Numerical Method

Assignment #4

20120383 Lee Hak-Hyun

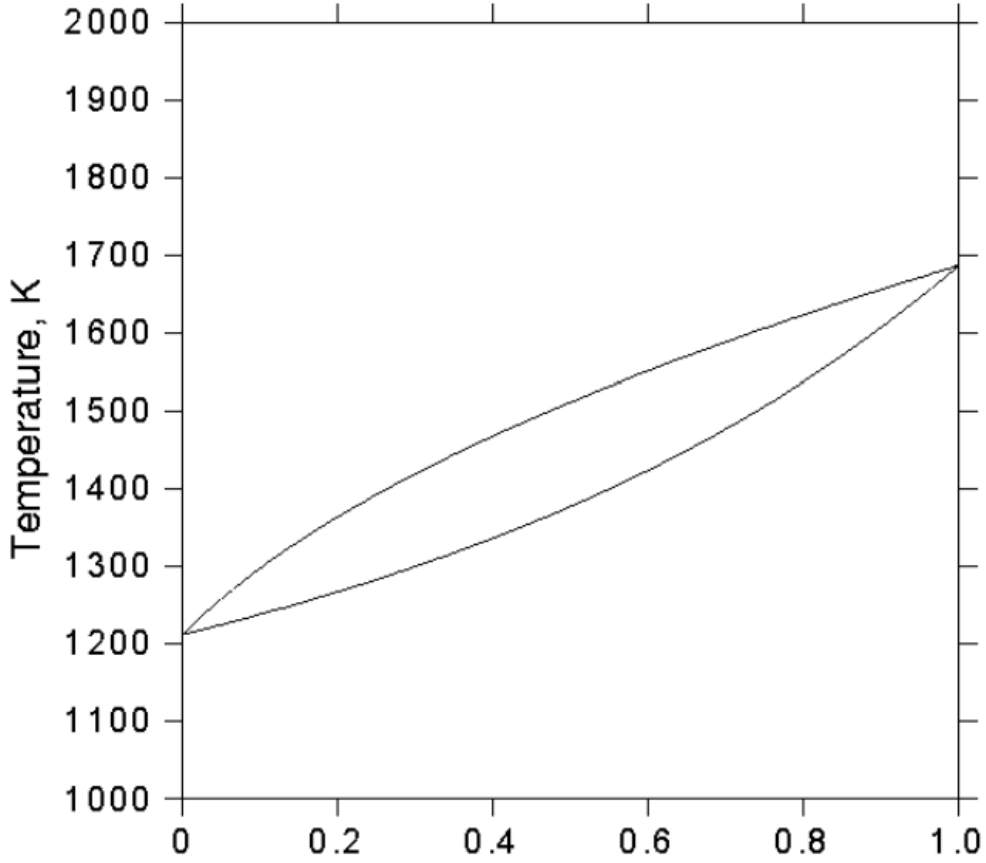
Problem

주어진 Gibbs energy 식을 이용하여 Ge-Si 2 원계 상태도를 계산으로 완성하시오.

$$^{o}G_{Ge}^{dia \rightarrow liquid} = 36944.72 - 30.4975\ T$$

$$^{o}G_{Si}^{dia \rightarrow liquid} = 50208.00 - 29.7617\ T$$

고상 (diamond 구조), 액상 모두에 대해 ideal solution 을 가정하시오.



Background

$$^{o}G_{Ge}^{dia\rightarrow liquid} = 36944.72 - 30.4975\ T$$

$$^{o}G_{Si}^{dia\rightarrow liquid} = 50208.00 - 29.7617\ T$$

Equilibrium Condition: $\mu_{Si}^{L} = \mu_{Si}^{S}$ $\mu_{Ge}^{L} = \mu_{Ge}^{S}$

$$G_m^P = x_{Si}\Delta^o G_{Si}^{ref\rightarrow P} + x_{Ge}\Delta^o G_{Ge}^{ref\rightarrow P} + RT(x_{Si}\ln x_{Si} + x_{Ge}\ln x_{Ge}) + x$$

$$\mu_i^P = \Delta^o G_i^{ref\rightarrow P} + RT\ln x_i + (1-x_i)^2 L^P$$

$$\mu_{\mathrm{Si}}^{\mathrm{L}} - \mu_{Si}^{S} = {}^{\circ}G_{Si}^{dia\rightarrow liquid} + RTln\left(\frac{x_{Si}^{L}}{x_{Si}^{S}}\right) = 0$$

