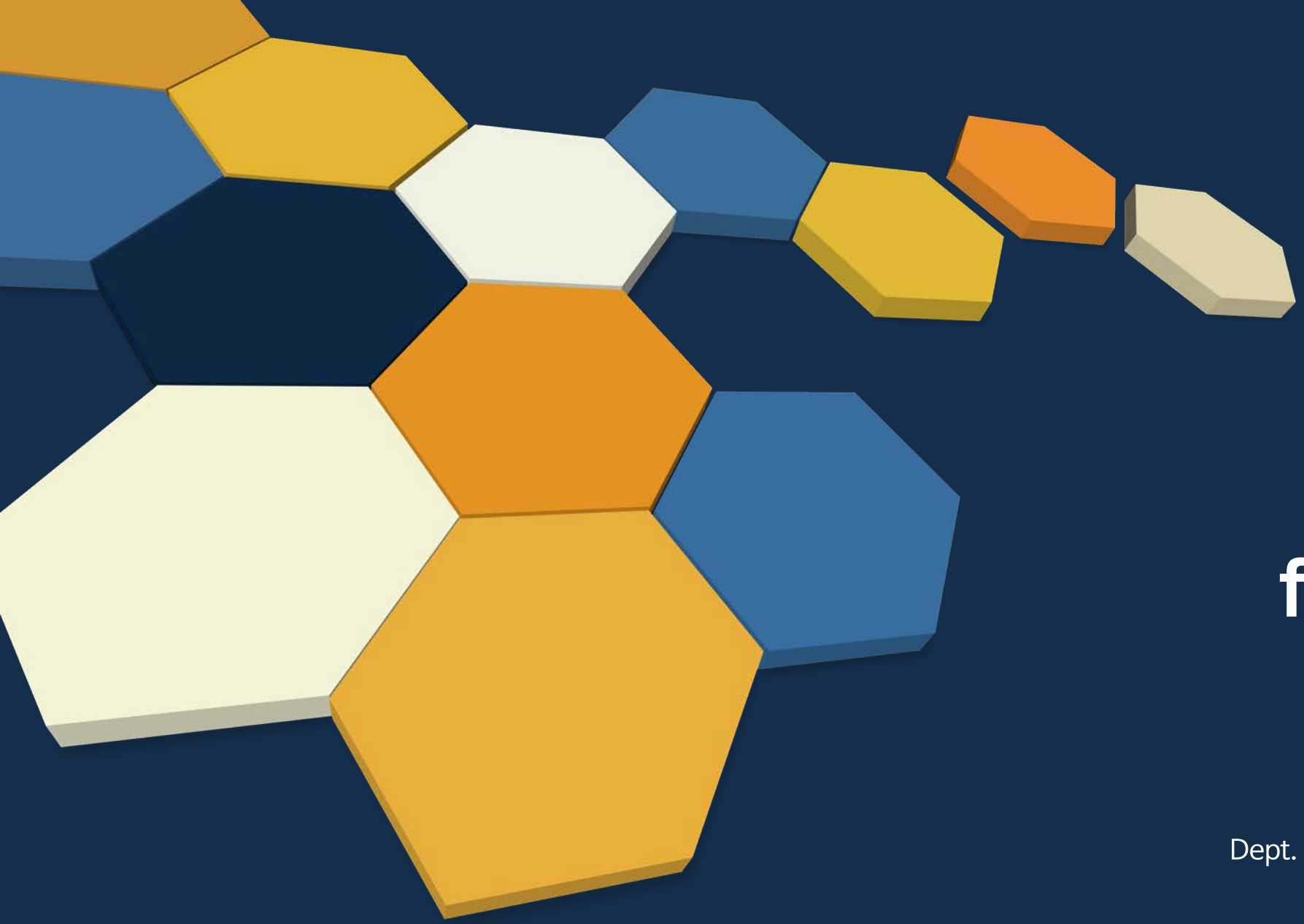

Numerical Analysis for Materials

Midterm

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Thermodynamics(L Parameter, Chemical Potential)

$\Delta G_{ex}=X_{Tk}(1-X_{Tk})\{L_0+(1-2X_{Tk})\ L_1\}$ $\Delta G_{ex}=X_{Tk}(1-X_{Tk})\{L_0+(1-2X_{Tk})\ L_1\}=X_{Tk}(1-X_{Tk})\ \Omega$

