(-286000/(R*T))/(R*T)
Ohm_Si=9.05*10**-3*np.exp(-322465/(R*T))/(R*T)
def Ohm_C(c):
    return 4.529*(10**-7)*np.exp(-(1-2.221*(10**-4)*T)*(-72007*c+147723*(1-c))/
################################################################################
############################Diffusion Coefficients############################
def DiffC(si, c):
    G_FeVa = 0
    G_SiVa = 51000 - 21.8*T
    G_SiC = -20510 + 38.7*T
    G_FeC = 77207 - 15.877*T
#L values
    L_FeSiVa = -125248 + 41.116*T - 142708*(1 - 2*si) + 89907*((1- 2*si)**2)
    dL_FeSiVa= 142708*2-4*89907*(1-2*si)
    L_FeSiC= 143219.9 + 39.31*T -216320.5*(1-2*si)
    dL_FeSiC= 216320.5*2
    L_FeCVa = -34671
    ddL_FeSiVa = 8*89907
#Chemical Potentials
    dGm_dyC=-(1-si)*G_FeVa-si*G_SiVa+(1-si)*G_FeC+si*G_SiC+R*T*(np.log(c/(1-c))
    ddGm_dyC2= R*T*(1.0/c + 1/(1-c)) - 2*(1 - si)*(-34671)
    ddGm_dySidyC=G_FeVa-G_SiVa-G_FeC+G_SiC-(1-2*si)*L_FeSiVa+(1-2*si)*L_FeSiC-(
#   dGm_dySi= (c-1)*G_FeVa+(1-c)*G_SiVa- c*G_FeC+c*G_SiC + R*T*(np.log(si)-np.l
    ddGm_dySi2=R*T*(1/si-1/(1-si)) -2*(1-c)*L_FeSiVa+2*(1-2*si)*(1-c)*dL_FeSiVa

    DiffusionCoeffients.append(c*(1-c)*Ohm_C(c)*ddGm_dyC2)
    DiffusionCoeffients.append(c*(1-c)*Ohm_C(c)*ddGm_dySidyC)
    DiffusionCoeffients.append(si*(1-si)*(dGm_dyC*(Ohm_Si-Ohm_Fe) + ddGm_dySidy
    DiffusionCoeffients.append(si*(1-si)*((1-si)*Ohm_Si+si*Ohm_Fe)*ddGm_dySi2)

    return DiffusionCoeffients

def Plot(ct, si, p):
    wt_C,wt_Si=[],[]
    for i in range(0, n):
        Cf = ct[i]/(1+ct[i])
        Sif= si[i]/(1-Cf)
```

C:₩WINDOWS₩system32₩cmd.exe

```
5 day
450000
480000
510000
540000
570000
600000
630000
660000
690000
8 day
720000
750000
780000
810000
840000
10 day
870000
900000
930000
960000
990000
1020000
1050000
1080000
1110000
13 day
Iterate time:  448.07254362106323

C:₩Users₩Administrator₩Desktop>python ex.py
```

Diffusion Coefficient Function으로 구할 때

5. Results

0.py | 00.py* | 1.py | a.py* | ex.py* | f.py

```python
'''


#    plt.axis([-40, 40, 0.3, 0.6])


G_FeVa = 0
G_SiVa = 51000 - 21.8*T
G_SiC = -20510 + 38.7*T
G_FeC = 77207 - 15.877*T
while(1):
    time += dt
    #print(time)
    for i in range(0, n):
        L_FeSiVa[i] = -125248 + 41.116*T - 142708*(1 - 2*si[i]) + 89907*((1- 2*
        dL_FeSiVa[i]= 142708*2-4*89907*(1-2*si[i])
        L_FeSiC[i]= 143219.9 + 39.31*T -216320.5*(1-2*si[i])
        dL_FeSiC= 216320.5*2
        L_FeCVa = -34671
        ddL_FeSiVa = 8*89907

        dGm_dyC[i]=-(1-si[i])*G_FeVa-si[i]*G_SiVa+(1-si[i])*G_FeC+si[i]*G_SiC+R
        ddGm_dyC2[i]= R*T*(1.0/c[i] + 1/(1-c[i])) - 2*(1 - si[i])*(-34671)
        ddGm_dySidyC[i]=G_FeVa-G_SiVa-G_FeC+G_SiC-(1-2*si[i])*L_FeSiVa[i]+(1-2*
        dGm_dySi[i]= (c[i]-1)*G_FeVa+(1-c[i])*G_SiVa- c[i]*G_FeC+c[i]*G_SiC + R
        ddGm_dySi2[i]=R*T*(1/si[i]-1/(1-si[i])) -2*(1-c[i])*L_FeSiVa[i]+2*(1-2*

