STRUCTURE PROPERTIES OF AMORPHOUS MATERIALS

M. Davidović and Đ. Jović
"Boris Kidrič" Institute of Nuclear Sciences, Vinča, Beograd

Abstract:

Relaxation processes in crystalline solids and amorphous materials during structural changes can be studied by method of thermal annealing. In the case of amorphous ferromagnetics, for instance, the changes which appear during the annealing involve an increase in T_c and density n. The change in density n (i.e. a uniform shortening of bond lenghts) means a change in the topology of the amorphous materials, which is associated with the recombination of the structure defects.

By measuring the structure factor S(Q) or calculating their Fourier transform g(r), before and after the thermal annealing one can study the structure properties (i.e. the regularity and the irregularity) of armophous materials. On the other hand, the elastic stress on the atomic scale $\bar{p}$ (atomic level stress), the quantity which directly describes the fluctuations in the local density, can be calculated for a corresponding interatomic potential $\varphi(r)$ and pair correlation function g(r). In this paper we calculated quantify f(r) which is proportional to $\bar{p}$ for binary amorphous alloy $Fe_{0.8}B_{0.2}$.

1. INTRODUCTION

The relaxation processes in amorphous materials can be explored by the thermal annealing if one measures the structure factor S(Q) in wide Q region before and after temperature treatment[1]. From the S(Q) measurements, by the neutron or X-ray diffraction method[2] we can calculate the pair correlation function g(r) or radial distribution function RDF(r), using the Fourier transform procedure

$$RDF(r) = 4\pi r^2 n + \frac{2r}{\pi} \int_0^\infty [S(Q)-1]\, Q.\sin(Qr)dQ \qquad (1)$$

or

$$G(r) = 4\pi rn\,[g(r) - 1] = \frac{2r}{\pi}\int_0^{\infty} [S(Q) - 1]\, Q.\sin(Qr)dQ \qquad (2)$$

Function RDF(r) modulates about $4\pi r^2 n$ and usually has about four to five peaks before becoming equal to $4\pi r^2 n$. This actually means that short-range topological order exists in amorphous materials. The most effective function in the study of the structural relaxation of amorphous materials (instead g(r) or RDF(r)) is the so-call reduced RDF(r) G(r). In the case of binary or multi-component amorphous materials the partial pair functions $G_{ij}(r)$ are components of the total reduced RDF(r) G(r)[2]. Generally, all mentioned correlation functions show oscillations at low values of r which are spurious (the error limits of the experiment). For small values of S(Q) data, (equations 1 and 2), the quantity S(Q) – 1 becomes small and from the experimental point difficult to measure accurately, but the product Q[S(Q) – 1] may still be appreciable. From available S(Q) data[5] we calculated the pair correlation functions g(r) and G(r) for binary amorphous ferromagnetic $Fe_{0.8}B_{0.2}$, shown in Fig. 1.

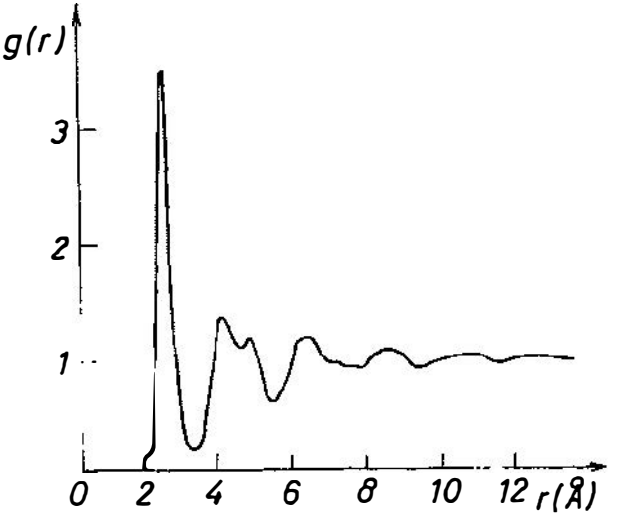

Fig. 1.
Pair correlation function g(r) at 300 K/

It is very easy to conclude that the structure of amorphous materials[3,4] is less ordered than in liquid metals.

