Modelling study of phase transitions in amorphous ultrathin films

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Abstract. The phase transition’s critical temperature dependence of the thickness and critical magnetic concentration are studied using the method of configuration averaging over the interaction fields in the framework of the Ising model in amorphous ultrathin film to define the transition from ferromagnetic state to paramagnetic one. It is shown that the Curie temperature increases quickly with a rise in number of monolayers and critical magnetic concentration decreases to bulk material value.

1. Introduction

The amorphous materials’ phase magnetic transitions have been studied theoretically for a long time (see for example [1, 2]) but it has been still timely [3]. The magnetic phase transition was studied in amorphous material by the method of random field in the framework of the Ising model in [1]. There was the phase transition’s temperature dependence of the ferromagnetic’s bulk concentration to study. Besides the critical magnetic concentration is calculated whereby the amorphous ferromagnetic becomes the paramagnetic. The Curie temperature dependence of the intensity of exchange interaction, the transverse and longitudinal susceptibilities and magnetization dependence of the temperature, the pyromagnetic coefficient dependence of the temperature was studied in the framework of the effective field theory in [2,3]. Particular attention is paid to the influence of the amorphization on the ferromagnetic’s hysteresis characteristics [3]. Kaneyoshi was made similar study much earlier [4, 5] where he studied the influence of the amorphization on the magnetic characteristics.

It should be noted that there are many experimental and theoretical studies [6-15] about size-effect’s influence on the crystalline ultrathin film’s magnetic characteristics near phase transition point. Experimental studies have been shown that phase transition’s relative change of the temperature decreases proportionally $L^{-1/\nu}$ with film thickness increasing where $\nu$-critical exponent of spin-spin correlations [14, 15].

Magnetic [16] and concentration [17] phase transitions’ theoretical studies have been shown that the dependence of the relative change in the Curie temperature of the thickness of an ultrathin film obeys a power law with an exponent equal to reverse critical exponent of spin-spin correlations $\nu = 0.69$. Moreover, the critical concentration of the transition from the ferromagnetic to the paramagnetic state decreases with increasing film thickness up to the percolation threshold [17].
It is assumed by the random interaction fields \([1, 12, 13, 17]\) to carry out the theoretical study of the size-effect’s influence on the magnetic and concentration phase transition.

2. The model
- Ultrathin film consists of \(N\) monolayers of diluted amorphous magnetic material with the bulk concentration of “magnetic atoms” \(c\);
- the direct exchange interaction occurs only between the nearest neighbors; moreover, the interaction fields \(h\) between the spin magnetic moments of the atoms are distributed in a random manner;
- spin magnetic moments are oriented along an axis \(Oz\) (approximation of the Ising model).

According to given a detailed account of formalism \([1, 12, 13, 17]\) the functions of random fields distribution \(W_n(h)dh = \frac{1}{\sqrt{2\pi b_n}} \exp\left[\frac{(h-h_n)^2}{2b_n}\right]\), \(1 \leq n \leq N\),

\[
W_n(h)dh = \frac{1}{\sqrt{2\pi b_n}} \exp\left[\frac{(h-h_n)^2}{2b_n}\right], \quad 1 \leq n \leq N, \tag{1}
\]

where \(m\) – atom’s magnetic moment, \(J_{1,1} = J_{1,k}\) is the exchange constant between atoms in the first layer and \(k\) –th layers and distribution parameters \((1)\) may be represented as follows:

\[
h_1 = c(\mu_1 + i\mu_2), \quad b_1 = c(1 + i^2), \quad h_n = c(i\mu_{n-1} + \mu_n + i\mu_{n+1}), \quad b_n = c(i^2 + \mu_n). \tag{2}
\]

In relations \((2)\) \(i_{n,k} = J_{n,k}/J_{1,k}\), \(J_{n,k}\) – the constant of the exchange interaction between atoms located in \(n\) –th and \(k\) –th layers. The average magnetic moment \(\mu_n = \langle\alpha_n\rangle - \langle\beta_n\rangle\) is defined as the difference between the average probabilities orientation of the magnetic moment of the atom \((\langle\alpha_n\rangle)\) and against \((\langle\beta_n\rangle)\) \(Oz\)-axis respectively:

\[
\langle\alpha_n\rangle = \int \alpha_n(h)W_n(h)dh = \int \frac{e^{m\mu/k_BT}}{e^{m\mu/k_BT} + e^{-m\mu/k_BT}} W_n(h)dh, \tag{3}
\]

\[
\langle\beta_n\rangle = \int \beta_n(h)W_n(h)dh = \int \frac{e^{-m\mu/k_BT}}{e^{m\mu/k_BT} + e^{-m\mu/k_BT}} W_n(h)dh, \tag{4}
\]

where \(m\) – atom’s magnetic moment, \(T\) – temperature, \(k_B\) – Boltzmann constant. We obtain a system of self-consistent equations according to the definition of the average magnetic moment quoted above:

\[
\mu_1 = \int \tan\left(\frac{h}{t}\right)W_n(h,\mu_1,\mu_2)dh, \quad \mu_n = \int \tan\left(\frac{h}{t}\right)W_n(h,\mu_{n-1},\mu_n,\mu_{n+1})dh, \tag{5}
\]

where \(t = k_B T/m\).

