Modeling of nanocrystallization process in $Fe_{85}B_{15}$ amorphous alloy

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Formation of structures with nanoscale grain size during crystallization of metallic glasses is of a great interest from both fundamental and technical points of view. In part, fundamental studies of the mechanisms of crystal nucleation and growth as well as kinetics of transformation will aid in optimizing structure and excellent physical (magnetic and mechanical) properties of nanostuctured materials attractive for applications [1-3].

The process of formation of the α-Fe solid solution crystals at first stage of crystallization of $Fe_{85}B_{15}$ amorphous alloy under constant rate heating has been studied by means of X-ray diffractometry and differential scanning calorimetry (DSC). The experimental kinetic curves shown in (Fig. 1) have been analyzed using the proposed analytical model based on the combination of Kolmogorov equation:

$$X(T) = 1 - \exp\left\{ -\left(\frac{\pi}{3}\right) I U_D^3 \left[\frac{T^2}{(qQ)} \right]^4 \right\} \tag{1}$$

(with I being the nucleation frequency) and the relation describing the dependence of the rate of diffusion-controlled crystal growth $U_D(T)$ on temperature and heating rate[1]:

$$U_D(T) = \left(\frac{\lambda_n}{2}\right) \left[D(T) \left(\frac{qQ}{T^2} \right) \right]^{\frac{1}{2}} \tag{2}$$

where D is the volume diffusion coefficient $D = D_0 \exp\left(-\frac{Q}{T}\right)$ and λ_n is a dimensionless parameter depending on the matrix concentration at and far from the interface and that of the crystal. Assuming the homogeneous mode of nucleation and using the numerical values of the parameters determined for description of crystallization of $Fe_{84}B_{16}$ glass [2] the $X(T)$ curves have been calculated with λ_n being as an adjustable parameter. As it is seen from (Fig. 1) a good quantitative agreement between the experimental kinetic crystallization data and the calculated one has been achieved in assumption that the value of λ_n is lowered with the heating rate. It implies that the boron concentration in α-Fe increases with q (Fig. 3) which is in general accordance with the results presented in [3]. The calculations within the model has shown that the grain size d of α-Fe solid solution formed during primary crystallization in binary $Fe_{85}B_{15}$ glass is monotonically decreased as the heating rate increases (Fig. 2) and, in part, becomes as small as 48 nm at q=10^4 K/s. The results of simulations are in good agreement with the TEM data for q=10^4 K/s [3].

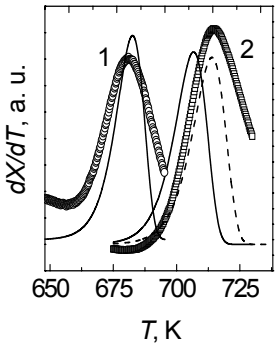

Fig. 1. A comparison of the experimental (dots) and calculated (lines) dependencies of the crystallization rates *dX/dT* of α-solid solution in $Fe_{85}B_{15}$ metallic glass at heating rates of 0.167 K/s (1) and 0.67 K/s (2). The calculated curves were obtained using nonisothermal kinetic equation (1) and values of parameter λ_n equal to 1.4 (solid lines) and 0.86 (dashed line)

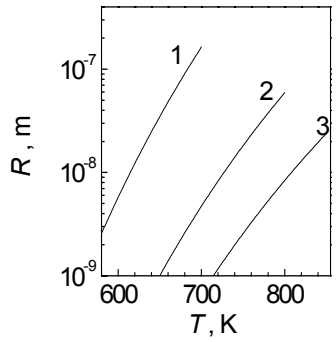

Fig. 2. Variations of the radius of α-Fe solid solution grains in metallic glass $Fe_{85}B_{15}$ versus temperature calculated for different heating rate: 1 – 0.167 K/s; 2 - 200 K/s; 3 - 10^4 K/s.

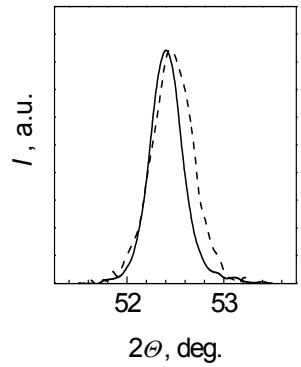

Fig. 3. Details of the (110) peaks of the X-ray diffractograms (Co K_α - radiation) for the samples of the $Fe_{85}B_{15}$ amorphous alloy heated to temperatures of the first stage of crystallization end at the rates of 0.167 K/s (solid line) and ~ 200 K/s (dashed line).

In conclusion, the analytical approach based on combination of the Kolmogorov equation and the relation for the rate diffusion-limited crystal growth rate *vs.* temperature and heating rate is developed for description of primary metallic glass crystallization kinetics at linear heating. Good agreement of the calculated dependencies of the crystallization rates on temperature with the experimental DSC thermograms for the $Fe_{85}B_{15}$ amorphous alloy is evidence for the validity of the proposed model. The results model calculations have shown that the size of α-Fe solid solution crystals formed during primary crystallization monotonically decreases as the heating rate increases and at heating with the rates above 10^3 K/s the nanocrystalline structure in the alloy investigated must be formed which is in accordance with the experimental data.

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[3] Abrosimova, G.Ye., Aronin, A.S., Stelmuh, V.A. (1991) Crystallization of $Fe_{85}B_{15}$ amorphous alloy above the glass transition temperature, *Fizika Tverdogo Tela* **33**, 3570-3576 (in Russian).

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