Alloy Disorder Scattering

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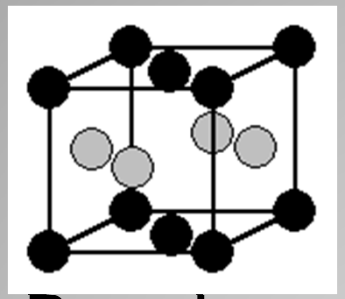
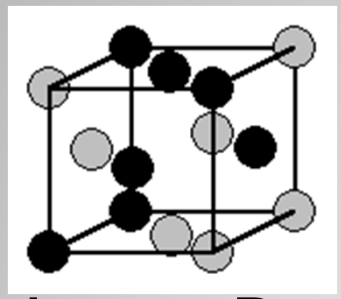
Alloys

- Ordered



- Random



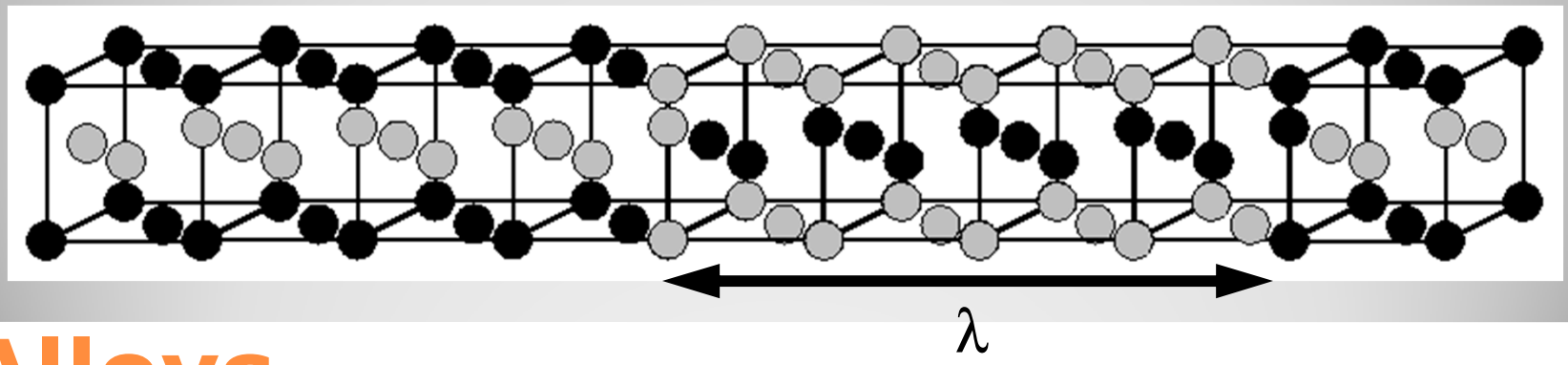
- Long Range Ordered

Example: CuAu

$T < 385^\circ$ C: CuAu-I ($L1_0$)

$T > 410^\circ$ C: Random

$385^\circ < T < 410^\circ$ CuAu-II



Malis and Ludwig PRB 60,14675 (1999).

Virtual Crystal Approximation

- VCA originated from tight binding methods
  - Replace atoms with effective atoms
  - Choose parameterization to return alloy properties
  - Works OK for some properties, not so well for others
- Coherent Potential Approximation (CPA)
  - Coherent Potential Approximation improvement over VCA replace disordered alloy medium with ordered effective medium. Determine effective medium self-consistently using the condition that the extra scattering from a cluster of atoms embedded in the medium for all possible positions of the cluster, be zero.

Virtual Crystal Approximation

- Many methods for averaging of potentials
  - Depend upon psuedopotential
- Two popular approaches general pseudopotentials
  - Modify the pseudpotentials
    - Ramer and Rappe 2000
  - Modify the DFT software
    - Bellaiche and Vanderbilt 2000

- Ramer and Rappe method
  - Average of all-electron potential and core charge density
  - Solve for eigenfunction that return eigenvalues
  - Any pseudopotential generator can be used with the

$$\varepsilon_l^{AVE} = (1-x)\varepsilon_{nl}^{A} + (x)\varepsilon_{n'l}^{B}$$

- The mechanics necessary for this appear to be available in the Opium pseudopotential package

Virtual Crystal Approximation

Virtual Crystal Approximation

- Averaging method works well for some situations but not great for others
  - Good for properties that are averaged over entire crystal
  - Little understanding local interactions
  - Cannot explain long range ordering

Binomial Distribution:

Let x be discrete random variable with two possible values: x=0 and x=1 that occur with probabilities p and q=1-p.

In our case that means that the unit cell will either have the cation A or the cation B

Now suppose that

$$Y = \sum_{i=1}^{n} x_i, \quad x_i = 1,2,\ldots N$$

are statistically independent and uniformly distributed random variables.

We want to find the pdf of Y. Since each of x_i can be either 0 or 1, the range of Y is from 0 to n. In our case this would mean characterizing the crystal and N would be the number of unit cells.

The probability of Y=0 is simply the probability that all x_i are zero. Then:

$$P(Y=0) = p^n = \binom{n}{0} p^n (1-p)^0 = \binom{n}{0} p^n q^0$$

The probability that Y=1 means that one of the xi's is 1 and the rest are zero. Therefore

$$P(Y=1) = np^{n-1}(1-p) = \binom{n}{1} p^{n-1} q$$

The probability of Y=k is simply:

$$P(Y=k)=\binom{n}{k}p^{n-k}q^{k}$$

The pdf is then simply given by:

$$P(y)=\sum_{k=0}^{n}\binom{n}{k}p^{n-k}q^{k}\delta(y-k)$$

The mean-square deviation is then given by:

$$E(Y^2)-[E(Y)]^2=np(1-p)$$

In our case:

$$\sigma / N_c=\left|V_A-V_B\right|\left[\frac{p(1-p)}{N_c}\right]^{1/2}$$

Matrix Element for Alloy Disorder Scattering

The matrix element for alloy disorder scattering is then given by:

$$M(k,k') = \frac{2\pi}{\hbar}\left|V_A - V_B\right|^2 \frac{x(1-x)}{N_c}\delta(k'-k \pm q)$$

The total scattering rate out of state k is given by:

$$\Gamma(k) = \frac{2\pi}{\hbar}\left|V_A - V_B\right|^2 x(1-x)\frac{1}{2}g_c(E)$$