        DCC[i] =c[i]*(1-c[i])*Ohm_C(c[i])*ddGm_dyC2[i]
        DCSi[i] = c[i]*(1-c[i])*Ohm_C(c[i])*ddGm_dySidyC[i]
        DSiC[i] = si[i]*(1-si[i])*(dGm_dyC[i]*(Ohm_Si-Ohm_Fe) + ddGm_dySidyC[i]
        DSiSi[i] = si[i]*(1-si[i])*((1-si[i])*Ohm_Si+si[i]*Ohm_Fe)*ddGm_dySi2[i

    for i in range(1, n-1):
        ct[0] = c_near0
        sit[0]= si_near0
        ct[n-1] = c_near100
        sit[n-1]= si_near100
        ct[i]= c[i] + dt/(dx**2)*(np.sqrt(DCC[i+1]*DCC[i])*(c[i+1]-c[i])-np.sqr
        sit[i] = si[i] +dt/(dx**2)*(np.sqrt(DSiC[i+1]*DSiC[i])*(c[i+1]-c[i])-np

```

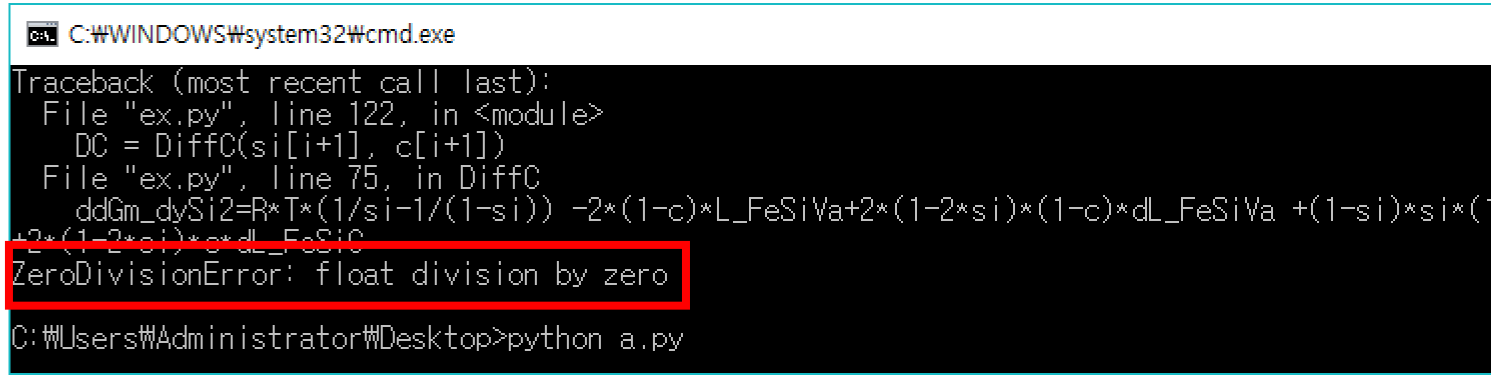
선택 C:₩WINDOWS₩system32₩cmd.exe

```
1047000
1050000
1053000
1056000
1059000
1062000
1065000
1068000
1071000
1074000
1077000
1080000
1083000
1086000
1089000
1092000
1095000
1098000
1101000
1104000
1107000
1110000
1113000
1116000
1119000
1122000
13 day
Iterate time: 266.377936

