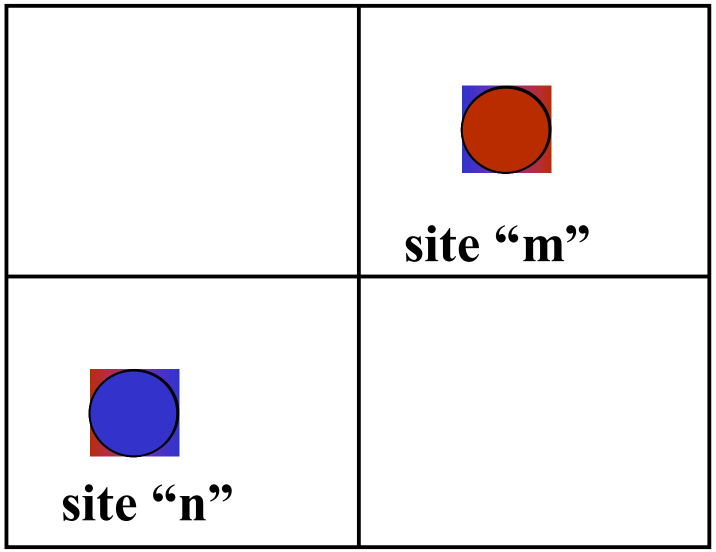
Correlation Length

- Chemical order & disorder in metallic alloy
- Calculation of Bragg and Diffuse Scattering
- Correlation length in the Mean-Field approach

Correlation Length

- Chemical order & disorder in metallic alloy A_xB_{1-x}



- Probability of having at any site:

  atom A : $p(A) = x$

  atom B : $p(B) = 1-x$

- Probability of having an atom B at site "m" knowing atom A at site "n": $P_B(m)$

- Probability of having an atom A at site "m" knowing atom B at site "n": $P_A(m)$

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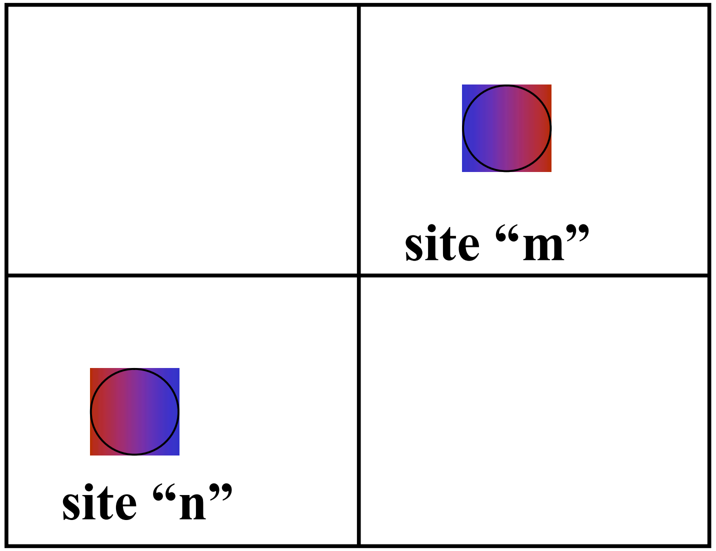


- **Pair probabilities**:
  - ✓ pair AB : $x \cdot P_B(m)$
  - ✓ pair AA : $x \cdot (1 - P_B(m))$
  - ✓ pair BA : $(1-x) \cdot P_A(m)$
  - ✓ pair BB : $(1-x) \cdot (1 - P_A(m))$

Correlation Length

- Scattering in metallic alloy A_xB_{1-x}
  - **Scattering intensity**:

$$I \propto \langle FF^* \rangle = \left\langle \sum_{nm} f_n f_m^* e^{-i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} \right\rangle = \sum_{nm} \langle f_n f_m^* \rangle e^{-i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)}$$

add and subtract $\langle f_n \rangle \langle f_m^* \rangle e^{-i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)}$

$$I \propto \sum_{n,m} \left|\langle f_n \rangle\right|^2 e^{-i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} + \sum_{n,m} \left(\langle f_n f_m^* \rangle - \left|\langle f_n \rangle\right|^2 \right) e^{-i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)}$$

$$I \propto N \times \left\{ \sum_{m} \left|\langle f_o \rangle\right|^2 e^{-i\vec{Q}\cdot(\vec{r}_o - \vec{r}_m)} + \sum_{m} \left(\langle f_o f_m^* \rangle - \left|\langle f_o \rangle\right|^2 \right) e^{-i\vec{Q}\cdot(\vec{r}_o - \vec{r}_m)} \right\}$$

