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Short Range Order Change at Structural Relaxation in $Fe_{75}Si_6B_{14}Mo_5$ Amorphous Alloy

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Structural relaxation process in $Fe_{75}Si_6B_{14}Mo_5$ amorphous alloy has been studied by means of X-ray diffraction method. Structure parameters, obtained from analysis of structure factors and pair correlation functions are used in order to clarify this phenomenon on the short range order scale. More detailed analysis was done for profile of second maxima in structure factors. Results showed that rearrangement of atomic clusters occurs at high temperature relaxation.The structure relaxation is accompanied by formation the clusters of less size due to which an atomic distribution becomes more close to perfect amorphous structure.

Keywords: Amorphous alloys, structural relaxation, structure factors**.**

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Introduction

Amorphous alloys are similar to liquid ones because the characteristic of both phases is lack of short range order. But, contrary to liquid alloys an amorphous ones reveal a higher sensitivity to heating due to existence of metastable structure units, formed upon rapid cooling of melt. Numerous studies evidently showed that heating of amorphous alloys is accompanied by two main processes: structural relaxation and crystallization. There are two kinds of structural relaxation – low- temperature relaxation and high-temperature one[1].

Structural relaxation process in amorphous alloys is related with changes of main physical- chemical properties, most of which are important at practical application of those materials. It is clear that such changes should be analyzed with relation to short range order structure because arrangement of nearest neighbors and their interactions are responsible for formation of properties. In this work we represent the results on structure changes at high-temperature relaxation in $Fe_{75}Si_6B_{14}Mo_5$ amorphous alloy, which is promising from viewpoint of advanced soft magnetic materials [2,3]. We attempt to use more structure parameters, derived from structure factors and pair correlation functions in order to make a deeper understanding the structural relaxation process and its relation with nanocrystalization, occurring at higher temperatures[4].

I. Experimental

Samples for studies of temperature changes of short range order and relaxation process in $Fe_{75}Si_6B_{14}Mo_5$ amorphous alloy have been prepared by means of rapid cooling from liquid state using the copper disk, rotating with high speed. Information on atomic arrangement was obtained with help of X-ray diffraction method (XRD) using DRON-3 diffractometer, attached with high temperature chamber (Cu-radiation, Bragg-Brentano focusing geometry) [5]. Angular dependences of scattered intensitieswere corrected by polarization factor and incoherent scattering was taking into account. These intensity functions were analyzed and main structure parameters have been obtained from them. Namely, we have measured the half peak-height width, used to estimate the correlation radius. This characteristic parameter of topologically disordered materials is commonly considered as the size of structural units – clusters. From intensity curves,the structure factors (SF) have been calculated. The principal peak's position and its height were the main parameters used in interpretation of SF.

Another structure characteristics-pair correlation functions (PCF) and radial distribution function (RDF) were calculated from SF's using the integral Fourier-transformation. The first peak position of PCF interprets as the most probable distance to nearest neighbors, and the area under first peak of RDF was interpreted as number of atoms in first spherical shell (coordination number). Besides the first peak of SF and RDF we also focused our attention on second peak of these functions,

which is most sensitive to structural relaxation process in amorphous alloys.

II. Results and discussion

The structure changes in $Fe_{75}Si_6B_{14}Mo_5$ amorphous alloy at heating within temperature range 383-683 K can be seen in Fig. 1. One can see that principal peak position

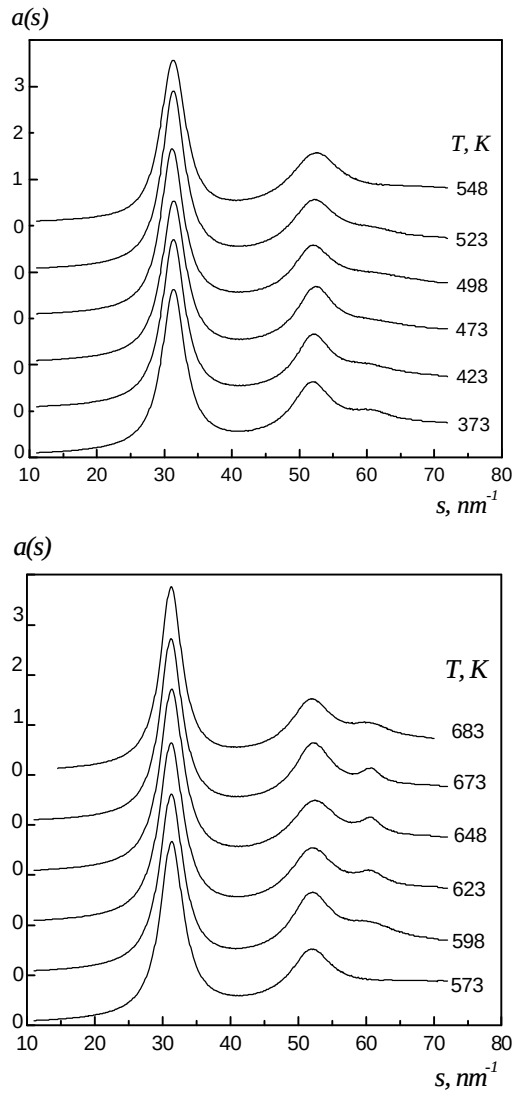

Fig. 1. SF for $Fe_{75}Si_6B_{14}Mo_5$ amorphous alloy at different temperatures.

and their height slightly depend on temperature, whereas the second maximum reveals the more significant changes within investigated temperature region. Namely, this maximum shows the subpeak, which just is most sensitive to annealing temperature and becomes most pronounced at annealing within temperature range 598-673 K. The similar behavior was observed in early studied other amorphous alloys that permits to consider such subpeak as a most important characteristic of structural relaxation process [6-8]. For that reason in order to have a more knowledge and understanding of this process in amorphous alloys the detailed analysis of subsidiary maximum profile and its evolution with temperature should be carried out. We have analyzed such parameter as half height width at different annealing temperatures, which was used for estimation of such structural parameter as cluster size. From experimental data follows that temperature dependence of this parameter has a maximum at temperature about 550 K.

