Anelastic relaxation in non-crystalline metals: geometrical aspects

Yu V Barmin, I L Bataronov, A V Bondarev and V V Ozherelyev
Voronezh State Technical University, 14 Moskovski prospekt, Voronezh 394026, Russia
E-mail: bondarev@vmail.ru

Abstract. Using the molecular dynamics method we constructed a model of atomic structure of amorphous Ta. On the basis of Voronoi–Delaunay tessellation the study of interatomic voids in the model was conducted. Information on the spatial arrangement of voids was obtained and distribution of voids by sizes was calculated. According to the obtained results, we made a conclusion of principal impossibility of anelastic relaxation of interstitial metalloid atoms, which is connected with geometrical difference of the structure of crystalline and amorphous metals.

1. Introduction
In metallic glasses it was not obtained decisive experimental evidence of anelastic relaxation, caused by interstitial atoms – the point defects of atomic structure (the counterpart of Snoek-type relaxation in crystals [1]), in spite of considerable efforts, undertaken in this direction. The unique exception is relaxation caused by hydrogen atoms discovered by B.S. Berry [2]. This suggests that there obviously exists some prohibition of fundamental nature on the realization of this type of anelastic relaxation mechanisms in metallic glasses [3].

For metallic glasses, in the absence of the necessary theoretical approach and incompleteness of the experimental data, the only possibility of analysis of relaxation mechanisms on the atomic level is the application of computer simulation methods which are successfully applied in the present time for solving of such problems in crystals.

For investigation of possibility of existence of the Snoek-type relaxation in amorphous metals it is necessary to have data on the spatial arrangement of large voids in which metalloid atoms can locate. In this paper on the basis of Voronoi–Delaunay approach we studied interatomic voids in the molecular-dynamics model of amorphous tantalum.

2. Simulation technique
Simulation of atomic structure of amorphous Ta was performed by molecular dynamics method. As an initial configuration, 7000 Ta atoms were randomly placed into the cubic cell with periodic boundary conditions. Dimensions of the cube were chosen so that density of the model structure corresponded to the real density of the material. For numerical integration of equation of motion the Verlet algorithm in the velocity form was applied. The integration step was $2 \times 10^{-15}$ sec. Relaxation was conducted during 5000 time steps at the constant temperature 300 K.
For description of interatomic interaction we used the spherically symmetrical pair potential having the form of a polynomial of the fourth power which was successfully applied earlier for simulation of atomic structure of amorphous alloys of the Re-Ta system [4].

Analysis of interatomic space structure was performed using the Voronoi–Delaunay approach [5]. An initial element for void description is Delaunay simplex. It is determined by four mutually nearest atoms and represents a tetrahedron with vertices in the centers of these atoms. With the help of the Delaunay simplex one can determine a simplest (simplicial) void: it is an empty volume between these four spheres. On the edges of the simplex the gaps are situated which lead into the simplex.

The main tool for interatomic space study is a Voronoi network – a set of edges and vertexes of the Voronoi polyhedra constructed for all atoms of the system. Each node of the Voronoi network is a center of a circumscribed sphere of some Delaunay simplex and at the same time it is a center of an interstitial sphere, i.e. the sphere inscribed between the four atoms.

The nodes of the Voronoi network are locally the “deepest” points of the interatomic space, they are most distant from the nearest spheres. The network node indicates some elementary void which can be characterized by the value of the radius of the corresponding interstitial sphere [5].

3. Results and discussion
For quantitative description of the voids in the structure of amorphous Ta we used the radiiuses if interstitial spheres. On the distributions of the radii of interstitial spheres (figure 1) and of the radii of gaps of simplicial voids (figure 2) two maxima present which correspond to the tetrahedral and octahedral atomic configurations.

![Figure 1. Distribution of radii of interstitial spheres $R_S$ (in the units of diameter of Ta atom).](image1)

![Figure 2. Distribution of gaps of simplicial windows $R_W$.](image2)

The first maximum of distribution of the radii of simplicial gaps $R_W$ falls on $0.11 d$ ($d = 0.292$ nm is diameter of Ta atom) and corresponds to passageways between dense atomic triplets. The second maximum falls on approximately $0.22 d$, which is close to a radius of a sphere inscribed into a regular octahedral configuration of hard spheres. From figures 1 and 2 it is also seen the presence of long tail of the distribution in the region of big radiuses which indicates the presence of large voids in the model. The maximum radius of interstitial spheres is about $0.21$ nm ($0.75 d$).

In figure 3 we show the spatial arrangement of voids with radii exceeding $0.075$ nm ($0.26 d$). Such voids are sufficiently large and the metalloid atoms, for example, the carbon atoms, can locate in them. From the figure it is seen that the largest voids in the amorphous system are arranged irregularly in contrast to a crystalline system. An interstitial metalloid atom in an octahedral void of a bcc metal al-
ways have possibility to jump in a similar neighbouring void (the Snoek-type relaxation is sequent of this), but in the case of amorphous structure it proves to be impossible.

![Figure 3. Arrangement of interatomic voids in the model of amorphous Ta. Radii of the voids exceed 0.075 nm.]

In the previous works it was revealed that anelastic relaxation of interstitial metalloid atoms (B, C, Si) in non-crystalline metals was not observed experimentally and, probably, is impossible due to the following obvious circumstances:

(i) A point defect connected with an interstitial atom is not a dipole in amorphous metals because distortions generated in arrangement of surrounding atoms have no symmetry axis;

(ii) It is not elastic dipole in the strict sense because the stresses arising on the atomic level rapidly decrease to the values much smaller than in crystals, due to insignificant cooperative displacement of surrounding atoms, i.e. the interstitial atom becomes a matrix atom.

In this paper we presented the third, the most obvious and simple proof connected with geometrical difference in the structure of crystalline and amorphous metals.

References

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