Bragg peaks

$$I_{Bragg}(\vec{Q}) \propto \left|\langle f_n \rangle\right|^2 \cdot \sum_{\vec{G}} \delta(\vec{Q} - \vec{G})$$

Reciprocal lattice vectors

"Diffuse scattering"

$$I_{diff} \propto \sum_{m} \left(\langle f_o f_m^* \rangle - \left|\langle f_o \rangle\right|^2 \right) e^{-i\vec{Q}\cdot(\vec{r}_o - \vec{r}_m)}$$

Correlation Length

- Scattering in metallic alloy $A_x B_{1-x}$
  - **Bragg Scattering** : $I_{Bragg}(\vec{Q}) \propto \left|\langle f_n \rangle\right|^2 \cdot \sum_{\vec{G}} \delta(\vec{Q} - \vec{G})$

$$I_{Bragg}(\vec{G}) \propto \left|\langle f_n \rangle\right|^2 = \left| x \cdot f_A + (1-x) \cdot f_B \right|^2$$

$$I_{Bragg}(\vec{G}) \propto \left|\langle f_n \rangle\right|^2 = x^2 \cdot f_A f_A^* + x(1-x) \cdot (f_A f_B^* + f_B f_A^*) + (1-x)^2 \cdot f_B f_B^*$$

Spherical atoms: f_A *and* f_B *are real.*

$$I_{Bragg}(\vec{G}) \propto \left|\langle f_n \rangle\right|^2 = x^2 \cdot f_A^2 + 2x(1-x) \cdot f_A f_B + (1-x)^2 \cdot f_B^2$$

Case $x = ½ = (1-x)$: $I_{Bragg} \propto \left(\frac{f_A + f_B}{2} \right)^2$

Correlation Length

- Scattering in metallic alloy $A_x B_{1-x}$

  - Diffuse Scattering :
  $$I_{diff} \propto \sum_m \left(\langle f_o f_m^* \rangle - |\langle f_o \rangle|^2 \right) e^{-i\vec{Q}\cdot(\vec{r}_o - \vec{r}_m)}$$

$$I_{diff} \propto \langle f_o f_o^* \rangle - |\langle f_o \rangle|^2 + \sum_{m \neq o} \left(\langle f_o f_m^* \rangle - |\langle f_o \rangle|^2 \right) e^{-i\vec{Q}\cdot(\vec{r}_o - \vec{r}_m)}$$

sole non zero term
when no correlation

correlation effect

$$\sum_{m \neq 0} \left(\langle f_o f_m^* \rangle - |\langle f_n \rangle|^2 \right) e^{i\vec{Q}\cdot\vec{r}_m}$$

Correlation Length

- Scattering in metallic alloy $A_x B_{1-x}$

  - **Diffuse Scattering** :

$$I_{diff} \propto \sum_m \left(\left\langle f_o f_m^* \right\rangle - \left| \left\langle f_o \right\rangle \right|^2 \right) e^{-i\vec{Q}\cdot(\vec{r}_o - \vec{r}_m)}$$

$$\begin{cases} f_A, f_B \quad \textit{real} \\ x \cdot P_B(m) = (1-x) \cdot P_A(m) \end{cases}$$

$$A = \left\langle f_o f_m \right\rangle - \left\langle f \right\rangle^2$$

$$A = x(1-x) \cdot (f_A - f_B)^2 \cdot \left(1 - \frac{P_A(m)}{x} \right)$$

$$I_{diff}^o = x\,(1-x) \cdot (f_A - f_B)^2$$

$$I_{diff} = I_{diff}^o \cdot \left(1 + \sum_{m \neq 0} \left(1 - \frac{P_A(m)}{x} \right) \cdot e^{i\vec{Q}\cdot\vec{r}_m} \right)$$

Correlation Length

- Scattering in metallic alloy A_xB_{1-x}

  - **Diffuse Scattering** :

$$I_{diff} = I^{o}_{diff} \cdot \left(1 + \sum_{m \neq 0} \left(1 - \frac{P_A(m)}{x} \right) \cdot e^{i\vec{Q}\cdot\vec{r}_m} \right)$$

Case $P_A(m) = x$, *totally disordered alloy :* $I_{diff} = I^{o}_{diff} \propto (f_A - f_B)^2$

