

CONCENTRATION DEPENDENCE OF CURIE TEMPERATURE OF TWO-SORT AMORPHOUS MAGNETS

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The Curie temperature of two-component amorphous ferromagnet is found using the expansion of the free energy in powers of order parameter. For the model with liquid-type disorder introduced via hard spheres structure factor the explicit expression for the concentration dependence of ferromagnetic ordering temperature is obtained.

Keywords: amorphous ferromagnets, critical concentration, critical temperature, wave number, Curie temperature, disorder, exchange integral, exchange interactions, ferromagnets disordered, Heisenberg mode, Heisenberg ferromagnet.

1. INTRODUCTION

Theoretical investigations of amorphous magnets mainly were performed during study of thermodynamical and dynamical properties of one-component magnetic systems [1-4]. Nevertheless the great number of experimental investigations of physical properties of amorphous magnets were devoted to the systems, containing two or more kinds of magnetic atoms [1]. So the problem of theoretical study of such systems arises. The present paper is devoted to theoretical determination of Curie temperature of amorphous two-component magnet and to investigation of its concentration dependence.

2. Theory

The system of magnetic atoms of M sorts with N_a atoms of sort a , which are randomly distributed in volume V , is considered. The Heisenberg Hamiltonian [5], generalized on the case of many-component system was considered as the effective Hamiltonian causing magnetic properties.

With the help of functional integration method magnetic part of the amorphous many-component magnet free energy was calculated [6] in the non-interacting spin and structure fluctuations approximation:

$$F_s^{\text{am}} = F_{\text{mol}} + \frac{1}{2} \sum_a \sum_k J_k^{\text{aa}} \frac{N_a}{V} s_a (s_a + 1) + \frac{1}{2\beta} \sum_{k \neq 0} \ln \det (\hat{I} - \hat{\alpha}_k \hat{M}^{(2)}) + \frac{1}{2\beta} \sum_{k \neq 0} \sum_{\omega} \ln \det \hat{\Delta}(k, \omega) - \frac{1}{2\beta} \sum_{a,b} \sum_{k \neq 0} S_{ab}^{\text{am}}(k) \left[\hat{M}^{(1)} (\hat{I} - \hat{\alpha}_k \hat{M}^{(2)})^{-1} \hat{\alpha}_k \hat{M}^{(1)} \right]_{ab} \quad (1)$$

where F_{mol} is the part of free energy in the molecular field approximation [6], J_k^{ab} is the exchange integral Fourier coefficient, s_a is the spin value of atom of sort a , k is the wave vector. $\beta=1/T$ is the reciprocal temperature in energy units. Matrix

$$(\hat{\alpha}_k)_{ab} = \beta J_k^{ab} \sqrt{N_a N_b} / V \quad (2)$$

and

$$\hat{\Delta}(\mathbf{k}, \omega) = \left(\hat{1} - \hat{M}^{(1)} \hat{K}_+(\omega) \hat{\alpha}_k \right)^2 - \left(\hat{1} - \hat{M}^{(1)} \hat{K}_+(\omega) \hat{\alpha}_k \right) \times \hat{M}^{(1)} \hat{K}_-(\omega) \hat{\alpha}_k \left(\hat{1} - \hat{M}^{(1)} \hat{K}_+(\omega) \hat{\alpha}_k \right)^{-1} \hat{M}^{(1)} \hat{K}_-(\omega) \hat{\alpha}_k,$$

$$\hat{K}_{\pm}(\omega) = \frac{\hat{K}(\omega) \pm \hat{K}(-\omega)}{2} \quad (3)$$

where the matrixes

$$M_b^{(l+1)} = \left(\frac{d}{dy_b} \right)^l M_b^{(l)}, l = 0, 1, \dots, y_b = \beta \mu_b \tilde{h}_b, \quad (4)$$

$$M_b^{(1)} = s_b B_b(y_b s_b) \quad (5)$$

$$B_b = \left(1 + \frac{1}{2s_b} \right) \text{cth} \left(1 + \frac{1}{2s_b} \right) y - \frac{1}{2s_b} \text{cth} \frac{y}{2s_b} \quad (6)$$

is the Brillouin function, \tilde{h}_b is the effective magnetic field; the function

$$K_b(\omega) = \beta \mu_b h - (i\beta\omega)^{-1}, \quad (7)$$

where h is the external magnetic field. And $S_{ab}^{am}(k)$ are the partial structure factors.

