Exchange interactions of ordered and disordered FeCo

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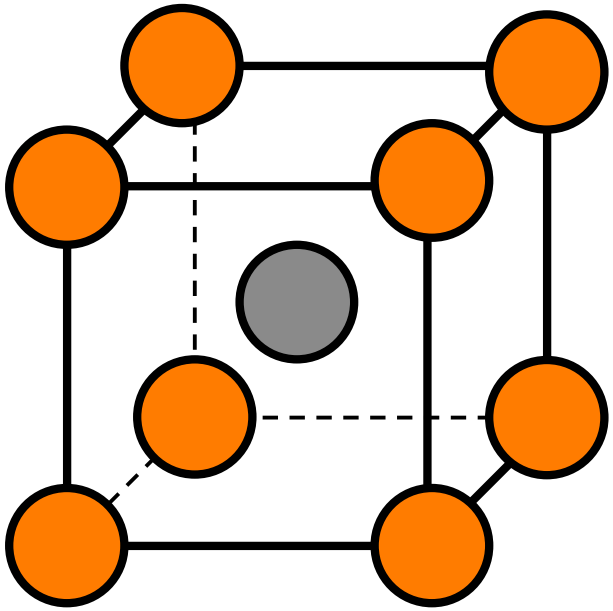
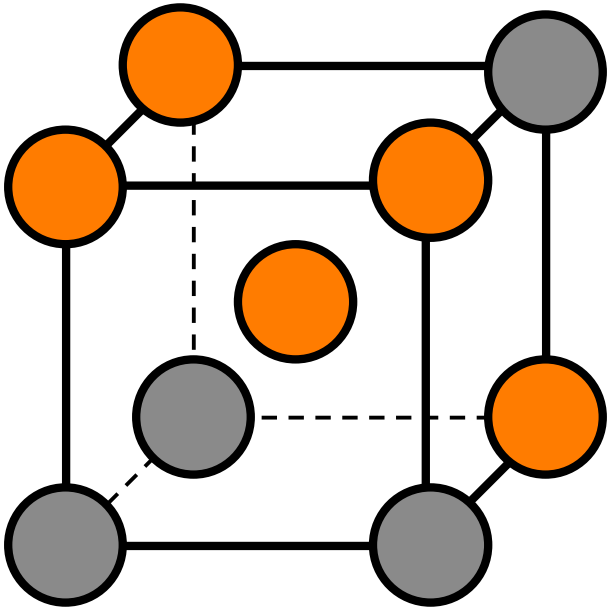
FeCo



B2

T < 1000 K



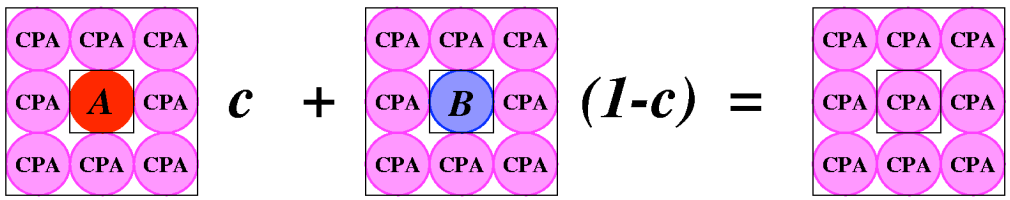
BCC

1000 K < T < 1250 K

Large Curie temperature (~1500K) predicted for BCC FeCo (MacLaren et al. 1999)

The Method in General: LKKR-CPA

- **Basic Framework: *Local Spin Density Approximation* (LDA) to density functional theory.**
- **Solving Kohn-Sham Equations: Layer-KKR *multiple scattering* technique to find *Green's function* of the ground state.**
- **Treat disorder: Single site *Coherent potential Approximation* (CPA) to treat substitutional disorder**



Replace the alloy $A_cB_{(1-c)}$ by a periodic medium chosen in such a way that when an atom A or B is embedded on a single site one recovers on average the Green's function of the medium.

