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Correlation Between the Electronic Structure and Thermostability of the Fe-Based Soft Magnetic Glasses

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The temperature dependencies of magnetic susceptibility $\chi(T)$ for amorphous $Fe_{85}B_{15}$-based alloys with Co and Cr dopants have been investigated in the range of 300-850 K using the Faraday technique. The crystallisation of the studied amorphous alloys is accompanied by an essential increasing of χ. Co and Cr dopants were shown to increase the temperature range of amorphous state stability in $Fe_{85}B_{15}$-based soft magnetic glasses. The computer simulation of the electronic states density n(E) of $Fe_{85}B_{15}$ amorphous alloy displayed that the Fermi level is located in the vicinity of local maximum of n(E) curve. Co and Cr dopants were shown to decrease n(E) at the Fermi level. The comparison of the experimental $\chi(T)$ curves and the data of electronic structure simulation proved the applicability of the Nagel-Tauc electronic criterion to describe the thermal stability of the investigated alloys.

Keywords: amorphous systems alloys; thermal stability, electronic structure; soft magnetic materials.

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I. Introduction

The interest in amorphous metallic materials (AMM) is caused by the fact that AMM possess the unique combination of physical properties [1-3]. In particular, Fe-based amorphous alloys possess high level of soft magnetic properties: low coercive force and hysteresis losses, higher magnetic penetrability that makes these materials perspective to use them as the elements of magnetic circuits. Therewith the thermal-time stability of the AMM`s basic service characteristics often is not high enough for their industrial applications. So, one of the key problems in this field is to work out the methods of AMM`s stability enhancement and monitoring. The common way to solve this problem is to choose the appropriate AMM composition. It is necessary to emphasise that there are a lot of facts [4] evidencing the peculiarities of AMM electronic structure being the dominant factor determining the level of their thermal stability and key service characteristics. The correlation between the crystallisation temperature and electronic states density at the Fermi level known as the Nagel-Tauc criterion has been revealed for a series of amorphous metallic systems [5].

But till now the applicability of the Nagel-Tauc electronic criterion to transition metal-based amorphous alloys is still discussed. To clarify this question we carried out the systematic magnetometric investigation of the $Fe_{85-x}TM_xB_{15}$-amorphous alloys (TM are Co and Cr) paying special attention to their thermal stability and perform appropriate calculations of their electronic structure.

II. Experimental and calculation procedure

$Fe_{80}TM_5B_{15}$ glassy ribbons were obtained by the melt spinning technique. The amorphous structure was verified by the X-ray diffraction. Temperature dependencies of magnetic susceptibility $\chi(T)$ were investigated in 300-850 K region using the Faraday magnetometer with automatic microbalance. The heating rate was equal to 8 K/min. The sensitivity of the method was equal to 10^{-11} cm^3/g. The accuracy of the susceptibility measurements $\Delta\chi/\chi$ was better than 1.5 % and of the temperature $\Delta T \leq 0.5$ K.

The calculation of the electronic states density were performed on the basis of an extension of a s-d band model of the coherent potential approximation in the case of the topologically disordered alloy [6]. We have calculated the electronic density of states for pure amorphous metal using the *fcc* tight-binding energy spectrum as input data. Only 3d and 4s states of Fe have been considered, because the others are located too far from the Fermi level. The radial distribution function has been obtained from the X-ray diffraction measurements [7].

III. Results and discussion

For better understanding the factors stabilising the Fe-B-based amorphous alloys the systematic magnetometric investigation of $Fe_{85-x}TM_xB_{15}$-amorphous alloys (TM are Co and Cr) and the theoretical investigation of their electronic structure peculiarities have been performed. The experimental temperature dependencies of magnetic susceptibility