Putting the free energy (1) into series over the powers of the order parameters $\overline{\langle \varphi_0^{z,a} \rangle_{av}}$ we get the next expression for the free energy in zero external field $h = 0$:

$$F_s^{am} = -\frac{1}{\beta} N a \ln(2s_a + 1) + \frac{3}{2\beta} \sum_{k \neq 0} \ln \det \left(\hat{1} - \hat{M}^{(2)}(0) \hat{\alpha}_k \right) + \frac{1}{2\beta} \sum_{a,b} \left(\hat{\alpha}_0^{1/2} \hat{A} \hat{\alpha}_0^{1/2} \right)_{ab} \overline{\langle \varphi_0^{z,a} \rangle_{av}} \overline{\langle \varphi_0^{z,b} \rangle_{av}} \quad (8)$$

where the matrix $\hat{M}^{(2)}(0)$ is diagonal with the elements (4), when $y_b = 0$

$$M_b^{(2)}(0) = \frac{s_b(s_b + 1)}{3} \quad (9)$$

The elements of matrix \hat{A} are:

$$A_{ab} = \left(\alpha_0^{-1} \right)_{ab} - \delta_{ab} M_a^{(2)}(0) - \frac{1}{\sqrt{N_a N_b}} \sum_{k \neq 0} M_a^{(2)}(0) M_b^{(2)}(0) g_{ab}(k) \times \left[S_{ab}^{am}(k) - \delta_{ab} \right] + \frac{\delta_{ab}}{6\sqrt{N_a N_b}} \sum_{k \neq 0} M_a^{(2)}(0) [g_{ab}(k) - \alpha_{aa}(k)] \times \frac{1}{12\sqrt{N_a N_b}} \sum_{k \neq 0} M_a^{(2)}(0) M_b^{(2)}(0) \alpha_{ab}^2(k), \quad (10)$$

where the matrix of screened exchange interactions is

$$\hat{g}(k) = \hat{\alpha}_k (\hat{1} - \hat{M}^{(2)}(0) \hat{\alpha}_k)^{-1}. \quad (11)$$

From the conditions of stationary of the free energy (8) we come to the system of linear uniform equations for the quantities $\overline{\langle \varphi_0^{z,a} \rangle}_{av}$ (order parameters), in which coefficients are matrix elements $(\hat{\alpha}_0^{1/2} \hat{A} \hat{\alpha}_0^{1/2})_{ab}$. From the condition of non-triviality of solution of this system we come to the condition

$$\det(\hat{\alpha}_0 \hat{A}) = 0 \quad (12)$$

which is the equation for the critical temperature. This equation has M solutions, which determine the temperatures of transition to the different types of magnetic ordering. First of all creates the ordering with the highest temperature of transition. And this temperature- we shall take into account, determining the Curie temperature of amorphous ferromagnet. Our equation (12) for the Curie temperature is nonlinear. Throwing off the integral items we get the equation for the Curie temperature in the molecular field approximation:

$$\det(\hat{1} - \hat{\alpha}_0 \hat{M}^{(2)}(0)) = 0 \quad (13)$$

Let us determine the Curie temperature for two-sort amorphous magnetic system. From the equation (13) we got next solution for the Curie temperature in the m f a:

$$T_c^{*(0)} = \frac{T_c^{(0)}}{\rho J_0^{11} \frac{s_1(s_1+1)}{3}},$$

$$T_c^{*(0)} = \frac{1}{2} \left\{ 1 - x + xIs + \left[(1 - x - xIs)^2 + 4x(1-x)J^2s \right]^{1/2} \right\}, \quad (14)$$

where

$$\rho = \frac{N}{V}, x = \frac{N_2}{N}, N = N_1 + N_2$$

$$s = \frac{s_2(s_2+1)}{s_1(s_1+1)}, I = \frac{J_0^{22}}{J_0^{11}}, J = \frac{J_0^{12}}{J_0^{11}}, \quad (15)$$

In the expression (14) the Curie temperature is determined in units of Curie temperature in m f a of one-sort system. The Curie temperature, that is obtained in the m f a, doesn't take into account the fluctuations of structure and magnetic moment.

For the investigation of influence of structure disorder of amorphous magnet on the critical temperature one has to make calculation in the higher approximation.