$$\mu_{\mathrm{Ge}}^{\mathrm{L}} - \mu_{Ge}^{S} = {}^{\circ}G_{Ge}^{dia\rightarrow liquid} + RTln\left(\frac{1-x_{Si}^{L}}{1-x_{Si}^{S}}\right) = 0$$

$$f_1(x_1, x_2, \cdots, x_n) = 0$$

$$f_2(x_1, x_2, \cdots, x_n) = 0$$

$$\cdots \quad \cdots$$

$$f_n(x_1, x_2, \cdots, x_n) = 0$$

$\Rightarrow$ F(X) = 0

$$F(X) = \begin{bmatrix} f_1(x_{Si}^{L}, x_{Si}^{S}) \\ f_2(x_{Si}^{L}, x_{Si}^{S}) \end{bmatrix} = \begin{bmatrix} \mu_{\mathrm{Si}}^{\mathrm{L}} - \mu_{Si}^{S} \\ \mu_{\mathrm{Ge}}^{\mathrm{L}} - \mu_{Ge}^{S} \end{bmatrix}$$

Background

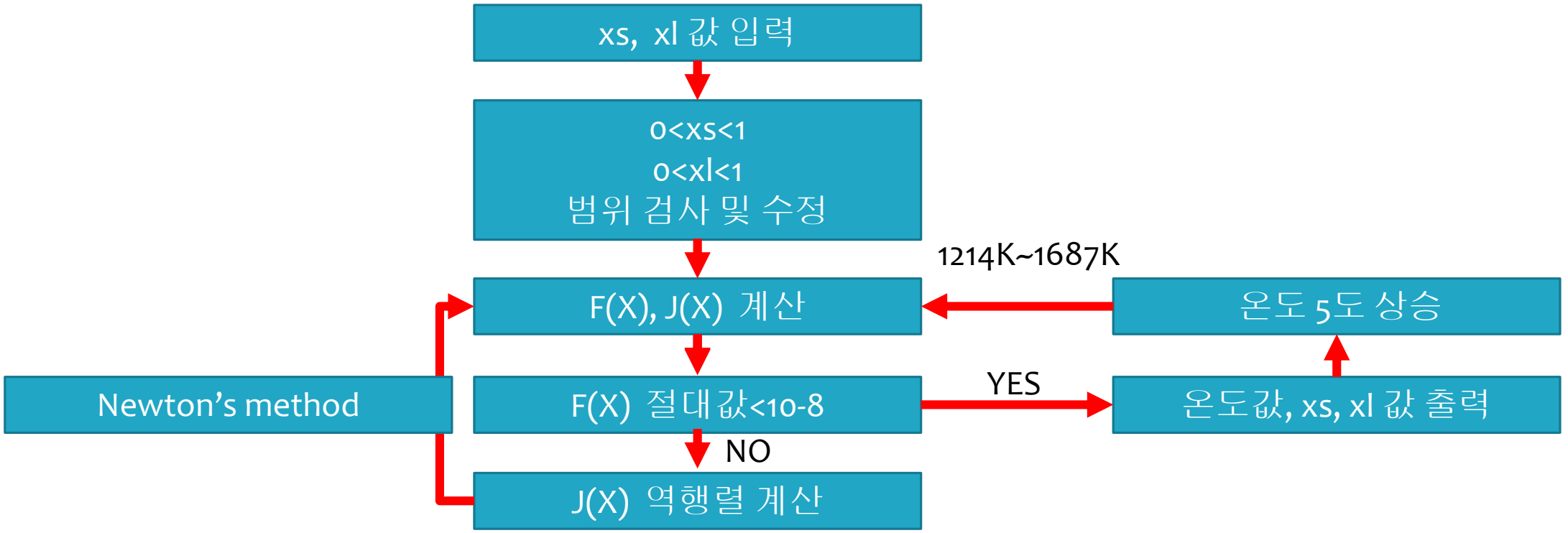
Jacobian matrix $J(X)$

$$J(X) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_3} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

$$J(X) = \begin{bmatrix} \frac{RT}{x_{Si}^L} & \frac{-RT}{x_{Si}^S} \\ \frac{-RT}{1-x_{Si}^L} & \frac{RT}{1-x_{Si}^S} \end{bmatrix}$$

$$P_{(k)} = p_{(k-1)} - [J(P_{(k-1)})]^{-1} F(P_{(k-1)})$$

Algorithm


xs, xl 값 입력
0<xs<1
0<xl<1
범위 검사 및 수정
F(X), J(X) 계산
F(X) 절대값<10-8
YES
NO
Newton's method
J(X) 역행렬 계산
1214K~1687K
온도 5도 상승
온도값, xs, xl 값 출력

