Magnetic properties of amorphous alloys in a random field model

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Abstract

In this study, an attempt was made to sequentially calculate the Curie temperature of iron-containing alloys based on the theory of random fields of exchange interaction. This method makes it possible to determine the conditions for the occurrence of ferromagnetism in an amorphous alloy depending on the concentration of exchange-interacting ions, their Holschmidt radius, and the type of crystal lattice of the transition metal.

Introduction

Despite many publications on the research topic [1-5], there are gaps in the explanation of some magnetic properties of amorphous metal alloys, including the behaviour of the Curie point depending on the concentration and type of metalloids. From general considerations, the Curie point of an amorphous iron-based alloy should be lower than that of a crystalline analogue since the number of neighbours in the first and second coordination spheres, which make the main contribution to the field of exchange interaction in the bcc lattice, is greater than in objects with random close packing, for which the average coordination number is z*≈12 [6]. In this study, an attempt was made to sequentially calculate the Curie temperature of iron-containing alloys based on the theory of random fields of exchange interaction [7-8].
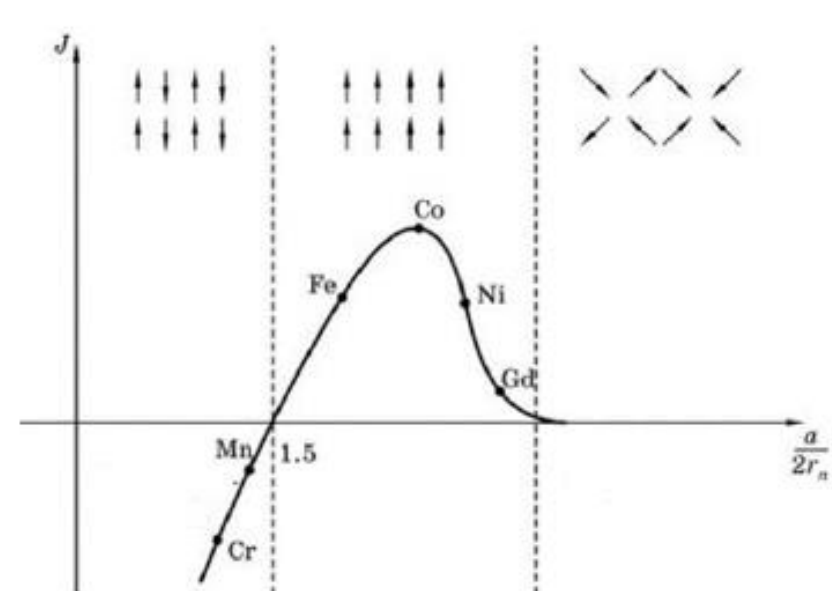

FIG. 1. The Bethe-Slater dependence [10] of the exchange integral J on the ratio of the distance between ion a to the diameter of the unfilled shell $2r_n$

The method of random fields of exchange interaction

Following [9], we considered a system of interacting particles randomly distributed over the volume. The projection of the field H_i on the z axis (the axis of symmetry in the Ising model), created at the origin by one arbitrary particle located at a point with coordinate r_i with a magnetic moment $\boldsymbol{m}_i$, can be determined by means the law:

$$H_i = \varphi(r_i, \boldsymbol{m}_i). \tag{1}$$

Given the known distribution of particles over r_i and $\boldsymbol{m}_i$, the distribution density of the interaction field on a particle located at the origin of coordinates is a δ-function of the form:

$$\delta[H_i - \textstyle\sum_i \varphi(r_i, \boldsymbol{m}_i)]. \tag{2}$$

Considering the probability of particle distribution over volume and magnetic moment, the distribution density of the random interaction field H can be represented as

$$W(H) = \frac{1}{\sqrt{\pi}\,B} \exp\left(-\frac{(H - H_0(\alpha - \beta))^2}{B^2}\right). \tag{3}$$

$$H_0 = n \int \varphi(\boldsymbol{r})\,\mathrm{d}V, \quad B^2 = 2n \int \varphi^2(\boldsymbol{r})\,\mathrm{d}V. \tag{4}$$

where value $n=N/v$ is the "effective" number of particles per unit volume, α and β are the relative number of particles oriented "up" and "down".
Similar relationships for crystalline ferromagnets are as follows:

$$H_0 = p \textstyle\sum \varphi_k , \quad B^2 = 2p(1 - m^2 p) \textstyle\sum \varphi_k^2, \tag{5}$$

where p is the concentration of exchange-interacting ions at the sites of the crystal lattice. Near the Curie point, $B^2 \approx 2p \sum \varphi_k^2$.