3. RESULTS AND CONCLUSIONS.

In the case of two-component system with the model exchange integral $J_k^{ab} = J_0^{ab} J_k^*$, (J_k^* is dependent on atomic sort function, $J_0^* = 1$) and structure factor $S_{ab}^{am}(k)$ in the substitution approximation the expression for the Curie temperature (using the iteration method) reads:

$$T_c^* = \frac{B + \sqrt{B^2 - 4C}}{2}, \quad T_c^* = \frac{T_c}{\rho J_0^{11} \frac{s_1(s_1+1)}{3}}, \quad (16a)$$

$$B = (1-x)m_{11}^* + 2J\sqrt{x(1-x)}m_{12}^* + xIm_{22}^*, \quad (16b)$$

$$C = x(1-x)(I - J^2) \left[m_{11}^* m_{22}^* - (m_{12}^*)^2 \right], \quad (16c)$$

$$I = \frac{J_0^{22}}{J_0^{11}}, \quad I = \frac{J_0^{12}}{J_0^{11}}, \quad x = \frac{N_2}{N} \quad N = N_1 + N_2, \quad (16d)$$

m_{ab}^* are given by formulas:

$$m_{11}^* = 1 + (1-x)t(x)P_1 - [2Q_1 + t(x)(1-x)R] \frac{t(x)}{4s_1(s_1+1)}, \quad (17a)$$

$$m_{22}^* = s[1 + Ixt(x)sP_2] - \frac{sIt(x)}{4s_1(s_1+1)}, [2Q_2 + sIt(x)R], \quad (17b)$$

$$m_{12}^* = sJt(x)\sqrt{x(1-x)} \left[P - \frac{Jt(x)}{4s_1(s_1+1)} R \right] \quad (17c)$$

where

$$P_a = \frac{1}{N} \sum_{k \neq 0} [S^{am}(k) - 1] \frac{J_k^*(1 - J_k^* \Delta_a)}{(1 - J_k^*)(1 - J_k^* \Delta)}, \quad (18a)$$

$$Q_a = \frac{1}{N} \sum_{k \neq 0} J_k^* \left[\frac{1 - J_k^* \Delta_a}{(1 - J_k^*)(1 - J_k^* \Delta)} - 1 \right] \quad (18b)$$

$$P = \frac{1}{N} \sum_{k \neq 0} [S^{am}(k) - 1] \frac{J_k^*}{(1 - J_k^*)(1 - J_k^* \Delta)}, \quad (18c)$$

$$R = \frac{1}{N} \sum_{k \neq 0} (J_k^*)^2. \quad (18d)$$

The rest notations read:

$$t(x) = \frac{1}{T_c^{*(0)}}, \quad (19)$$

$T_c^{*(0)}$ is the Curie temperature in molecular field approximation,

$$\Delta = st^2(x)x(1-x)(I - J^2), \quad \Delta_1 = sxt(x)(I - J^2), \quad (20a)$$

$$\Delta_1 = (1-x)t(x) \left(1 - \frac{J^2}{I} \right), \quad s = \frac{s_2(s_2+1)}{s_1(s_1+1)}. \quad (20b)$$

When the concentration of one component is equal to zero ($x=0$ or $x=1$) the equation (16a) gives the known result [4] for one-component amorphous ferromagnet. Considering structure factor

$S^{am}(k)$ to be known and using numerical calculations one can due to (16)-(20) investigate concentration dependence of two-component amorphous ferromagnet Curie temperature in the case of different values of spins, exchange interactions and magnetic atoms densities. Amorphous body structure is well represented by the structure of the system of hard spheres, especially in the region, where $S^{am}(k)$ has the first maximum. This region gives the main contribution into integrals over wave vectors in (18a,b,c,d). Taking for the exchange integral the often used form $J^{ab}(r) = J^{ab} \exp[-\alpha(r/\sigma)]$, where σ is hard sphere diameter, α is numerical parameter, one can analytically calculate integrals in (18a,b,c,d) and reduce them to sums of Laplace-transforms of the magnetic atoms pair distribution function. When the atoms are considered to be hard spheres, then the Percus-Yevick theory [7,8] gives analytical expression for the Laplace-transformes. Finally we find:

$$P_a = \frac{\alpha^2}{2(1-\Delta)} \left\{ (1-\Delta_a) [G(0) - G(\alpha\sqrt{2})] + (\Delta - \Delta_a) [G(\alpha\sqrt{1+\sqrt{\Delta}})] \right\} - \frac{G(\alpha\sqrt{1-\sqrt{\Delta}})}{\sqrt{\Delta}}, \quad (21a)$$

$$Q_a = \frac{\alpha^3}{48\eta(1-\Delta)} \left[\sqrt{2}(1-\Delta_a) - 1 + \Delta + (\Delta - \Delta_a) \left(\sqrt{1-\sqrt{\Delta}} - \frac{\sqrt{1+\sqrt{\Delta}}}{\sqrt{\Delta}} \right) \right] \quad (21b)$$