Code

xs=x_{Si}^{S} , xl=x_{Si}^{L}
arr1=J(X), arr3=inverse

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#define R 8.3144621
```

R 값 global 변수 선언

```
void normalization(double **arr1,double **arr3,int x);
void pivoting(double **arr1,double **arr3,int x);
void gauss(double **arr1,double **arr3,int x);
void sub(double **arr1,double **arr3,int x);
void multiple(double **arr3,int x);
double function1(double xs,double xl, double T);
double function2(double xs, double xl, double T);
void Jacobian(double **arr1,double xs,double xl,double T);
```

Inverse matrix

$$F(X) = \begin{bmatrix} f_1(x_{Si}^L, x_{Si}^S) \\ f_2(x_{Si}^L, x_{Si}^S) \end{bmatrix} = \begin{bmatrix} \mu_{\mathrm{Si}}^{\mathrm{L}} - \mu_{Si}^{S} \\ \mu_{\mathrm{Ge}}^{\mathrm{L}} - \mu_{Ge}^{S} \end{bmatrix}$$

$$J(X) = \begin{bmatrix} \frac{RT}{x_{Si}^L} & \frac{-RT}{x_{Si}^S} \\ \frac{-RT}{1-x_{Si}^L} & \frac{RT}{1-x_{Si}^S} \end{bmatrix}$$

Code

```
int main(void)
{
    int x,i,j;
    double **arr1;
    double **arr3;
    double xs,xl;
    double T=1214;
    double f1,f2;
    int num=0;
```

F(X)의 element들

```
    FILE* outfile;

    outfile=fopen("result.txt","w");
```

결과 값 text로 저장

```
    printf("Matrix의 크기를 설정하시요:");
    scanf("%d",&x);
    arr1=(double**)malloc(sizeof(double*)*x);
    arr3=(double**)malloc(sizeof(double*)*x);

    printf("고상과 액상의 분율을 각각 입력하세요.₩n");

    scanf("%lf %lf",&xs,&xl);
```

초기 고상, 액상 분율 입력

```
for(T=1214;T<1687;num++)
{
    if(xs<0)
    {
        while(xs<0)
        {
            xs=xs+0.01;
        }
    }
    else if(xs>1)
    {
        while(xs>1)
        {
            xs=xs-0.01;
        }
    }
    if(xl<0)
    {
        while(xl<0)
        {
            xl=xl+0.01;
        }
    }
    else if(xl>1)
    {
        while(xl>1)
        {
            xl=xl-0.01;
        }
```

1214K~1687K
5도씩 상승

0<xs<1
0<xl<1
범위 검사 및 수정

Code

```
    if(xl==xs)
        xl=xs+0.005;
f1=function1(xs,xl,T);
f2=function2(xs,xl,T);
Jacobian(arr1,xs,xl,T);
```

역행렬이 없는 경우 xl값을 다시 설정

F(X), J(X) 계산

```
if(fabs(f1)<0.00000001&&fabs(f2)<0.00000001)
{
    printf("%.0lf   %lf %lf %.2E    %.2E    %d₩n",T,xs,xl,f1,f2,num);
    fprintf(outfile,"%.0lf   %lf %lf %d₩n",T,xs,xl,num);
    T=T+5;
    num=0;
    continue;
}
```

F(X)의 각 값이 10-8 이하일 경우 0으로 간주
각 값 출력 및 온도 5도 상승

```
for(i=0;i<x;i++)
{
    arr3[i]=(double*)malloc(sizeof(double)*x);
    for(j=0;j<x;j++)
    {
        if(i==j)
            arr3[i][j]=1;
        else
            arr3[i][j]=0;
    }
}
normalization(arr1,arr3,x);
pivoting(arr1,arr3,x);
gauss(arr1,arr3,x);
for(i=0;i<x;i++)
{
    for(j=0;j<x;j++)
    {
        if(fabs(arr1[i][j])<0.00000001)
            arr1[i][j]=0;
        if(fabs(arr3[i][j])<0.00000001)
            arr3[i][j]=0;
    }
}
xl=xl-((arr3[0][0]*f1)+(arr3[0][1]*f2));
xs=xs-((arr3[1][0]*f1)+(arr3[1][1]*f2));
```

오차 범위를 넘을 경우 역행렬 생성 후 Newton's method

Code

```
double function1(double xs,double xl, double T)
{
    double Si;

    Si=50208.00-(29.7617*T)+(R*T*log(xl/xs));

    return Si;
}
double function2(double xs,double xl, double T)
{
    double Ge;