This maximum shows the asymmetry and reveals the flat left hand side, whereas its right side drastically decreases at temperature increasing. Such behavior allows us to suppose that within observed temperature

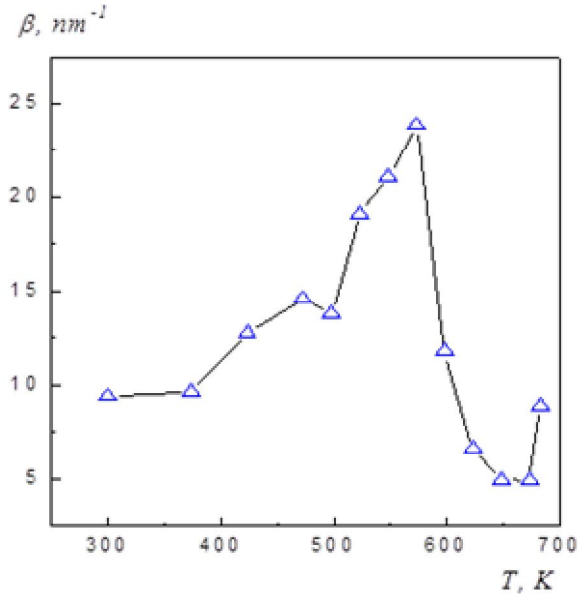

Fig. 2. Temperature dependence of half height width of subpeak in SF.

range the rearrangement of structural units (clusters) occurs [9].

Similar dependence was observed in the plot of half height peak width in pair correlation functions, but in this case the maximum has a symmetric profile contrary to one in structure factor. It is clear that increase of maxima width height, observed in SFs and PCFs is related with decrease of structural units size. Thus, the structure relaxation is accompanied by formation the clusters of less size due to which an atomic distribution becomes more close to perfect amorphous structure.

Pair correlation functions have been usedalso for estimation of mean interatomic distances <r>, $\sqrt{< r^2 >}$ and their temperature dependences according to formulas:

$$< r >= \frac{\int_{r_1}^{r_2} r g(r) dr}{\int_{r_1}^{r_2} g(r) dr}, \sqrt{< r^2 >} = \frac{\int_{r_1}^{r_2} r^2 g(r) dr}{\int_{r_1}^{r_2} g(r) dr}$$

r_1 and r_2 are the left and the right minima for principal peak of $g(r)$ Obtained results show almost unchangeable values of this paramer with temperature values that allowed us to conclude about existence of insignificant local thermal expansions at recrystalization process.

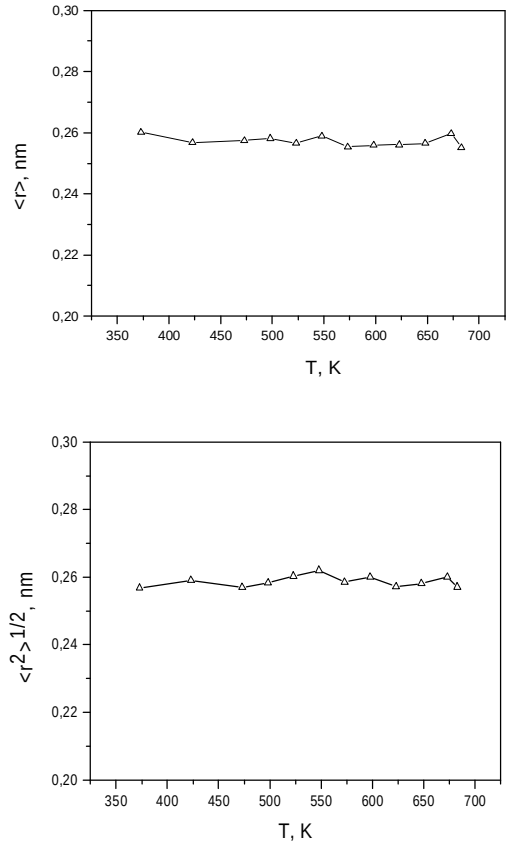

Fig. 3. Temperature dependence of meaninteratomic distance<r>-(a) and $\sqrt{< r^2 >}$ -(b).

Conclusions

It is shown that structural relaxation is accompanied by the formation of clusters of smaller size. Experimental data have shown that the temperature dependence of the cluster size has a maximum at about 550 *K*. This maximum has no symmetric profile and shows the flat left hand side, whereas its right one reveals the drastic decrease at temperature increasing. Such behavior allows us to suppose that within observed temperature range the rearrangement of structural units (clusters) occurs. Thus, the structure relaxation is accompanied by formation the clusters of less size due to which an atomic distribution becomes more close to perfect amorphous structure.

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