2. DISCUSSION AND RESULTS

Namely, two types of structure order exist: the short-range, which involves a rearrangement of the constituent ions and long-range, which involves a topological structure change[6]. The first one is a reversibile process and other one irreversible. Both of

tham can be studied using the diffraction method. The changes that occur in the reduced RDF(r) before and after temperature annealing is given as

$$\Delta G(r) = G(r)_{\text{annealed}} - G(r)_{\text{as quenched}} \tag{3}$$

and it describes the effect of structure relaxation. To extract information about the local structure the diffraction method analysis is insufficient since it is relatively intensitive to the detailed structure order. The different structure defects such as vacancies, corresponding to the free volume, exist in amorphous materials (like in liquids[7,8]). To study their influence on surrounding ions it is good to approximate the reduced RDF(r) G(r) as a function of local levels of stress p[9]. Namely G(r) can be expanded in Taylor's series in the neighbourhood of the minimum hydrostatic pressure value p as

$$G_p(r) = G_o(r) + \frac{\partial G(r)}{\partial r}\ \xi p + \frac{1}{2}\frac{\partial^2 G(r)}{\partial r^2}\ \xi^2 p^2 + ... \tag{4}$$

where ξ is constant beyond the first peak in S(Q) and $G_o(r)$ is the RDF(r) for atoms with p=o. According to the definition of G(r), and since the structure relaxation is a bulk quantity, one need's to calculate the average value of $G_o(r + \xi p)$ instead of G(r), where actually all odd terms in the above equ. vanish[9]

$$G_o(r + \xi p) \cong G_o(r) + \frac{\xi^2}{2}\frac{\partial^2 G(r)}{\partial r^2}\ \langle p^2 \rangle \ ..... \tag{5}$$

since $\langle p \rangle$ corresponds to the macroscopic external pressure. On the other hand, the atomic stress distribution $\langle p^2 \rangle$ is associated with the local atomic level stress (fairly large value), tensor $\sigma_i^{\alpha\beta}$. In case of central forces (isotropic system) tensor $\sigma_i^{\alpha\beta}$ can be written as[10]

$$\sigma_i^{\alpha\beta} = \frac{1}{2V_i}\sum_{j=1}^{N}\frac{\partial\varphi(r)}{\partial r}\Big/_{ij}\cdot\frac{r_{ij}^{\alpha}\, r_{ij}^{\beta}}{/\vec{r}_{ij}/} \tag{6}$$

where the atomic volume V_i is equal to $\frac{4\pi}{3}\cdot\bar{a}_i^3$ ($\bar{a}_i$ — is the effective atomic radius) and $\frac{\partial\varphi(r)}{\partial r} = \dot{\varphi}(r)$ is the first derivative of the interatomic potential $\varphi(r)$.

For macroscopically isotropic sistem, as is the case with amorphous materials, it is desirable to use the rotationally invariant parameter p instead of $\sigma_i^{\alpha\beta}$, where p can be defined[11] as

$$p \equiv \frac{1}{3}\sum_i \sigma_i = \frac{1}{6V_i}\sum_{j=1}^{N}\dot{\varphi}(r)\Big/_{ij}\, r_{ij} \tag{7}$$

where $p_i (i = 1, 2, 3)$ are three principal stresses. Parameter p is the local hydrostatic pressure which describes the fluctuation[9] as

$$\bar{p} \equiv \langle p^2 \rangle^{1/2} = \frac{1}{6V_i} \left[\int_0^\infty f(r)\, dr \right]^{1/2}; \text{ where } f(r) = g(r).r^4 \; |\dot{\varphi}(r)|^2 \qquad (8)$$

In order to study the structure changes (ie. the fluctuations of the local density), one needs to calculate the quantity f(r). To do that, as it is clear from equ. 8 one needs to know the structure factor S(Q) or its Fourier transform g(r) and the particular interatomic potential $\varphi(r)$. For many amorphous materials[12] S(Q) is usually measured, but the interatomic potential $\varphi(r)$ for disordered materials (like amorphous materials) can be described by pseudopotential method[12], Lennard-Jones (12–6) potential, Morse-type[13] and Jonson-type[14] interatomic potential $\varphi(r)$. Generally, every one of them has some parameter(s) which have to be fitted into some physical quantity which describes the material.