    Ge=36944.72-(30.4975*T)+(R*T*log((1-xl)/(1-xs)));

    return Ge;
}
```

```
void Jacobian(double **arr1,double xs,double xl,double T)
{
    int i,j;

    for(i=0;i<2;i++)
    {
        arr1[i]=(double*)malloc(sizeof(double)*2);
    }
    arr1[0][0]=(R*T)/(xl);
    arr1[0][1]=((-R)*T)/(xs);
    arr1[1][0]=((-R)*T)/(1-xl);
    arr1[1][1]=(R*T)/(1-xs);
}
```

F(X)의 element 및 J(X) 계산 함수

Result

각 Chemical potential 차이

Newton's method 시행 횟수

초기값에 따라 계산 속도 영향

```
Matrix의 크기를 설정하시요:2
고상과 액상의 분율을 각각 입력하세요.
0.1 0.9
Temperature      Xs          Xl          f1          f2          try
1214    0.010371    0.002571    1.82E-012   -2.05E-012   20
1224    0.049311    0.012732    0.00E+000   -1.08E-012   5
1229    0.068220    0.017972    -1.82E-012  -4.55E-013   5
1234    0.086769    0.023318    -1.82E-012  -9.09E-013   5
1239    0.104969    0.028771    0.00E+000   3.41E-013    5
1244    0.122830    0.034333    -1.82E-012  1.36E-012    5
1249    0.140361    0.040003    1.82E-012   0.00E+000    5
1254    0.157570    0.045782    -1.82E-012  2.27E-013    5
1259    0.174468    0.051670    -9.00E-009  -2.27E-012   4
1264    0.191062    0.057668    -6.09E-009  -2.73E-012   4
1269    0.207362    0.063777    -4.27E-009  -2.05E-012   4
1274    0.223374    0.069997    -3.08E-009  -2.50E-012   4
1279    0.239107    0.076329    -2.28E-009  -1.36E-012   4
1284    0.254568    0.082772    -1.73E-009  -1.36E-012   4
1289    0.269765    0.089328    -1.33E-009  4.55E-013    4
1294    0.284704    0.095997    -1.04E-009  0.00E+000    4
1299    0.299392    0.102779    -8.28E-010  2.73E-012    4
1304    0.313836    0.109675    -6.66E-010  -2.73E-012   4
1309    0.328042    0.116686    -5.44E-010  0.00E+000    4
1314    0.342016    0.123811    -4.46E-010  -2.27E-012   4
1319    0.355765    0.131051    -3.71E-010  0.00E+000    4
1324    0.369294    0.138407    -3.11E-010  -9.09E-013   4
1329    0.382608    0.145879    -2.60E-010  2.27E-012    4
1334    0.395713    0.153467    -2.24E-010  4.55E-013    4
```

1339	0.408615	0.161172	-1.93E-010	9.09E-013	4
1344	0.421318	0.168995	-1.64E-010	-4.55E-013	4
1349	0.433828	0.176934	-1.42E-010	-9.09E-013	4
1354	0.446149	0.184992	-1.24E-010	0.00E+000	4
1359	0.458285	0.193168	-1.07E-010	0.00E+000	4
1364	0.470242	0.201463	-9.64E-011	9.09E-013	4
1369	0.482023	0.209877	-8.55E-011	9.09E-013	4
1374	0.493633	0.218410	-7.28E-011	0.00E+000	4
1379	0.505077	0.227062	-6.55E-011	1.82E-012	4
1384	0.516357	0.235835	-5.82E-011	1.82E-012	4
1389	0.527478	0.244728	-5.28E-011	2.73E-012	4
1394	0.538444	0.253742	-4.91E-011	4.55E-012	4
1399	0.549258	0.262876	-4.37E-011	9.09E-013	4
1404	0.559924	0.272132	-4.00E-011	1.82E-012	4
1409	0.570445	0.281510	-3.46E-011	0.00E+000	4
1414	0.580825	0.291009	-3.18E-011	1.82E-012	4
1419	0.591066	0.300630	-3.00E-011	5.46E-012	4
1424	0.601173	0.310374	-2.82E-011	3.64E-012	4
1429	0.611147	0.320240	-2.36E-011	5.46E-012	4
