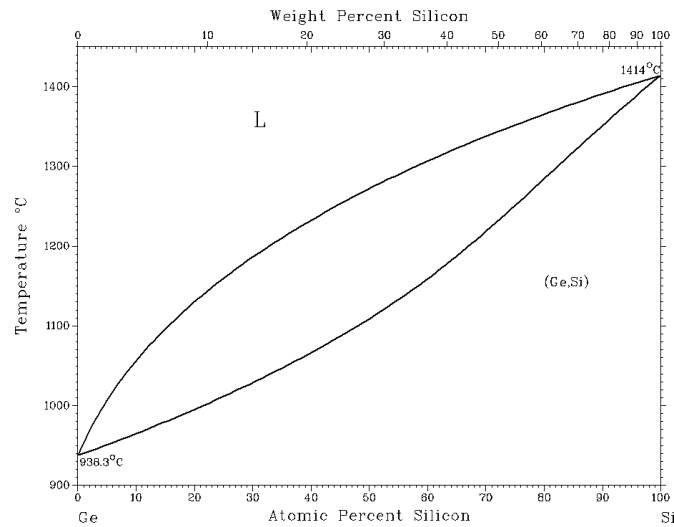


## 4. 비선형 연립 방정식

### Non-Linear Equation System

#### 1. 사용 예

- Multicomponent phase equilibria



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

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

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

- General form of a system of nonlinear equations

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

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

... ..

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

$$\Rightarrow F(X) = 0$$

## 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,  $F(\mathbf{X}) = 0$

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

Jacobian matrix  $J(\mathbf{X})$

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

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

## 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.

Calculate the Ge-Si phase diagram using the Gibbs energy values.

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

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

고상 (diamond 구조), 액상 모두에 대해 ideal solution 을 가정하시오.  
Assume ideal solution for both solid and liquid phases.