Equations \((5)\) and \((7)\) enable us to find the relative magnetic moment and the phase transition’s critical temperature dependence of the amorphous magnetic film’s number of layers and «magnetic» atom’s concentration.

3. The Curie temperature dependence of the film monolayers’ number and «magnetic» atoms’ concentration

The relative Curie temperature \(t_c = k_B T_c/J_{1,1}m\) dependence of the ultrathin amorphous film’s number of monolayers \(N\) is shown in figure 1. The Curie temperatures differ essentially for films less than 5 monolayers and practically don’t depend of the thickness for \(N > 8\).
The relative Curie temperature $t_c$ is $t_c = k_B T_c / J_{1,1} m$ dependence of the amorphous ultrathin film’s number of monolayers $N$ with «magnetic» atoms’ concentration $c = 1$. The calculation’s results of the relative Curie temperature $t_c(N)$ dependence of the crystalline film’s thickness with simple cubic lattice are shown in figure 2 for comparison [12]. It is evident that phase transition’s critical temperature of the amorphous and crystalline films varies similarly with increasing thickness $t_c(N) \to 1$ but the amorphous film’s Curie temperature varies faster. This is attributable to the large number of nearest neighbors $z$ in amorphous film than in a crystalline one ($z > 6$).

The «magnetic» atoms’ concentration markedly affects the magnetic ordering as in the case of the crystalline ultrathin films [16, 17] (see for example figure 3).

Fig 1. The relative Curie temperature $t_c = k_B T_c / J_{1,1} m$ dependence of the amorphous ultrathin film’s number of monolayers $N$ with «magnetic» atoms’ concentration $c = 1$.

Fig 2. The relative Curie temperature dependence $t_c(N) = T_c(N)/T_c(N \to \infty)$ of the amorphous (blue curve 1) and crystalline (purple curve 2) [12] ultrathin films’ number of monolayers $N$ with «magnetic» atoms’ concentration $c = 1$.

Fig 3. The relative Curie temperature $t_c = k_B T_c / J_{1,1} m$ dependence of the «magnetic» atoms’ concentration $c$ for the films with different thickness $N$. From left to right: blue curve-$N = 10$, green curve-$N = 5$, light brown curve-$N = 3$, purple curve-$N = 2$, blue curve-$N = 1$.
Moreover the ferromagnetic’s critical concentration $c_{cr}$ decreases with increasing film thickness up whereby the ferromagnetic becomes the paramagnetic. The amorphous film’s critical concentration $c_{cr}$ varies through bigger range in comparison with crystalline films [16, 17].

4. Conclusion
It is shown as the theoretical study’s result of the influence of size-effect on the magnetic and concentration phase transition in ultrathin amorphous films:

1) the Curie temperature increases with increasing monolayers’ number of the ultrathin amorphous films where the Curie temperature’s type of the dependence is similar in behavior of crystalline one;
2) magnetic atoms’ critical concentration decreases with increasing film thickness up whereby the magnetic phase transition occurs.

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References
[1] Belokon V and Semkin S 1992 Journal of Experimental and Theoretical Physics 101 (10) 1254-1258
[2] Ainame A, El-Atri A and Saber M 1995 Journal of Magnetism and Magnetic Materials 145 139-146
[3] Essaoudi I, Ainame A, Saber M and J J de Miguel 2009 Journal of Magnetism and Magnetic Materials 321 38-42
[4] Kaneyoshi T 1985 Journal of the Physical Society of Japan 54 3514-3525
[5] Kaneyoshi T 1992 Introduction to Amorphous Magnets (Singapore: World Scientific) p 87
[6] Ambrose T and Chien C L 1996 Physical Review Letters 76 (10) 1743-1746
[7] Ambrose T and Chien C L 1996 Journal of Applied Physics 79 5920-5922
[8] Bramfeld T S and Willis R F 2008 Journal of Applied Physics 103 07C718
[9] Willis R F, Bramfeld T S, Podolak K R 2007 Journal of Applied Physics 101 09G119
[10] Gradman U 2001 Encyclopedia of Materials: Science and Technology 5832-5837
[11] Marques M I and Gonzalo J A 2000 Acta Physica Polonica A 97 1033-1038
[12] Afremov L L and Kirienko Y V 2013 Journal of Physics:Conference Series 410 012017
[13] Afremov L L and Petrov A A 2014 Journal of Physics:Conference Series 490 012021
[14] Huang F, Mankey G J, Kief M T and Willis R F 1993 Journal of Applied Physics 73(10) 6760-6762
[15] Huang F, Mankey G J, Kief M T and Willis R F 1994 Journal of Applied Physics 49(6) 3962-3971
[16] Afremov L L, Kirienko Y V 2013 Applied Mechanics and Materials 328 823-826
[17] Afremov L L, Il’yushin I G 2013 Advanced Materials Research 683 69-72