1434	0.620993	0.330229	-2.18E-011	6.37E-012	4
1439	0.630713	0.340342	-2.09E-011	3.64E-012	4
1444	0.640309	0.350577	-1.82E-011	3.64E-012	4

Result

1444	0.640309	0.350577	-1.82E-011	3.64E-012	4
1449	0.649786	0.360937	-1.73E-011	3.64E-012	4
1454	0.659144	0.371420	-1.55E-011	6.37E-012	4
1459	0.668387	0.382027	-1.73E-011	5.46E-012	4
1464	0.677517	0.392758	-1.27E-011	7.28E-012	4
1469	0.686538	0.403614	-1.27E-011	5.46E-012	4
1474	0.695450	0.414595	-1.18E-011	2.73E-012	4
1479	0.704257	0.425700	-1.00E-011	4.55E-012	4
1484	0.712960	0.436931	-1.18E-011	1.09E-011	4
1489	0.721563	0.448287	-1.09E-011	9.09E-012	4
1494	0.730067	0.459768	-9.09E-012	5.46E-012	4
1499	0.738473	0.471375	-8.19E-012	9.09E-012	4
1504	0.746786	0.483107	-7.28E-012	5.46E-012	4
1509	0.755005	0.494966	-8.19E-012	1.27E-011	4
1514	0.763133	0.506950	-8.19E-012	1.27E-011	4
1519	0.771173	0.519061	-5.46E-012	1.46E-011	4
1524	0.779125	0.531298	-4.55E-012	1.27E-011	4
1529	0.786992	0.543661	-7.28E-012	1.64E-011	4
1534	0.794775	0.556152	-5.46E-012	1.82E-011	4
1539	0.802477	0.568768	-5.46E-012	2.00E-011	4
1544	0.810098	0.581512	-4.55E-012	2.18E-011	4
1549	0.817640	0.594383	-4.55E-012	2.36E-011	4
1554	0.825105	0.607381	-3.18E-012	2.36E-011	4
1559	0.832495	0.620506	-3.64E-012	3.09E-011	4
1564	0.839811	0.633758	-2.73E-012	3.64E-011	4
1569	0.847054	0.647137	-5.00E-012	4.55E-011	4
1574	0.854226	0.660644	-5.91E-012	5.28E-011	4
1579	0.861328	0.674279	-3.18E-012	5.46E-011	4
1584	0.868361	0.688041	-5.46E-012	7.46E-011	4

1589	0.875328	0.701931	-4.55E-012	8.37E-011	4
1594	0.882229	0.715948	-4.09E-012	9.28E-011	4
1599	0.889065	0.730094	-1.36E-012	1.13E-010	4
1604	0.895837	0.744367	-3.64E-012	1.53E-010	4
1609	0.902548	0.758768	-3.64E-012	1.89E-010	4
1614	0.909197	0.773297	-3.64E-012	2.35E-010	4
1619	0.915787	0.787953	-5.23E-012	3.20E-010	4
1624	0.922318	0.802738	-4.55E-012	4.15E-010	4
1629	0.928791	0.817651	-2.73E-012	5.49E-010	4
1634	0.935208	0.832692	-3.87E-012	7.77E-010	4
1639	0.941569	0.847861	-2.05E-012	1.13E-009	4
1644	0.947875	0.863158	-4.32E-012	1.72E-009	4
1649	0.954128	0.878583	-5.46E-012	2.76E-009	4
1654	0.960329	0.894136	-4.66E-012	4.74E-009	4
1659	0.966478	0.909817	-5.46E-012	8.89E-009	4
1664	0.972576	0.925627	-1.48E-012	5.46E-012	5
1669	0.978624	0.941564	-5.68E-013	2.73E-011	5
1674	0.984624	0.957629	-2.84E-013	-2.00E-011	5
1679	0.990575	0.973823	-4.26E-013	-4.55E-011	5
1684	0.996479	0.990144	-1.31E-012	1.06E-010	5

계속하려면 아무 키나 누르십시오 . . .

Result

result - 메모장

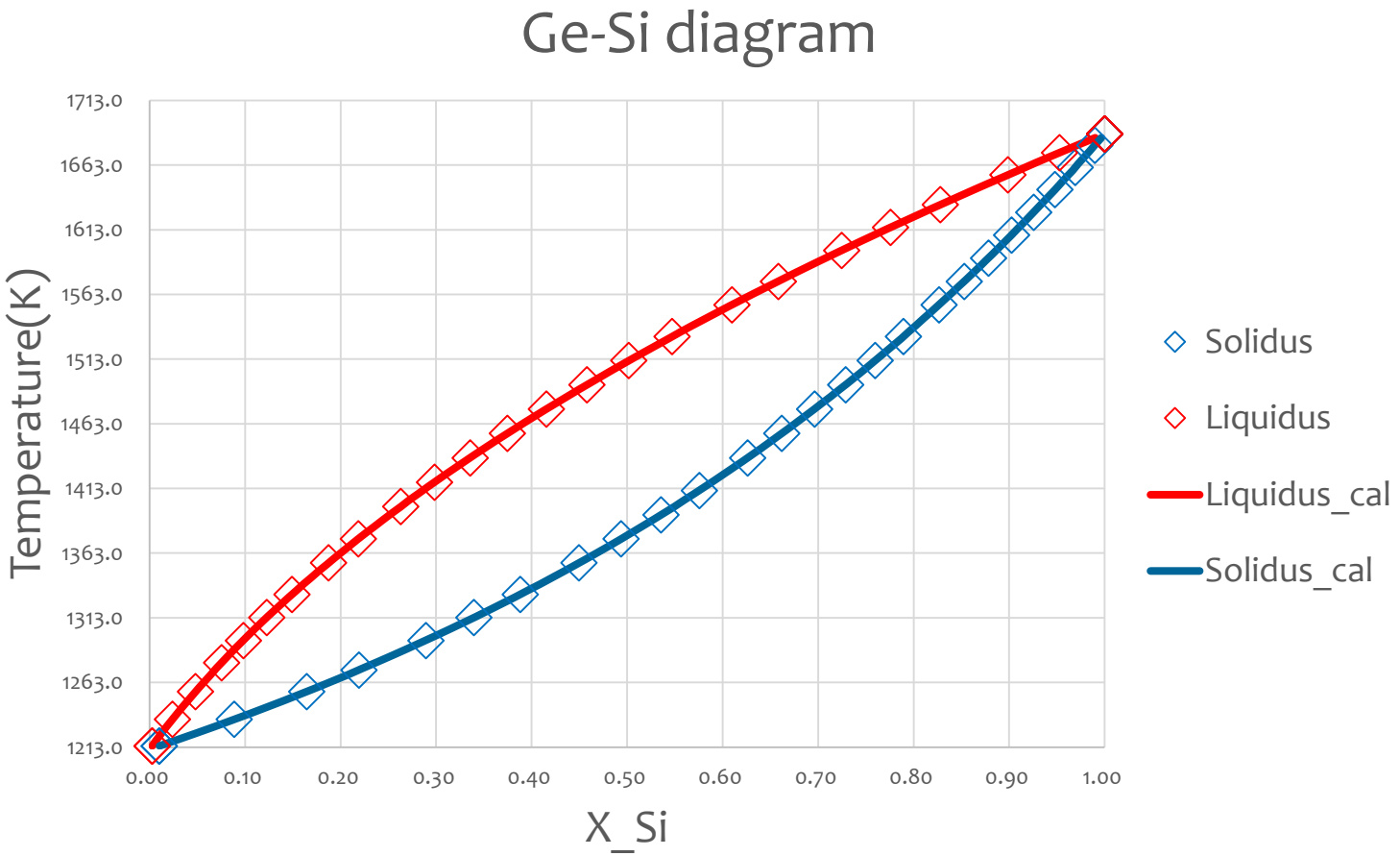
파일(F) 편집(E) 서식(O) 보기(V) 도움말(H)

1214	0.010371	0.002571	20
1219	0.030032	0.007599	5
1224	0.049311	0.012732	5
1229	0.068220	0.017972	5
1234	0.086769	0.023318	5
1239	0.104969	0.028771	5
1244	0.122830	0.034333	5
1249	0.140361	0.040003	5
1254	0.157570	0.045782	5
1259	0.174468	0.051670	4
1264	0.191062	0.057668	4
1269	0.207362	0.063777	4
1274	0.223374	0.069997	4
1279	0.239107	0.076329	4
1284	0.254568	0.082772	4
1289	0.269765	0.089328	4
