11th International Conference on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

Phase transition of the Spin- 1/2 Ising Ferromagnetic Thin Films

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Abstract – The phase transition and magnetization in the Ising ferromagnetic thin films were studied by Mont Carlo simulation. The Curie temperature was calculated as a function of the exchange interaction and the effective nearest neighbour. Results showed that the Curie temperature decreased by increasing the vacancies in the ferromagnetic thin film.

A three dimensional ferromagnetic thin film was considered as atomic monolayers with localized spins-1/2 in a simple cubic (SC) structure. The Hamiltonian of this model is given by:

$$E = -2\sum_{i=1}^{N_X}\sum_{j=1}^{N_Y}\sum_{k=1}^{L}\varepsilon_{i,j,k}S_{i,j,k}[J_0\varepsilon_{i,j+1,k}S_{i,j+1,k} + J_0\varepsilon_{i+1,j,k}S_{i+1,j,k} + J_1\varepsilon_{i,j,k+1}S_{i,j,k+1}]. \quad (1)$$

Where the summation is carried out only over the nearest neighbour pairs of spins, N_x and N_y are number of atoms in each monolayer, L is number of monolayers and S is spin variable. J_0 *and* J_1 denote the nearest neighbour exchange interaction in the monolayer and between the monolayers respectively and ε is occupation number. If $\varepsilon = 1$ the atomic site will occupied with one atom and otherwise with zero.
By the mean field theory for spins-1/2 the Curie temperature obtained as below equation:

$$T_C = \frac{J_o z_o^{eff}}{k_B} + \frac{2J_1 z_1^{eff}}{k_B} \quad (2)$$

Where z_0^{eff} and z_1^{eff} are effective nearest neighbour in the monolayer and between the monolayers respectively:

$$z_o^{eff} = 2\frac{\sum_{i=1}^{N_X}\sum_{j=1}^{N_Y}\sum_{k=1}^{L}\left[\varepsilon_{i,j+1,k} + \varepsilon_{i+1,j,k}\right]}{N_x \times N_y \times L}, \qquad z_1^{eff} = \frac{\sum_{i=1}^{N_X}\sum_{j=1}^{N_Y}\sum_{k=1}^{L}\varepsilon_{i,j,k+1}}{N_x \times N_y \times L}. \quad (3)$$

Systems with N_x=N_y=50, 100, 1000 and L=1, 2, 5 were studied for several vacancies. Mont Carlo method were used to investigate the Curie temperature in iron thin films**.** Results showed that the Curie temperature decreased by increasing the vacancies in structure of thin film.

Table 1: The effective nearest neighbour for different structures without vacancy.

	Fcc(111)	Fcc(001)	Bcc(111)	Sc
z_0^{eff}	6	4	6	4
z_1^{eff}	3	4	1	1

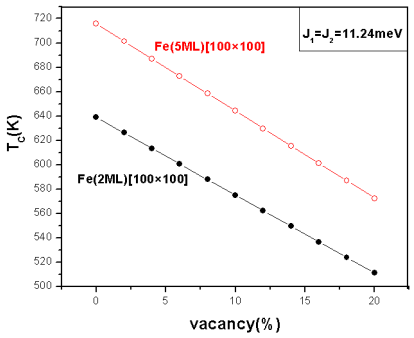

Figure 1: The dependence of the Curie temperature as a function of the vacancies in Fe (2ML) and Fe (5ML) with 100×100 atoms.

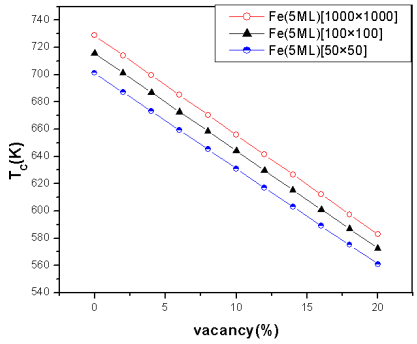

Figure 2: The effect of finite size on the Curie temperature in Fe (5ML) as a function of the vacancies.