C:₩Users₩Administrator₩Desktop>
```

Diffusion Coefficient Array로 구할 때

5. Results

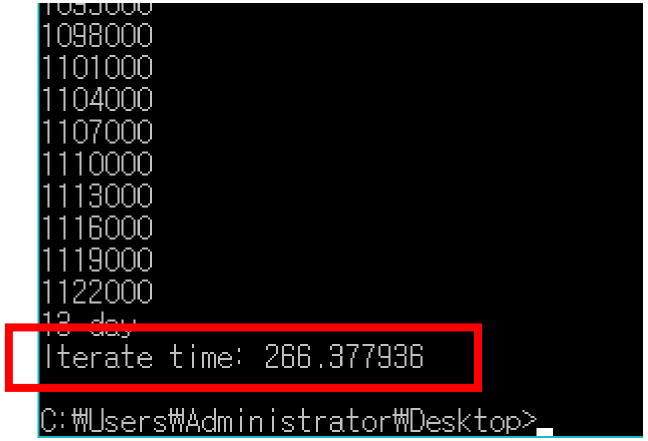
W_Si = 0

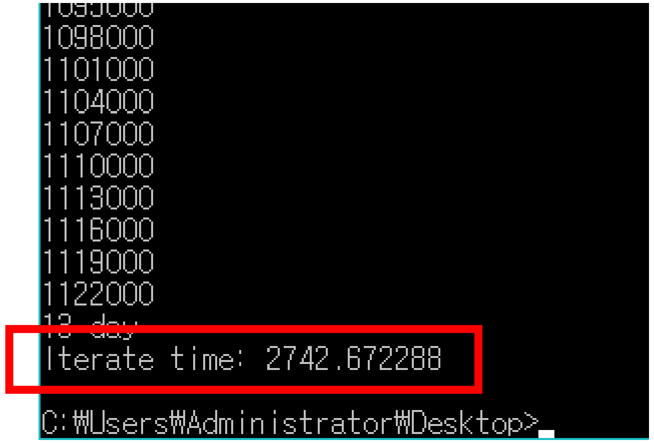


N=100

dx = 0.1/N (m)

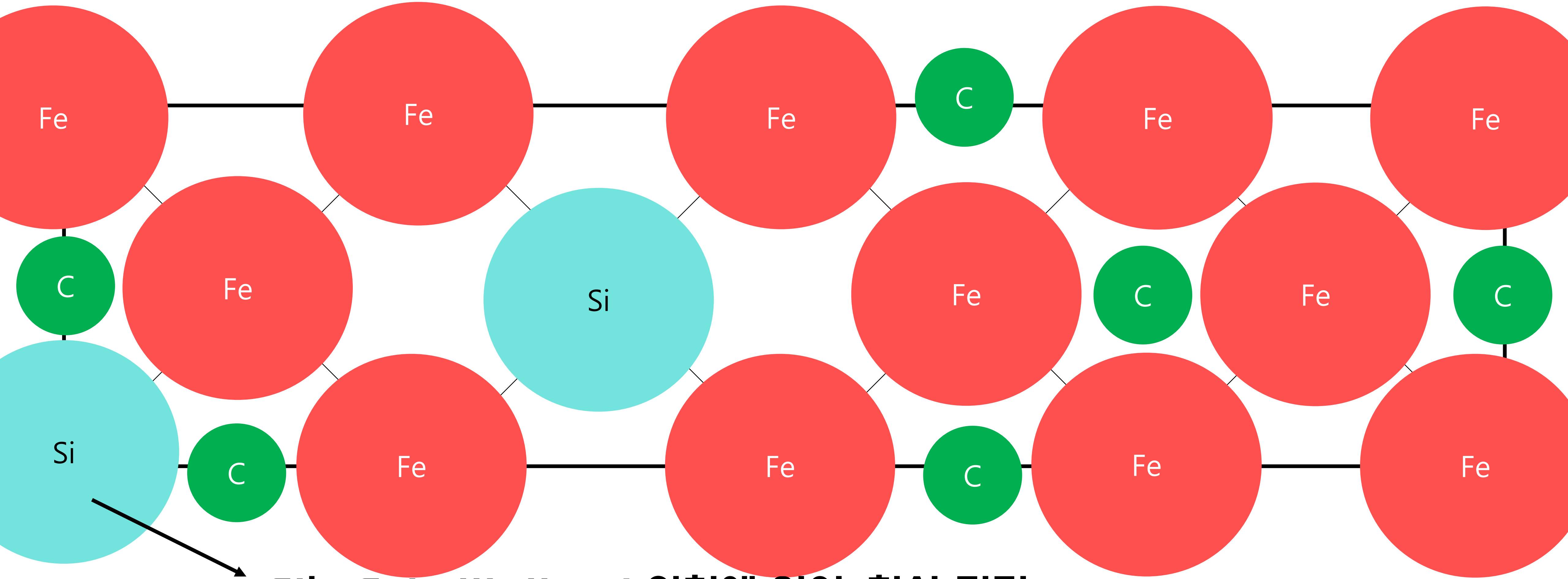
N=1000





6. Conclusion

세 원소의 Chemical Potential에 의해 일반적인 확산과 달리
Uphill Diffusion이 일어남을 확인(농도 보다는 Chemical Potential 때문!)



Si는 Substitutional 위치에 있어, 확산 더딤

6. Conclusion

소재 수치 해석
꿀 잼