Using the measured structure factor data for amorphous alloy[5] $Fe_{0.8}B_{0.2}$ we calculated functions g(r) and G(r), (equ. 2) and using Morse-type interatomic potential[13] we calculate $|\dot{\varphi}(r)|^2$

$$\varphi(r) = \epsilon \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right]; \quad |\dot{\varphi}(r)|^2 = 4\alpha^2 \epsilon^2 \left| e^{-\alpha(r-r_0)} \; e^{-2\alpha(r-r_0)} \right| \qquad (9)$$

where coefficients: α — the softness of the interatomic potential $\varphi(r)$ and the ϵ — depth of the $\varphi(r)$ were chosen as 4 and 0.5 eV, respectively. A problem occured in determining the r_0 parameter since we used S(Q) data for a total structure (summ of partial structure factors) which means that we had to use the equilibrium distance r_0 between pairs Fe-Fe, Fe-B and B-B (in average r_0 was chosen as 0.276 Å). For the mentioned parameters the quantity f(r) was calculated and plotted in Figure 2. The curve shows an oscillating beha-

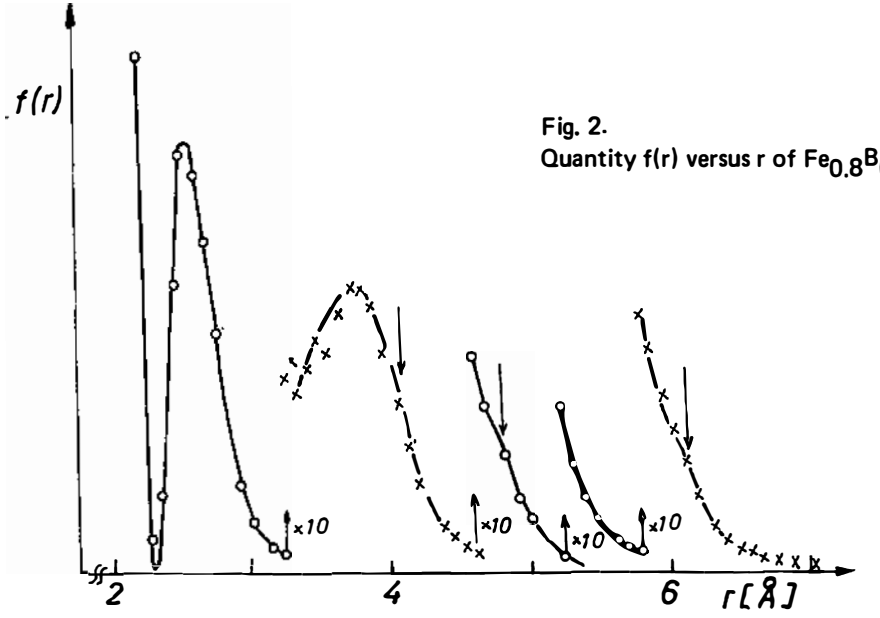

Fig. 2.
Quantity f(r) versus r of $Fe_{0.8}B_{0.2}$

viour with a singularity at $r = r_o$. The shape of the second peak is different compared to the symmetric first one, due to different relaxation preocesses in $Fe_{0.8}B_{0.8}$. Namely, relaxation processes in amorphous materials are caused by different structure arrangements of the pairs, (three atoms for multi-components materials). Also, one needs to expedt structure rearrangement around the structure defects such as vacancies. One way to study experimentally the influence of the defects in relaxation processes (the defects are trapped in amorphous materials during their production) is thermal anealling study[14]. This kind of study is now in progress and we expect some results very soon.

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