Thus, the main characteristics of the distribution function H_0 and B are interconnected through the interaction law $\varphi(\boldsymbol{r})$. As for the exchange interaction of two particles, its energy can be determined as follows:
$$E_{ij} = -m_i m_j J_{ij} = -m \cdot mJ(r_{ij}) = -m\,\varphi(r_{ij}).$$

The Curie point is determined by the relation:

$$\frac{H_0}{B} \tanh\left(\frac{mB}{k_B T_c}\right) = 1. \tag{6}$$

Obviously, the relation $\frac{H_0}{B}$ must be greater than 1. And the condition $\frac{H_0}{B} = 1$ determines the critical concentration p_c of exchange-interacting ions. In the case of a crystalline ferromagnet and interaction between particles of only the first coordination sphere, $\varphi_k = f = $ const. From here,

$$\gamma = \frac{H_0}{B} = \frac{p_c z f}{f\sqrt{2p_c z}} = 1, \tag{7}$$
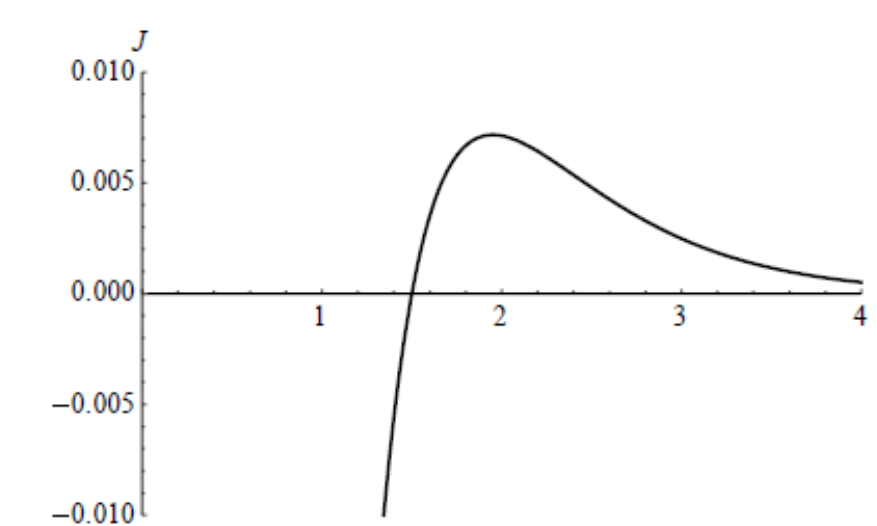
$$p = \frac{2}{z}, \tag{8}$$

FIG. 2. Dependence of the exchange integral J on the ratio of the distance between ion a to the diameter of the unfilled shell $2r_n$ $(x = \frac{a}{2r_n} = \frac{a}{d})$. The results for function (10) are shown.

Magnetic phase transition in an amorphous alloy

The greatest difficulty for calculating the exchange interaction fields in an amorphous alloy is the calculation of the exchange integral J between neighbouring atoms (ions) as a function of the distance between them. Perhaps the only exact result was obtained when calculating the exchange interaction energy of an ionized hydrogen molecule [10]. The exchange energy, up to sign, is proportional to the exchange integral and has the form

$$E_0 \sim \frac{1}{r_0}\left(1 - \frac{2}{3}r_0{}^2\right)\exp(-r_0), \tag{9}$$

where $r_0 = \frac{a}{c}$, c is the radius of the first Bohr orbit, and a is the distance between the nuclei.

We consider the Bette–Slater dependence of the exchange integral J on the ratio of the distance between ion a to the diameter of the unfilled shell $2r$, which qualitatively correctly reflects the dependence of the exchange integral on the distance. Ferromagnetic elements Fe, Co, and Ni have the highest value of the exchange integral. Based on such a scheme, it is possible to explain not only the ferromagnetism of Fe, Co, and Ni but also the antiferromagnetism of alloys, and so forth.