$$P = P_a, \quad \Delta_a = 0 \quad (21c)$$

$$R = \frac{\alpha^3}{384\eta} \quad (21d)$$

$$G(p) = p \left[\left(1 + \frac{\eta}{2} \right) p + (1 + 2\eta) \right] \left\{ 12\eta \left[\left(1 + \frac{\eta}{2} \right) p + (1 + 2\eta) \right] + e^p \left[(1-\eta)^2 p^3 + 6\eta(1-\eta)p^2 + 18\eta^2 p - 12\eta(1+2\eta) \right] \right\}^{-1} - \frac{1}{p^2} \quad (22a)$$

$$G(0) = - \left(\frac{1}{2} - \frac{\eta}{10} + \frac{\eta^2}{20} \right) / (1 + 2\eta), \quad (22b)$$

η is the packing parameter. For $\Delta < 0$ expressions (21a,b,c,d) are valid as well, but in this case it is necessary to write $G(p)$ in explicit form for complex parameter p .

The numerical calculations of the Curie temperature in the random phase approximation, that takes into account the structural and magnetic fluctuations for two-sort amorphous magnets, show that the critical concentration x_c of one of magnetic components ($T_c^*(x_c) = 0$) exists when the parameter α increases (it corresponds to decrease of effective radius of exchange interaction in the model exchange integral). The account of fluctuations at the decrease of α^{-1} leads to existence of bound magnetic atoms packing density. Phase transition into ferromagnet phase is absent below this value.

REFERENCES

1. Handrich. K., Kobe S. *Amorphe Ferro- and Ferrimagnetika*. - Berlin: Akademie-Verlag. 1980. - 293 p.
2. Петраковский Г.А. *Аморфные магнетики // Успехи физических наук*. - 1981. - Т.134, № 2. - С.305-331.

3. Вакарчук И.А., Рудаковский Ю.К., Понедилок Г.В. К проблеме магнетизма в топологически неупорядоченных системах // Проблемы современной статистической физики / Отв. ред. Боголюбов Н.Н. – Киев: Наук. Думка, 1985. – С.63-72.
4. Vakarchuk I.A., Rudavsky Yu.K., Ponedllok G.W. Free energy of the amorphous ferromagnets with Heisenberg exchange interaction and liquid-like disorder // *Phys.status solidi(b)*. – 1985. –V.128. – P.231-242.
5. Тябликов С.В. Методы квантовой теории магнетизма. М.: Наука, 1975. – 528 с.
6. Вакарчук И.А., Марголыч И.Ф. К теории многокомпонентных неупорядоченных магнетиков // Теор. и мат. физика. – 1987. – Т.72, № 3. – С.462-476.
7. Юхновский И.Р., Головкин М.Ф. Статистическая теория классических равновесных систем. – Киев: Наукова думка, 1980. – 372 с.
8. Балееску Р. Равновесная и неравновесная статистическая механика. Т.1. М.: Мир, 1978. – 405 с.

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ELEMENTS OF THE SILICON TCD DESIGN AND TECHNOLOGY

Key words: model, design, technology, silicon, detector

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Silicon TCD (Thermal Conductivity Detector, katarometer) chip analytical model, elements of the design and technology are presented. Detector was designed for the μ TAS (Micro Total Analysis System) application to recognize the composition of the different gas mixtures. TCD consists of the two pieces : glass plate and silicon chip. Two parallel flow channels 15 000 μm long, 400 μm wide and 50 μm deep were etched in the silicon chip and milled in the glass plate. Some of resistors were designed to act as a heaters and the other ones as a thermo resistors. Composition changes of the mixture flowing throughout the channel cause the temperature distribution changes and thermo resistors electrical response. Distance between the heaters and thermo resistors is of the great importance to the TCD sensitivity. VLSI silicon technology was applied to reduce geometrical dimensions and micromechanical technology to over-hange resistors across the flow channels to reduce thermal capacity and heat loses to the bulk and environment.

ANALYTICAL MODEL

Analytical model [1,2,3] is based on the heat transfer from the heater to the gas stream and environment. It can be expressed by the following second order differential equation (1). This model can be easily applied for the fast calculations even on the standard PC unit. One can estimate every individual parameter influence on the temperature distribution along the channel. Lost power (Q) from the heater to the TCD bulk and environment, caused by the resistor paths thermal conduction, were taken into account, too.