The method is adequate to predict ground state magnetic properties of substitutionally disordered alloys

Calculated Moments

	Ferromagnetic	*Paramagnetic*
BCC	***Fe*** = *2.66* μ_B ***Co*** = *1.74* μ_B	***Fe*** = *2.65* μ_B ***Co*** = *0* μ_B
B2	***Fe*** = *2.50* μ_B ***Co*** = *1.77* μ_B	

Agrees with experiments and previous calculations

FeCo (previously: Mac Laren et al. JAP 99)

- **LKKR-CPA, map onto Heisenberg model**

$$\delta E_{i\alpha,j\beta} = \frac{1}{\pi}\int^{\varepsilon_F} d\varepsilon \,\mathrm{Im}\left\{\mathrm{Tr}\left(\Delta_{i\alpha}\tau_c^{ij}\Delta_{j\beta}\tau_c^{ji}\right)\right\}$$

(Liechtenstein et al. JMMM 87)

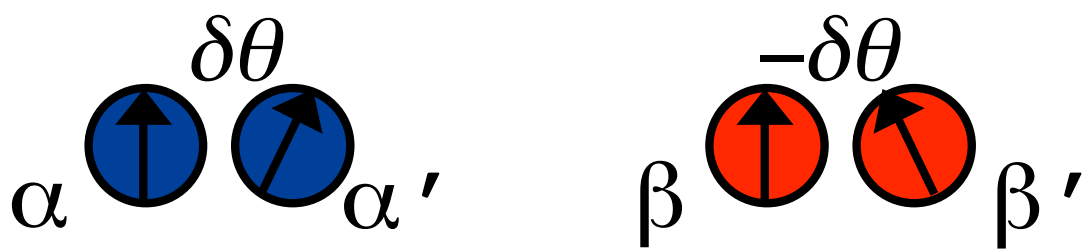
- **Estimate Curie temperature in mean field**

$$T_c \sim 1500\mathrm{K}$$

- **Higher than Co (T_c=1300K)**
  - **if BCC FeCo was stable to high temperature**
  - **Formula used not quite right for random alloys**

Interaction energy of two impurities

Impurity: Chemical and magnetic perturbation



$$\Delta E_{i\alpha,j\beta} = \left(\delta E_{i\alpha',j\beta'} - \delta E_{i\alpha,j\beta}\right) - \left(\delta E_{i\alpha',j\beta} - \delta E_{i\alpha,j\beta}\right) - \left(\delta E_{i\alpha,j\beta'} - \delta E_{i\alpha,j\beta}\right)$$

New formulation

After a lengthy derivation …
to second order in $\delta\theta$

$$\delta E_{i\alpha,j\beta} = \frac{1}{\pi}\int^{\varepsilon_F} d\varepsilon \,\mathrm{Im}\left\{\mathrm{Tr}\left(\Delta_{i\alpha}\boldsymbol{\tau}_{c\uparrow}^{i\alpha,j\beta}\Delta_{j\beta}\boldsymbol{\tau}_{c\downarrow}^{j\beta,i\alpha} + \Delta_{i\alpha}\boldsymbol{\tau}_{c\downarrow}^{i\alpha,j\beta}\Delta_{j\beta}\boldsymbol{\tau}_{c\uparrow}^{j\beta,i\alpha}\right)\right\}$$

$$\hat{\boldsymbol{\tau}}_c^{i\alpha,j\beta} = \left[1 - \hat{\boldsymbol{\tau}}_c^{i}\left(\hat{t}_{i,c}^{-1} - \hat{t}_{i,\alpha}^{-1}\right)\right]^{-1}\hat{\boldsymbol{\tau}}_c^{ij}\left[1 - \hat{\boldsymbol{\tau}}_c^{j}\left(\hat{t}_{j,c}^{-1} - \hat{t}_{j,\beta}^{-1}\right)\right]^{-1}$$

J_{ij} Ferromagnetic Order

	BCC	B2	
		Fe	Co
(1/2, 1/2, 1/2)	*26.17*	*27.42*	*27.42*
(0, 0, 1)	*1.46*	*0.21*	*0.76*
(0, 1, 1)	*1.09*	*1.02*	*0.67*
(1/2, 1/2, 3/2)	*0.93*	*1.24*	*1.24*
(1, 1, 1)	*-1.86*	*-2.23*	*-0.43*
T_c	1800 K	1890 K	

Conclusions

- Calculate exchange interactions for random alloys within CPA
- High Curie temperature for BCC FeCo still holds (larger than Co)
- Stabilizing BCC FeCo phase could lead to record Curie Temperature

J_{ij} Paramagnetic Order

	B2	
	Fe	Co
(1/2, 1/2, 1/2)	*0*	*0*
(0, 0, 1)	*-7.69*	*0*
(0, 1, 1)	*2.1*	*0*
(1/2, 1/2, 3/2)	*0*	*0*
(1, 1, 1)	*-5.86*	*0*

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