We tried to approximate the Bette–Slater curve based on formula (9). Assuming the dependence of the exchange integral on the ratio of the distance between ions a to the diameter of the unfilled shell $2r$ in the form:

$$J(x) = \frac{e^{-2x}\left(-1 + \frac{4x^2}{9}\right)}{\frac{x}{a}}, \tag{10}$$

where $x = \frac{a}{2r} = \frac{a}{d}$.

Using the approach described above, consider an amorphous alloy containing iron in an amount of 70% of the total composition. The volume of the crystal cell in accepted units is $V = x^3 = \left(\frac{a_0}{d}\right)^3 = 7.26$. The volume occupied by two ions is $NV_0 = 2\frac{4}{3}\pi\left(\frac{r_g}{r}\right)^3 = 4.93$, where $r_g = 0.124 \cdot 10^{-9}$ m is the Holschmidt radius and $r = 74 \cdot 10^{-12}$ m is the iron ion radius. The volume fraction occupied by ions is defined as $\frac{NV_0}{V} = \frac{4.93}{7.26} = 0.68$. Thus, the effective density can be found as $n = 0.7\frac{NV_0}{V}\left(1 + 0.7\frac{NV_0}{2V}\right) = 0.59$.

Using formula (4), we determine the moments of the distribution function by integrating over volume: $H_0 = 489\ T$, $B = 241\ T$.

Conclusion

From Eq. (6), one can determine the Curie temperature of an amorphous alloy with an iron concentration of 70% and a magnetic moment of iron ions, $m = 1.9\mu_B$. We considered that the average magnetic moment of bulk iron changes to $1.9\mu_B$ when passing from a crystalline compound to its amorphous counterpart. We find that the Curie temperature in the case of an amorphous alloy was $T_c \approx 570\ \mathrm{K}$, which is consistent with the result shown in [11].

Therefore, the result obtained can be considered approximate. Using the values H_0 and B obtained by us, we can estimate the "effective number of nearest neighbours" z of iron ions for an amorphous alloy using the ratio $z = \left(\frac{H_0}{B}\right)^2 \frac{2}{p}$. Then, $z = 13.9$, which also agrees with the result obtained experimentally in [11].

The Curie point can significantly depend on the magnetic moment of iron ions, which in turn, is determined by the concentration and type of metalloids that make up the alloy. The data known to us indicate that in alloys with an iron ion concentration of 70%–80%, the magnetic moment per atom ranges from $1.2\ \mu_B$ to $1.9\ \mu_B$. The effective number of the nearest neighbours at an iron ion concentration of 70% during amorphization turns out to be approximately 12.66, which corresponds to the experimental data.
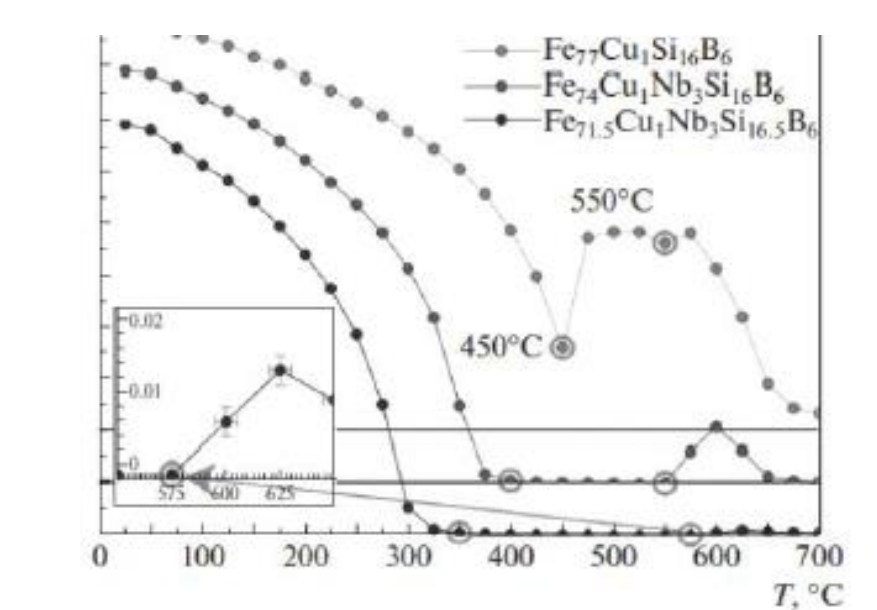

FIG. 3. The curve of dependence $I_s/I_s o = f(T)$ of spinning tapes based on Fe [11].

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