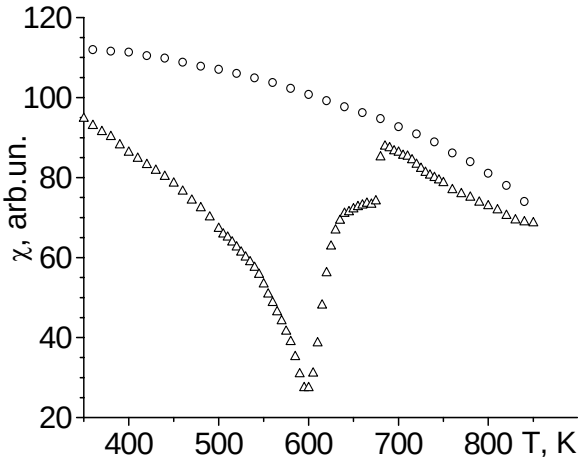

Fig. 1. The temperature dependence of magnetic susceptibility for $Fe_{80}Co_5B_{15}$ AMM (triangles – heating, circles – cooling).

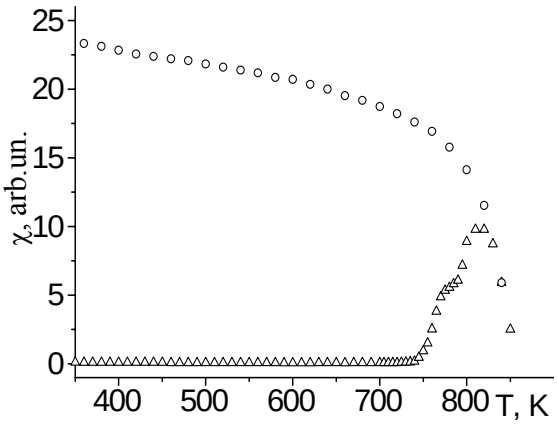

Fig. 2. The temperature dependence of magnetic susceptibility for $(Fe_{0,62}Cr_{0,38})_{85}B_{15}$ AMM (triangles – heating, circles – cooling).

Table

The crystallization temperature T_X of $Fe_{85-x}Co_xB_{15}$ amorphous aloys for the first and second stages of crystallization process

x, %	T_X, K	
	1-stage	2-stage
0	650	675
5	615	680
12	605	695
15	615	690
17	615	690
21	600	680
25	645	726

χ(T) were proved to be the curves of the similar shape for all investigated glasses, with the exception of Curie temperature value T_c. For AMM with Co T_c is higher than crystallisation temperature T_X and the paramagnetic region is not observed within the amorphous state. On the other hand the Cr dopants

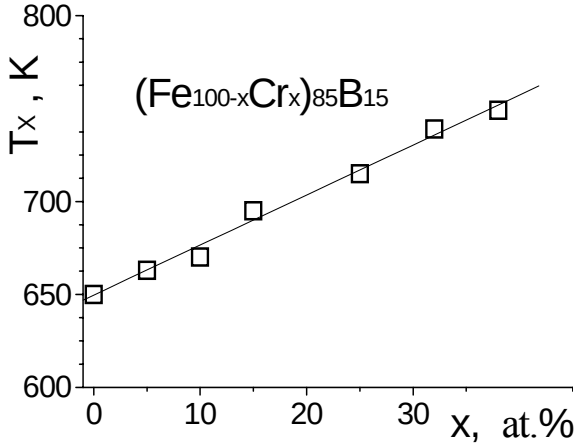

Fig. 3. The crystallization temperature of $(Fe_{100-x}Cr_x)_{85}B_{15}$ amorphous alloys.

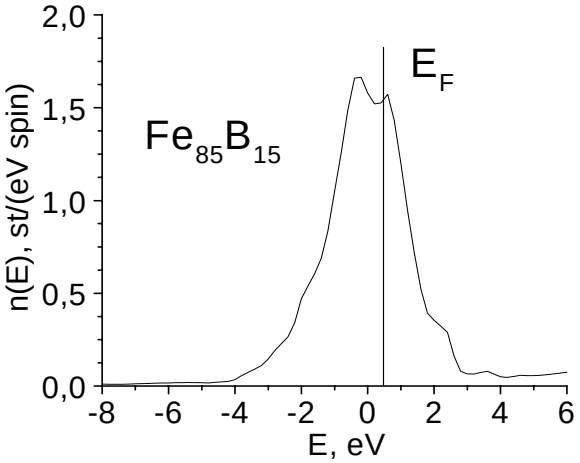

Fig. 4. The energy dependencies of electronic states density n(E) for the amorphous $Fe_{85}B_{15}$ (the position of the Fermi energy is indicated by vertical line).