1294	0.284704	0.095997	4
1299	0.299392	0.102779	4
1304	0.313836	0.109675	4
1309	0.328042	0.116686	4
1314	0.342016	0.123811	4
1319	0.355765	0.131051	4
1324	0.369294	0.138407	4
1329	0.382608	0.145879	4
1334	0.395713	0.153467	4
1339	0.408615	0.161172	4
1344	0.421318	0.168995	4
1349	0.433828	0.176934	4
1354	0.446149	0.184992	4
1359	0.458285	0.193168	4
1364	0.470242	0.201463	4
1369	0.482023	0.209877	4
1374	0.493633	0.218410	4
1379	0.505077	0.227062	4
1384	0.516357	0.235835	4
1389	0.527478	0.244728	4
1394	0.538444	0.253742	4
1399	0.549258	0.262876	4

1394	0.538444	0.253742	4
1399	0.549258	0.262876	4
1404	0.559924	0.272132	4
1409	0.570445	0.281510	4
1414	0.580825	0.291009	4
1419	0.591066	0.300630	4
1424	0.601173	0.310374	4
1429	0.611147	0.320240	4
1434	0.620993	0.330229	4
1439	0.630713	0.340342	4
1444	0.640309	0.350577	4
1449	0.649786	0.360937	4
1454	0.659144	0.371420	4
1459	0.668387	0.382027	4
1464	0.677517	0.392758	4
1469	0.686538	0.403614	4
1474	0.695450	0.414595	4
1479	0.704257	0.425700	4
1484	0.712960	0.436931	4
1489	0.721563	0.448287	4
1494	0.730067	0.459768	4
1499	0.738473	0.471375	4
1504	0.746786	0.483107	4
1509	0.755005	0.494966	4
1514	0.763133	0.506950	4
1519	0.771173	0.519061	4
1524	0.779125	0.531298	4
1529	0.786992	0.543661	4
1534	0.794775	0.556152	4
1539	0.802477	0.568768	4
1544	0.810098	0.581512	4
1549	0.817640	0.594383	4
1554	0.825105	0.607381	4
1559	0.832495	0.620506	4
1564	0.839811	0.633758	4
1569	0.847054	0.647137	4
1574	0.854226	0.660644	4
1579	0.861328	0.674279	4

1469	0.686538	0.403614	4
1474	0.695450	0.414595	4
1479	0.704257	0.425700	4
1484	0.712960	0.436931	4
1489	0.721563	0.448287	4
1494	0.730067	0.459768	4
1499	0.738473	0.471375	4
1504	0.746786	0.483107	4
1509	0.755005	0.494966	4
1514	0.763133	0.506950	4
1519	0.771173	0.519061	4
1524	0.779125	0.531298	4
1529	0.786992	0.543661	4
1534	0.794775	0.556152	4
1539	0.802477	0.568768	4
1544	0.810098	0.581512	4
1549	0.817640	0.594383	4
1554	0.825105	0.607381	4
1559	0.832495	0.620506	4
1564	0.839811	0.633758	4
1569	0.847054	0.647137	4
1574	0.854226	0.660644	4
1579	0.861328	0.674279	4
1584	0.868361	0.688041	4
1589	0.875328	0.701931	4
1594	0.882229	0.715948	4
1599	0.889065	0.730094	4
1604	0.895837	0.744367	4
1609	0.902548	0.758768	4
1614	0.909197	0.773297	4
1619	0.915787	0.787953	4
1624	0.922318	0.802738	4
1629	0.928791	0.817651	4
1634	0.935208	0.832692	4
1639	0.941569	0.847861	4
1644	0.947875	0.863158	4
1649	0.954128	0.878583	4
1654	0.960329	0.894136	4
1659	0.966478	0.909817	4
1664	0.972576	0.925627	5
1669	0.978624	0.941564	5
1674	0.984624	0.957629	5
1679	0.990575	0.973823	5
1684	0.996479	0.990144	5

Result


Ge-Si diagram
Temperature(K)
1713.0
1663.0
1613.0
1563.0
1513.0
1463.0
1413.0
1363.0
1313.0
1263.0
1213.0
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
X_Si
Solidus
Liquidus
Liquidus_cal
Solidus_cal

Result

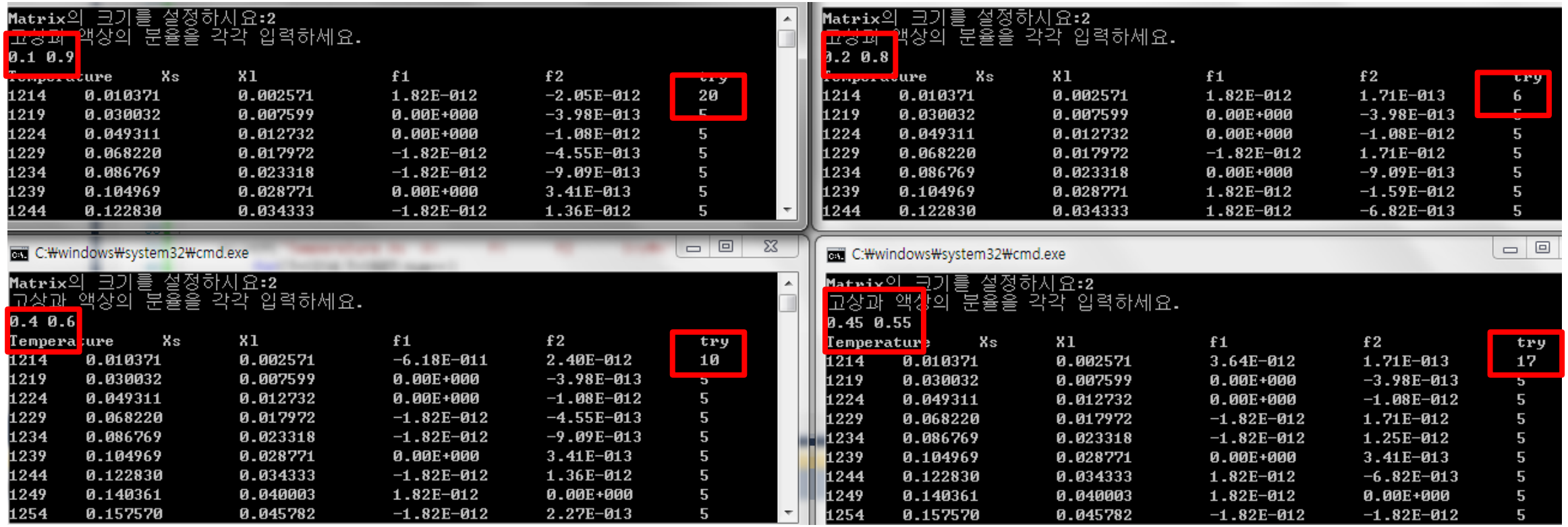
T=1214K부터 시행 했을 때와 T=1400K부터 시작햇을 때

