Computer simulation of atomic structure of rhenium-based amorphous alloys

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Abstract. Using the molecular dynamics method, we constructed the computer models of Re$_{100-x}$Tb$_x$ (x=13–89 at. %) amorphous alloys. The statistical geometry analysis of the structure on the basis of Voronoi polyhedra was conducted. We calculated the topological characteristics of the Voronoi polyhedra constructed around Re and Tb atoms and studied their dependence on the composition of the alloys.

1. Introduction
Binary amorphous alloys of rhenium with transition metals (V, Nb, Ta, Hf, W) are of great interest because they have the very high thermal stability [1]. Atomic structure of amorphous alloys of Re-Ta, Re-Hf and Re-Tb systems was studied earlier by X-ray diffraction method [2–4]. But it became evident that only experimental results (structure factors, radial distribution functions and parameters of topological short-range order) are insufficient for complete understanding of atomic structure of these materials. This encourages us to construct and analyze computer models of these binary amorphous alloys. Earlier we reported on the results of computer simulation of Re-Ta [5] and Re-Hf [3] amorphous alloys. In this paper we present the results of statistical geometry analysis of molecular-dynamics models of Re-Tb amorphous alloys in the wide compositional region.

2. Computational technique
Simulation of atomic structure of Re$_{100-x}$Ta$_x$, Re$_{100-x}$Tb$_x$ and Re$_{100-x}$Hf$_x$ was carried out using the molecular dynamics method. As an initial atomic configuration we chose random distribution of 7000 atoms inside the basic cube with periodical boundary conditions. For numerical solving equations of motion the Verlet algorithm in the velocity form was used. Integration step was 2·10$^{-15}$ s, relaxation was conducted during about 5000 time steps. Simulation was conducted at constant temperature 300 K with correction of temperature on each time step by means of velocity scaling.

For the description of interatomic interaction in amorphous metallic alloys we constructed the model potential represented as a polynomial of the fourth power [5]:

$$U(r) = \begin{cases} C_1 \cdot (r - r_k)^4 + C_2 \cdot (r - r_k)^3 + C_3 \cdot (r - r_k)^2 & \text{at } r \leq r_k \\ 0 & \text{at } r > r_k \end{cases}.$$  (1)
Here \( r_k \) is a cut-off radius of the potential. Coefficients \( C_1, C_2, C_3 \) were found as a solution of the system of three linear equations which connect the potential energy, its first and second derivatives with parameters for crystalline analogues:

\[
\begin{align*}
\varphi(a) &= -A \cdot E_a, \\
\varphi'(a) &= 0, \\
\varphi''(a) &= \frac{18Kv}{a^2},
\end{align*}
\]

where \( \varphi(r) \) is potential energy of a crystal calculated per atom as a sum of pair potentials [6] defined by formula (1), \( E_a \) is atomization energy, \( A \) is coefficient of order of unity, \( a \) is equilibrium interatomic distance, \( K \) is bulk modulus, \( v_a \) is volume per atom.

Introduction of the coefficient \( A \) is caused by the fact that potential energy in amorphous and crystalline state is not equal. The value of \( A \) was chosen so that coincidence of the model and experimental RDF would be achieved.

The numerical values of the coefficients for the Re-Tb system are given in Table 1.

\[
\begin{array}{cccccc}
\text{Sort of the potential} & C_1 \ (10^3 \text{ eV nm}^{-4}) & C_2 \ (10^3 \text{ eV nm}^{-3}) & C_3 \ (10^2 \text{ eV nm}^{-2}) & r_k \ (\text{nm}) & A \\
U_{\text{Re-Re}} & -6.4188 & -3.9867 & -4.5543 & 0.3699 & 1.82 \\
U_{\text{Re-Tb}} & -2.2434 & -1.6204 & -2.1293 & 0.4239 & 1.49 \\
U_{\text{Tb-Tb}} & 0.1062 & -0.2214 & -0.4441 & 0.4779 & 0.70
\end{array}
\]

The Voronoi polyhedra were constructed as the space regions where all points are closer to the center of the given atom than of the center of any other atom of the system [7]. The center of each atom was connected by line segments with its 30 nearest neighbours, through the centers of these segments we draw the perpendicular planes, each of them divides the space into two half-spaces. The Voronoi polyhedron is found as intersection of all half-spaces containing the center of the given atom.

### 3. Results and discussion
We studied atomic structure of amorphous alloys of the Re\(_{100-x}\)-Tb\(_x\) system with six compositions: \( x = 13, 18, 36, 53, 71 \) and 89 at. % Tb. The reduced distribution functions for these alloys are in a good agreement with the experimental ones [4].