T-dependent L parameters

- Liquid(1500K): $\Omega = (12496.767886 - 7.996993T) + (1 - 2X_{Tk})(2397.462734 + 5.616841 \times 10^{-3}T)$
- FCC(600K): $\Omega = (8997.620500 - 4.994669T) + (1 - 2X_{Tk})(3599.988962 - 6.622663 \times 10^{-3}T)$
- BCC(600K): $\Omega = (7000.661574 - 4.057468T)$

$$\mu_{Tk}{}^{L} = 6000 - 10T + RTlnx_{Tk} + (1 - x_{Tk})^2 \{L_0{}^{L} + (1 - 4x_{Tk})L_1{}^{L}\}$$

$$\mu_{Tk}{}^{Fcc} = 7500 + RTlnx_{Tk} + (1 - x_{Tk})^2 \{L_0{}^{Fcc} + (1 - 4x_{Tk})L_1{}^{Fcc}\}$$

$$\mu_{Tk}{}^{Bcc} = RTlnx_{Tk} + (1 - x_{Tk})^2 \{L_0{}^{Bcc} + (1 - 4x_{Tk})L_1{}^{Bcc}\}$$

$$\mu_{Ps}{}^{L} = 12000 - 10T + RTln(1 - x_{Tk}) + (x_{Tk})^2 \{L_0{}^{L} + (3 - 4x_{Tk})L_1{}^{L}\}$$

$$\mu_{Ps}{}^{Fcc} = RTln(1 - x_{Tk}) + (x_{Tk})^2 \{L_0{}^{Fcc} + (3 - 4x_{Tk})L_1{}^{Fcc}\}$$

$$\mu_{Ps}{}^{Bcc} = 4000 + RTln(1 - x_{Tk}) + (x_{Tk})^2 \{L_0{}^{Bcc} + (3 - 4x_{Tk}) * L_1{}^{Bcc}\}$$