```
Matrix의 크기를 설정하시요:2
고상과 액상의 분율을 각각 입력하세요.
0.1 0.9
Temperature      Xs          Xl          f1          f2          try
214     0.010371    0.002571    1.82E-012   -2.05E-012  20
1219    0.030852    0.007577    0.00E+000   -3.78E-013  5
1224    0.049311    0.012732    0.00E+000   -1.08E-012  5
1229    0.068220    0.017972    -1.82E-012  -4.55E-013  5
1234    0.086769    0.023318    -1.82E-012  -9.09E-013  5
1239    0.104969    0.028771    0.00E+000   3.41E-013   5
```

```
Matrix의 크기를 설정하시요:2
고상과 액상의 분율을 각각 입력하세요.
0.1 0.9
Temperature      Xs          Xl          f1          f2          try
1400    0.551403    0.264718    -3.64E-012  1.82E-012   7
1405    0.562057    0.273778    -3.64E-011  0.00E+000   4
1410    0.572532    0.283400    -3.46E-011  0.00E+000   4
1415    0.582884    0.292923    -2.82E-011  2.73E-012   4
1420    0.593098    0.302569    -2.64E-011  9.09E-013   4
1425    0.603178    0.312337    -2.46E-011  3.64E-012   4
1430    0.613127    0.322228    -2.27E-011  3.64E-012   4
```

초기 온도 시작 값에 따라 시도 횟수의 차이를 보임

Result



초기 고상과 액상 분율의 차이가 작아질수록 계산속도가 빠른 경향,
but 어느 일정 범위 안으로 들어가면 오히려 계산이 느려짐

Result