For the models of different compositions we constructed the Voronoi polyhedra of three types: total and partial, around the Re atoms and around the Tb atoms. We calculated the distributions of the polyhedra by the number of faces, of faces by the number of sides (figure 1), and distributions of the polyhedra by topological indexes \( n_3-n_4-n_5-n_6-n_7 \), where \( n_3 \) is the number of triangular faces, \( n_4 \) is the number of quadrangular faces etc (figure 2). We calculated the average values of the number of faces, which gives the geometrical coordination number, and the average number of sides (table 2).

\[
\begin{array}{cccc}
\text{Table 1. Parameters of the polynomial potential.} \\
\text{Sort of the potential} & C_1 \ (10^3 \text{ eV nm}^{-4}) & C_2 \ (10^3 \text{ eV nm}^{-3}) & C_3 \ (10^2 \text{ eV nm}^{-2}) & r_k \ (\text{nm}) & A \\
U_{\text{Re-Re}} & -6.4188 & -3.9867 & -4.5543 & 0.3699 & 1.82 \\
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\end{array}
\]

\[
\begin{array}{cccc}
\text{Table 2. Average number of faces} \langle F \rangle \text{ and average number of sides} \langle S \rangle \text{ of the faces of the Voronoi polyhedra for the models of Re-Tb amorphous alloys.} \\
\text{Parameters} & \text{Re\(_{87}\)Tb\(_{13}\)} & \text{Re\(_{47}\)Tb\(_{53}\)} & \text{Re\(_{11}\)Tb\(_{89}\)} \\
\text{Around Re} & \text{Around Tb} & \text{Around Re} & \text{Around Tb} & \text{Around Re} & \text{Around Tb} \\
\langle F \rangle & 13.60 & 16.10 & 13.11 & 14.76 & 11.32 & 14.26 \\
\langle S \rangle & 5.12 & 5.25 & 5.08 & 5.19 & 4.94 & 5.16
\end{array}
\]
Figure 1. Distributions of Voronoi polyhedra by the number of faces (on the left) and distributions of faces by the number of sides (on the right): (a) – Re\textsubscript{87}Tb\textsubscript{13}, (b) – Re\textsubscript{47}Tb\textsubscript{53}, (c) – Re\textsubscript{11}Tb\textsubscript{89} amorphous alloys. White circles correspond to polyhedra constructed around Re, black circles – around Tb atoms.

We studied dependence of these distributions on composition of the alloys. The distribution of faces by the number of sides does not depend on the composition and of the sort of atom on which the polyhedra were constructed. When approaching to the middle of the concentration interval the total number of polyhedron types increases. The latter is explained by increasing of topological disorder in atomic arrangement and correlates with increasing of mean-square deviation of atomic positions in the first coordination sphere [2, 3].

Amorphous alloys of all studied compositions are characterized by the same set of the most frequently occurring Voronoi polyhedra. The polyhedra with topological index 0-0-12-0, which is typical for local icosahedral environment, constitute up to 10 % of all polyhedra. The polyhedra with the indexes 0-1-10-2, 0-1-10-3, 0-2-8-2, 0-2-8-4 and 0-3-6-4 form the considerable part in the structure. They are obtained by slight modification of the 0-0-12-0 polyhedron and correspond to local coordination polyhedra that represent distorted icosahedra.
Figure 2. Distribution of the most frequently occurred types of Voronoi polyhedra (with the fraction more than 2 %) constructed around Re atoms (on the left) and Tb atoms (on the right).

(a) – Re\textsubscript{87}Tb\textsubscript{13}, (b) – Re\textsubscript{47}Tb\textsubscript{53}, (c) – Re\textsubscript{11}Tb\textsubscript{89} amorphous alloys.

References
[1] Barmin Yu V, Zolotukhin I V, Vavilova V V, Kovneristyi Yu K, Obvintsev Yu A and Stognie O V 1989 Doklady Physical Chemistry 2100
[2] Samoilov V G, Bataronov I L, Roshchupkin S A and Barmin Yu V 1995 Bulletin of the Russian Academy of Sciences. Physics 591729
[3] Barmin Yu V, Lebedinskaya E V, Bataronov I L and Bondarev A V 2000 Mater. Sci. Forum 321-324519
[4] Bondarev A V, Bataronov I L and Barmin Yu V 2004 Vestnik VGTU. Seriya Materialovedenie 1.1539 (in Russian)
[5] Bataronov I L, Bondarev A V, Barmin Yu V 2000 Bulletin of the Russian Academy of Sciences. Physics 641329
[6] Animalu A O E 1977 Intermediate Quantum Theory of Crystalline Solids (Englewood Cliffs: Prentice-Hall, Inc.)
[7] Medvedev N N 2000 The Voronoi–Dalauney method in investigation of the structure of non-crystalline systems (Novosibirsk: SO RAN, SRC OIGGM) (in Russian)