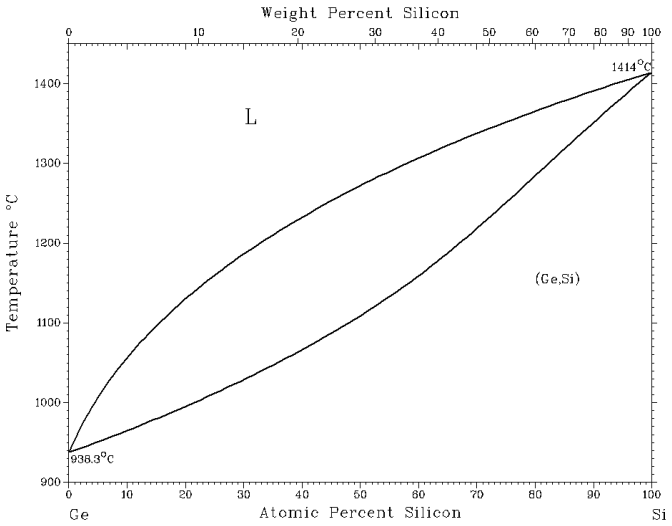
4. 비선형 연립 방정식

1. 사용 예

- Multicomponent phase equilibria



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

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

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

- General form of a system of nonlinear equations

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

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

$$\cdots \quad \cdots$$

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

$\Rightarrow$ F(X) = 0

2. Newton's Method

- Newton's method for single nonlinear equation

$$f(x) = 0$$

$$p_k = p_{k-1} - \frac{f(p_{k-1})}{f'(p_{k-1})}$$

- For nonlinear equation system, F(X) = 0

  Change in f_i due to the change in x_j : $\frac{\partial f_i}{\partial x_j}$

  Jacobian matrix J(X)

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

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

3. Quasi-Newton Method

Decrease the amount of computation

4. Steepest Descent method

Converge at any starting point

개인 과제물

- 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.