decrease the Curie temperature and the paramagnetic region exists within the amorphous state. Some typical $\chi(T)$ curves, as an example, are shown at figs. 1 and 2. It is necessary to note that crystallisation have the two-stage character. It is the evidence of primary crystallisation mechanism. According to the X-ray diffraction data α-Fe(TM) solid solution is formed at the first stage and the metastable $(Fe,TM)_3B$ boride is formed at the second stage of crystallisation process. The obtained results have shown that Co and Cr dopants generally expand the temperature range of solid phase formation compared to the basic $Fe_{85}B_{15}$ amorphous alloy.

The crystallisation temperature T_X was determined from $\chi(T)$ curves due to sharp rise of susceptibility value at crystallisation. The obtained T_X values in dependence of Co concentration are presented in table. One can conclude that crystallisation temperature T_X of $Fe_{85-x}Co_xB_{15}$-amorphous alloys varies non-monotonously and reaches the minimum at $x = 21$. On the other hand, when Cr content in the basic AMM increases the crystallisation temperature T_X is increased linearly (fig. 3). So the thermal stability of metallic glasses is improved with decreasing of electron number per atom and changed non-monotonously with increasing of electronic concentration.

To explain such behaviour we have analysed theoretically the electronic spectrum peculiarities of $Fe_{85}B_{15}$ glassy ribbon. The energy dependence of electronic density n(E) calculated according to the procedure described in Ref. [6] is presented at fig. 4. The main peculiarity of this curve is the presence of two sub-peaks distanced by 1 eV, that is a good agreement with experimental results stated in Ref. [8]. The Fermi level of $Fe_{85}B_{15}$ amorphous alloy is located slightly lower the right peak.

Reasoning from the data listed in Ref. [9] we considered that a few amount of Co and Cr dopants does not change essentially the shape of n(E). But the Fermi level position is shifted relatively to the local maximum (to the right side for alloys with Co dopants, to the left side – for alloys with Cr dopants). So, Cr dopants lead to a decreasing of the density of electronic states at the Fermi level and to an increasing the thermal stability of the investigated alloys. It means the Nagel-Tauc electronic criterion can be used to describe the thermal stability of $Fe_{85-x}B_{15}$ alloys. I.e. the alloy with the lower n(E) value at the Fermi level possesses the higher thermal stability.

In a case of Co dopants in $Fe_{85-x}Co_xB_{15}$-AMM the situation is more complicated. When the Fermi level is sifted to the higher energies the electronic state density

increases initially and then decreases passing through the maximum. Just this fact, in our opinion, causes the non-monotonic variation of crystallisation temperature T_X for $Fe_{85-x}Co_xB_{15}$-amorphous alloys (table).

IV. Conclusions

The main result of our investigation can be formulated as follows: the Nagel-Tauc electronic criterion mainly determines the thermal stability of the Fe-B – based soft-magnetic glasses. The dopants, which lead to a decreasing of electronic state density at the Fermi level (Co and Cr, in particular), should be used to stabilise their amorphous structure and, hence, the level of key service characteristics.

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Зв'язок між електронною структурою та термостабільністю магнітом'яких металевих стекол на основі заліза

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В температурному інтервалі 300-850 К методом Фарадея досліджено температурні залежності магнітної сприйнятливості χ(T) аморфних металічних сплавів на основі $Fe_{85}B_{15}$ з домішками Co and Cr. Процес кристалізації досліджуваних аморфних сплавів супроводжується суттєвим зростанням значення χ. Показано, що домішки Co та Cr збільшують температурний інтервал стабільності аморфного стану. Проведено розрахунки густини електронних станів n(E). Виявлено, що рівень Фермі знаходиться у локальному максимумі кривої n(E), а домішки Co і Cr зменшують значення n(E). Порівняння експериментальних кривих χ(T) та даних розрахунків електронної стркутури підтверджує застосовність електронного критерію Нагеля-Таука для описання термічної стабільності досліджених аморфних сплавів.