Strategy

1. Raw Phase Diagram

Liquid – FCC $\mu_{Ps}^{L} = \mu_{Ps}^{F}$ $\mu_{Tk}^{L} = \mu_{Tk}^{F}$

Liquid – BCC $\mu_{Ps}^{L} = \mu_{Ps}^{B}$ $\mu_{Tk}^{L} = \mu_{Tk}^{B}$

FCC – BCC $\mu_{Ps}^{F} = \mu_{Ps}^{B}$ $\mu_{Tk}^{F} = \mu_{Tk}^{B}$

Jacobian matrix $J(X)$

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

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

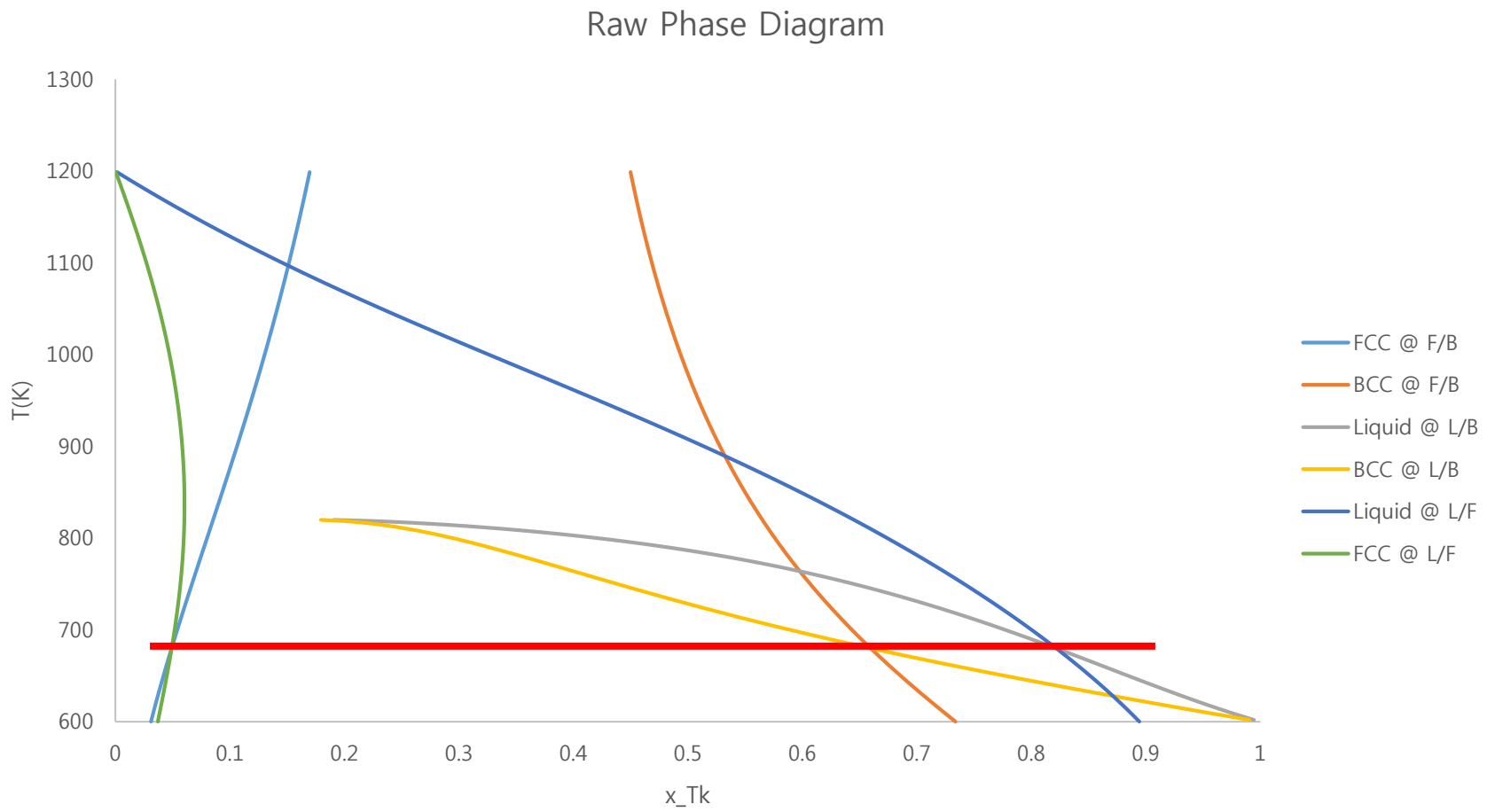
2. Peritectic Condition

$$\mu_{Ps}^{Liq} = \mu_{Ps}^{FCC} = \mu_{Ps}^{BCC}$$
$$\mu_{Ks}^{Liq} = \mu_{Ks}^{FCC} = \mu_{Ks}^{BCC}$$

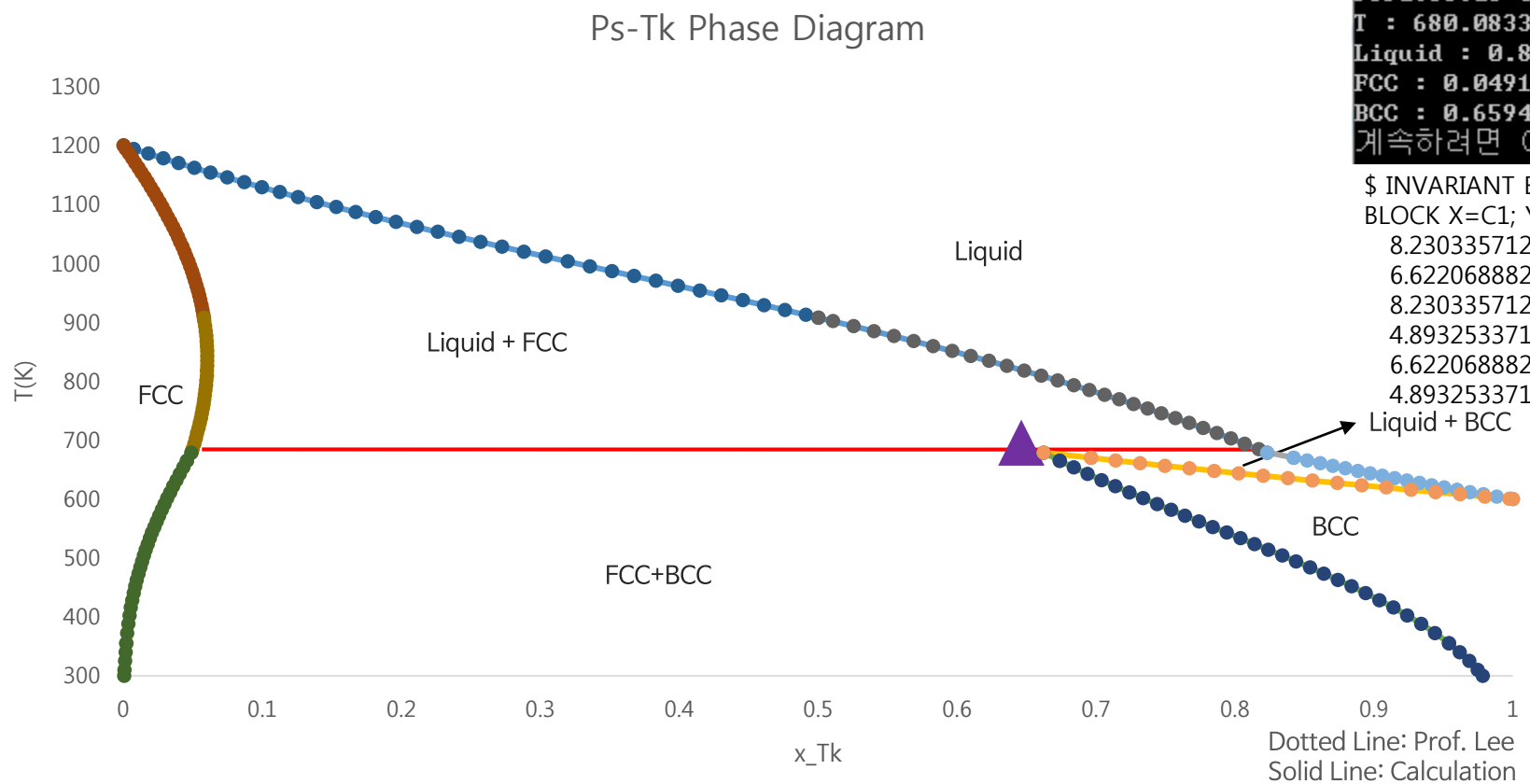
$$f_1 = \mu_{Ps}^{Liq} - \mu_{Ps}^{FCC} = 0$$
$$f_2 = \mu_{Ps}^{Liq} - \mu_{Ps}^{BCC} = 0$$
$$f_3 = \mu_{Tk}^{Liq} - \mu_{Tk}^{FCC} = 0$$
$$f_4 = \mu_{Tk}^{Liq} - \mu_{Tk}^{BCC} = 0$$