```
Matrix의 크기를 설정하시요:2
고상과 액상의 분율을 각각 입력하세요.
-5 8
Temperature      Xs          Xl          f1              f2              try
1214     0.010371        0.002571        -7.28E-012      2.40E-012       15
1219     0.030032        0.007599        0.00E+000       -3.98E-013      5
1224     0.049311        0.012732        0.00E+000       -1.08E-012      5
1229     0.068220        0.017972        -1.82E-012      -4.55E-013      5
1234     0.086769        0.023318        -1.82E-012      -9.09E-013      5
1239     0.104969        0.028771        0.00E+000       3.41E-013       5
```

```
Matrix의 크기를 설정하시요:2
고상과 액상의 분율을 각각 입력하세요.
0.4 0.4
Temperature      Xs          Xl          f1              f2              try
1214     0.010371        0.002571        1.82E-012       -2.05E-012      11
1219     0.030032        0.007599        1.82E-012       -3.98E-013      5
1224     0.049311        0.012732        0.00E+000       -1.08E-012      5
1229     0.068220        0.017972        3.64E-012       -4.55E-013      5
1234     0.086769        0.023318        -1.82E-012      1.25E-012       5
1239     0.104969        0.028721        1.82E-012       3.41E-013       5
```

초기 값이 범위를 벗어나거나 역행렬이 존재하지 않는 값이어도 예외 처리를 통해 올바른 값 출력

Conclusion

- Non-linear equation system을 Newton's method를 통해 풀 수 있었고, 이를 통해 Binary phase diagram 구현 또한 거의 정확히 구할 수 있다.
- 초기값 설정이 첫 계산 속도에 영향을 끼침을 알 수 있었다.
- 온도를 고정시킨 상태에서 Newton's method를 진행하여 변수를 바꿔주어야 한다.