Analysis of atomic structure of amorphous metals in the frame of percolation theory

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Abstract. Atomic structure of Re-Tb amorphous alloys (AA) was investigated by computer simulation method. The analysis of atomic structure of AA was performed within the framework of percolation theory and fractal geometry. Atomic clusters were determined as atomic groups of one type that are in the distances from each other not exceeding a percolation radius $r_c$. In the simplest case atoms belong to one cluster if they are in the immediate contact with each other. The size distribution of clusters, probability of belonging of the atom to the largest cluster, fractal dimensionality of the percolation cluster and concentration dependence of percolation radius were calculated. Correlation between magnetic properties of AA and their cluster structure was established.

1. Introduction

Atomic structure of amorphous metallic alloys is usually studied by X-ray diffraction method [1]. However, as it is known, the diffraction experiment allows us to obtain only averaged information on the atomic structure of amorphous alloys: such structural characteristics as radial distribution functions (RDF) and parameters of short-range order calculated from the RDF. This drawback encourages one to construct and analyze computer models of atomic structure of AA because the models give the atomic coordinates of the system.

However, even the traditional computer models as well as diffraction experiments do not allow one to establish the rules of atomic arrangement for amorphous materials. Such rules are well-known for crystals (translation symmetry) and for quasicrystals (rotational symmetry). But in amorphous structures the laws of spatial arrangement of atom are unknown. For this reason we used a new method for analysis of structure of AA based on application of percolation theory and fractal geometry [2-4].

2. Simulation technique

Simulations of atomic structure of Re-Tb AA were carried out using the molecular dynamics method [2]. As an initial atomic configuration we chose random distribution of 7000 atoms inside the basic cube with periodical boundary conditions. For numerical solving of equations of motion the Verlet algorithm in the velocity form was used. Integration step was 2.10-15 sec, relaxation was conducted during 5000 time steps. Simulation was conducted at constant temperature 300 K. For the description of interatomic interaction in amorphous metallic alloys we constructed the model polynomial potential [5]. Parameters of the potential were found from the atomization energy, bulk modules and atomic volumes for corresponding crystalline analogues.
The reduced RDF $G(r)$ calculated for the model of Re$_{82}$Tb$_{18}$ AA is in good agreement with the $G(R)$ function obtained from the X-ray diffraction experiment [6] (figure 1). For the models of the Re$_{100-x}$Tb$_x$ ($x=36, 53, 71$ and $89$ at. %) AA positions and shape of the first peaks and positions of the following peaks on the RDF also agree with the experiment.

![Figure 1](image-url). Reduced distribution functions $G(r)$ of Re$_{82}$Tb$_{18}$ AA. Solid lines – experiment, dotted lines – model.

3. Results and discussion

Atomic clusters were defined as follows: the cluster is a group of atoms of one type (terbium) which are in direct contact with each other, i.e. they are the nearest neighbours. The percolation radius $r_c$ (parameter which determines belonging of an atom to the cluster) was chosen equal to the distance to the first minimum of the partial RDF $g_{Tb-Tb}(r)$:

$$r_c = 0.4329\, \text{nm} = 1.22\,d_{Tb}.$$

We show in figure 2 the partial structure of the subsystem of the Tb atoms (the projection on the XY plane) for several compositions and the corresponding size distribution of clusters $N-nN$, where $N$ is the number of atoms in the cluster and $n$ is the number of clusters having the size $N$. The largest cluster is shown with links between the neighbouring atoms.

In figure 2a the subsystem of the Tb atoms for $10\%$ Tb is shown. Black circles represent atoms in the largest cluster in the model. White circles represent the rest of the Tb atoms. The Re atoms are not shown there. It is seen that at $10\%$ Tb a great number of small clusters exist, all the clusters are friable and extensive, and there are no compact ones.

Then we increased the concentration of the Tb atoms by $3\%$ only (figure 2(b)). At concentration of $13\%$ Tb one large cluster is formed which connects two opposite sides of the basic cube. Thus, near this concentration the percolation transition takes place. The shape of the size distribution of clusters changes when changing concentration of the Tb atoms. At $13\%$ Tb one large cluster is distinguished, the number of small clusters rapidly decreases.

Then we increased the concentration of the Tb atoms by $2\%$. In figure 2(c) the subsystem of the Tb atoms for $15\%$ Tb is represented. At this concentration almost all the atoms belong to the largest cluster. With increasing the concentration of the Tb atoms the number of small clusters rapidly decreases. The small clusters associate with the largest cluster. The large and then small pores in it disappear, the cluster becomes compact. The dependence of probability $P(x)$ that an atom belongs to the largest cluster with increasing concentration of the Tb atoms is shown in figure 3. It has the shape which is characteristic for geometrical phase transitions and represents a diffuse step. The value of $P(x)$ was determined as the ratio of the number of the Tb atoms in the largest cluster to the total number of the Tb atoms in the system.

As it is known from percolation theory, the percolation cluster is a fractal object [7, 8]. Fractal properties of the percolation cluster are connected with its scale invariance (self-similarity): the cluster
Figure 2. Projection of the subsystem of Tb atoms for Re$_{100-x}$Tb$_x$ (a – x=10, b – x=13, c – x=15 at. %) AA on the XY plane and size distribution of clusters. $N$ is the number of atoms in a cluster, $n$ is the number of clusters with the size $N$. 
Figure 3. Dependence of probability of belonging of an atom to the largest cluster on composition of the alloy.

Figure 4. Calculation of fractal dimensionality of the percolation cluster. \( R \) is the radius of the sphere, \( N \) is the number of atoms of the percolation cluster in the sphere of radius \( R \).

has the pores of all sizes, from the atomic diameter up to the size of the basic cube, as it is seen in figure 2(b). The value of fractal dimensionality of the percolation cluster is \( D=2.5; \) which was averaged over many realizations of the model (figure 4). It is close to the theoretical value \( D=2.54 \) for well-known lattice percolation problems [7, 8].

Since the value of dimensionality is closely connected with the values of critical exponents \( \beta \) and \( \nu \), then we can come to a conclusion that universality of critical exponents which takes place for lattice problems also extends to the amorphous structure.

The proposed percolation model is useful for the description of magnetic properties of amorphous alloys in which the atoms having their own magnetic moment are randomly distributed in the paramagnetic matrix.

In the Re-Tb AA in the wide compositional region a maximum on temperature dependence of dynamic magnetic susceptibility \( \chi(T) \) and irreversibility of magnetization \( M(T) \) are observed [9]. It is evidence of the spin-glass phase transition. Transition temperature \( T_f \) increases when increasing concentration of magnetic ions. The transition is observed only in the alloys containing more than 13% of magnetic atoms, i.e. the magnetic ordering is observed only above the percolation threshold in the system.

References
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