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial T} & \frac{\partial f_1}{\partial X_{Ks}^{Liq}} & \frac{\partial f_1}{\partial X_{Ks}^{FCC}} & \frac{\partial f_1}{\partial X_{Ks}^{BCC}} \\ \frac{\partial f_2}{\partial T} & \frac{\partial f_2}{\partial X_{Ks}^{Liq}} & \frac{\partial f_2}{\partial X_{Ks}^{FCC}} & \frac{\partial f_2}{\partial X_{Ks}^{BCC}} \\ \frac{\partial f_3}{\partial T} & \frac{\partial f_3}{\partial X_{Ks}^{Liq}} & \frac{\partial f_3}{\partial X_{Ks}^{FCC}} & \frac{\partial f_3}{\partial X_{Ks}^{BCC}} \\ \frac{\partial f_4}{\partial T} & \frac{\partial f_4}{\partial X_{Ks}^{Liq}} & \frac{\partial f_4}{\partial X_{Ks}^{FCC}} & \frac{\partial f_4}{\partial X_{Ks}^{BCC}} \end{bmatrix}$$

Raw Phase Diagram



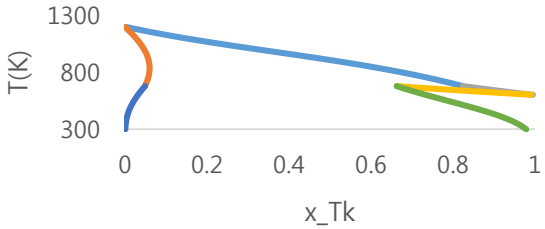
Peritectic Condition




```
Peritectic Condition
T : 680.083304
Liquid : 0.821584
FCC : 0.049136
BCC : 0.659490
계속하려면 아무 키나 누르십시오 . . .
```

```
$ INVARIANT EQUILIBRIUM
BLOCK X=C1; Y=C2;        GOC=C3,WAD;
   8.2303357124E-01   6.7871173096E+02   M
   6.6220688820E-01   6.7871173096E+02
   8.2303357124E-01   6.7871173096E+02   M
   4.8932533711E-02   6.7871173096E+02
   6.6220688820E-01   6.7871173096E+02   M
   4.8932533711E-02   6.7871173096E+02
```

Dotted Line: Prof. Lee
Solid Line: Calculation
Triangle: Peritectic Point



Investigation & Conclusion

Answers

1. Regression으로 구한 L parameter를 이용해 phase 별로 적합한 model을 적용, chemical potential을 계산할 수 있다.
2. Newton's Method를 이용하여 chemical potential로부터 raw phase diagram을 구성하는 data를 얻고 plot할 수 있다.
3. Newton's Method를 이용하여 Peritectic point(T, x_Tk)를 찾고 phase diagram을 완성할 수 있다.
4. Relative Error(T) = $\frac{680.083304K - 678.711731K}{678.711731K} \times 100(\%) = 0.202085\%$
5. Peritectic point를 찾을 때에는 초기 분율과 온도 설정이 매우 중요하다.