Case $P_A(m) > x$, *AB pairs are favored → cell doubling ≡ ordered alloy*

Case $P_A(m) < x$, *AA & BB pairs are favored → phase separation (A & B)*

Correlation Length

- Correlation length in the mean-field approach

  - 1D illustration

$$\left|\begin{array}{l} m \to \infty: \quad P_A(m) \to x \\ \\ m \to 0: \quad P_A(m) \to P_A(0) = 0 \end{array}\right.$$

$$\left|\begin{array}{l} 1 - \dfrac{P_A(m)}{x} \to 0 \\ \\ 1 - \dfrac{P_A(m)}{x} \to 1 \end{array}\right.$$

$$\left(1 - \frac{P_A(m)}{x}\right) \approx e^{-|m|a/\xi}$$

Correlation Length

- Correlation length in the mean-field approach

- 1D illustration

$$I_{diff} = I^{o}_{diff} \cdot \left(1 + \sum_{m \neq 0} e^{-ma/\xi} \cdot e^{2i\pi hm}\right)$$

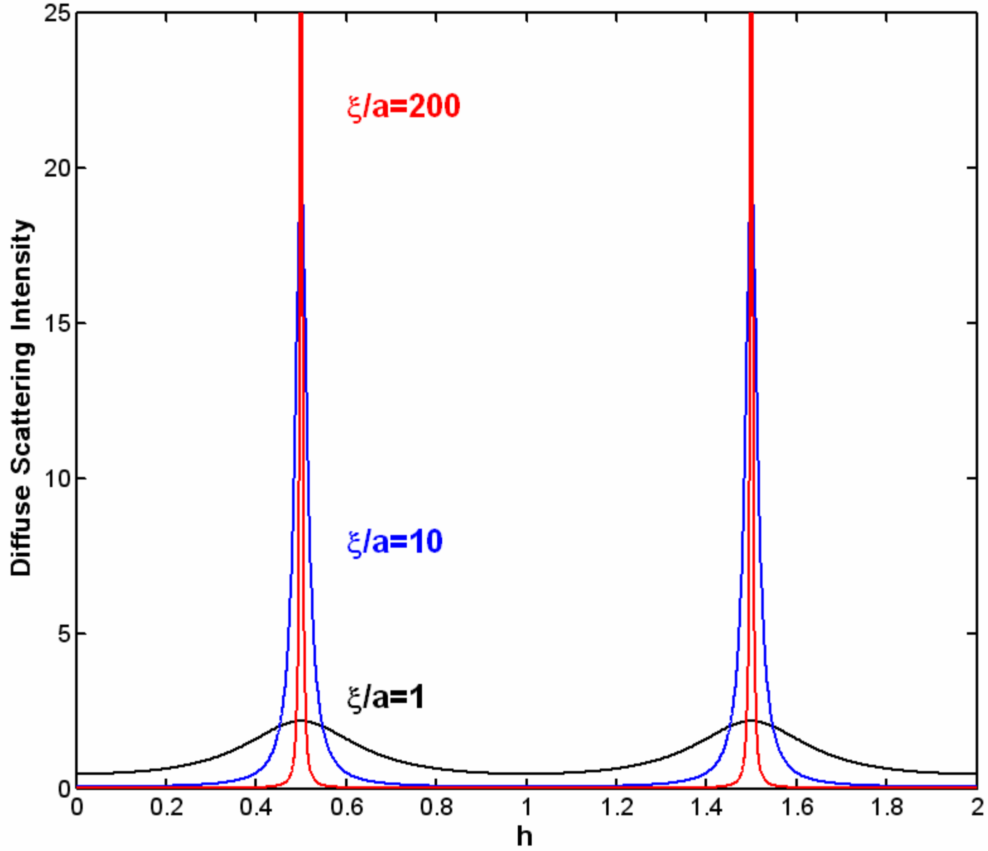
$$I_{diff} = I^{o}_{diff} \cdot \left(1 + 2\sum_{m>0} e^{-ma/\xi} \cdot \cos(2\pi hm)\right) = I^{o}_{diff} \cdot \left(1 + 2\sum_{1}^{N \to \infty} e^{-\alpha m}\right)$$

$$\alpha = a/\xi - 2i\pi h$$

$$I_{diff} = I^{o}_{diff} \cdot \left(1 - \frac{2}{1 - e^{+\alpha}}\right) = I^{o}_{diff} \cdot \left(1 - \frac{e^{-a/\xi} + \cos(2\pi h)}{ch(a/\xi) + \cos(2\pi h)}\right)$$

Correlation Length

- Correlation length in the mean-field approach
  - **1D illustration** $$I_{diff}(h) = I^{o}_{diff} \cdot \left(1 - \frac{e^{-a/\xi} + \cos(2\pi h)}{ch(a/\xi) + \cos(2\pi h)}\right)$$



$\xi \to 0$: $I_{diff} \to I_{Bragg}$

cell doubling