The research of the structure of amorphous metals by molecular dynamics method

G M Poletaev¹, V Yu Krasnov¹, M D Starostenkov¹ and N N Medvedev²

¹Altay State Technical University, Barnaul, Lenin Street, 46, 656038, Russia
²Biysk Pedagogical State University, Biysk, Korolenko Street, 53, 659333 Russia

E-mail: gmp@rol.ru

Abstract. The paper is concerned with the research of the dynamics of amorphous Ni structure by molecular-dynamics method. Ni was obtained from the melt state by a superrapid cooling. It was shown that the structure of amorphous metals could have at least two variants of the structure, depending on the velocity of cooling. The structure contained conjugated and variously deformed tetrahedrons at the cooling using velocities of $10^{14}–10^{15}$ K/s. Franck-Casper phase consisting of conjugated and variously deformed icosahedrons formed at the velocity of nearly $10^{13}$ K/s. The formation of FCC and HCP nanocrystals competing with Franck-Casper phase took place at the above mentioned velocity of cooling.

1. Introduction

Metallic glasses are obtained by a superfast cooling of the melt (spinning, centrifuging, flattening out the metal drop, extracting), or at the deposition of gaseous phase on a base layer using helium temperatures. In the first case, cooling velocities $10^4–10^7$ K/s are reached [1]. But it is shown in [2] that an amorphous state of Ag, Cu, Ni and Pb can be obtained at the velocities of $10^{11}–10^{13}$ K/s. At present, similar velocities are reached only at the deposition of a gaseous phase on a cold base layer. It is reported in paper [3] that in this case the following velocities of $10^{13}–10^{15}$ K/s are noticed.

The microstructure of amorphous metals is presented as a metastable non-polycrystal state with a high degree of short range ordering [4, 5]. Numerous X-ray data and the results of computer experiments testify to non-polycrystal glass metals and high degree of short range ordering [4, 6, 7]. It is also reported on the predominance of tetrahedron packing in such cases [4, 5, 7]. Numerous researches made mainly by computer simulation show that almost any amorphous metals contained large number of nearly ideal tetrahedrons. It is seen from papers [8, 9] that the conjunction of such nearly ideal tetrahedrons form the long chains (so-called Delon’s chains). But the paper [7] disproves that thesis and proves that clusters made of ideal tetrahedrons contain only two-three tetrahedrons.

Franck and Casper supposed that the structure of amorphous metals consisted of interpenetrated polyhedrons. There are four types of polyhedrons: 12, 14, 15 and 16-top log ones. The structures containing various combinations of conjugated Franck-Casper (F-C) figures were obtained by different researchers theoretically and by computer simulation method.

The present paper deals with the research of amorphous Ni structure by molecular-dynamics method. The structure is obtained by a superfast cooling from the melt state. The main objective of the paper is the determination of an amorphous metal structure in the dependence on velocity and method of cooling by the separation of known structural elements.
2. The methods of experiment

The calculated block of Ni contained 13500 atoms in the molecular-dynamics model. The interactions of atoms were described by Morse’s pair potential, it parameters were taken from paper [10]. Boundary conditions were given as periodical over two axes, free conditions were given over the third axis. The given model was presented as the section of a thin metallic film. Amorphous metal was obtained by a superfast cooling from the melt state to 0 K. The starting structure of the calculated block represented FCC crystal. The initial temperature of 5000 K was chosen that high to minimize the time of the crystal structure destruction and obtaining of the melt. The melting process was being carried out during 10 picoseconds (1000 iterations). Then the calculated block was cooled to 0 K. Three different velocities of cooling: $10^{13}$, $10^{14}$ and $10^{15}$ K/s were considered in the paper. The method of cooling consisted in the decrease of the velocity of atoms at every step of the computer experiment.

Two methods of cooling were used: a linear decrease of temperature of the calculated block ("Method1"), and a linear decrease of the velocities of atoms ("Method2").

The structure of Ni calculated blocks obtained was studied using various visualizers: radial distribution of atoms, and also using original visualizer of phase composition allowing studying the structure inside the calculated block in details, to observe the presence and location of different crystal, quasi-crystal phases and figures corresponding to amorphous structures.

The series of 10 experiments was carried out for each variant of cooling (60 experiments total).

3. Results and discussion

Figure 1 shows the dependencies of temperature on time at the cooling of Ni calculated blocks by two methods. The graphs corresponding to the cooling velocity of $10^{13}$ K/s (see figure 1a) have a horizontal section, the typical one for crystallization process. The coincidence of reference temperature (1728 K) of crystallization and temperatures obtained in the model (1680 to 1850 K) counts in favor of the right choice of interaction potential. During the cooling of melt using the velocities $10^{14}$ and $10^{15}$ K/s, the “step” was not observed on the graphs (figure 1b, 1c). Using structure visualizers, it was found that crystallization was not seen at such velocities.

![Figure 1](image1.png)

**Figure 1.** The dependencies of temperature on time during the cooling using the first (bold face line) and the second (thin line) methods with velocities: a) $10^{13}$ K/s; b) $10^{14}$ K/s; c) $10^{15}$ K/s.

The presence of FCC crystal phase in the cell obtained after the cooling with the velocity $10^{13}$ K/s is supported by the diagrams of radial distribution of atoms (see figure 2).

![Figure 2](image2.png)

**Figure 2.** The diagrams of a radial distribution of atoms for block cooled according to the “Method2” with velocities of: a) $10^{13}$ K/s; b) $10^{14}$ K/s; c) $10^{15}$ K/s. Grey lines - radial distribution of an FCC lattice.
The analysis of the presence of FCC and HCP phases, F-C figures was made. The percentage of elementary cells of FCC, HCP and F-C figures for three different velocities of cooling are shown in table 1. The ordered phase consisting of the conjugated elementary cells at the cooling velocity of $10^{13} \text{K/s}$ was noted. FCC and HCP phases, ordered F-C phase consisting of variously deformed icosahedrons (12-top logs) were observed. F-C structure consisting only of one type of polyhedrons contradicted to F-C model. It was described in papers as the model consisting of several types of polyhedrons. Nevertheless, the structure consisting only of icosahedrons was obtained in paper [11].

The ordered phase took from 80 to 95% of all the volume of the calculated block. Probably, it was amorphous-nanocrystal structure similar to one obtained in paper [12]. The amorphous phase was presented by the conjugated zones of F-C structures.

**Table 1.** Percentage of FCC and HCP elementary cells and F-C figures in the calculated blocks cooled with different velocities.

| Velocity of cooling | Elementary cells count | The part of FCC cells among all elementary cells | The part of HCP cells among all elementary cells | The part of F-C figures among all elementary cells |
|---------------------|------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| $10^{13} \text{K/s}$ | 29-79% | 2-80% | 0-59% | 7-94% |
| $10^{14} \text{K/s}$ | 29-33% | 42-49% | 19-26% | 27-34% |
| $10^{15} \text{K/s}$ | 27-29% | 46-50% | 21-23% | 28-32% |

A fault defect was often observed in FCC nanocrystals. Grains and corresponding grain boundary dislocations were less common. The sizes and positions of ordered zones were unique for each calculated block under study. It was not possible to study the structure of the conjunction of those areas (those transition areas took up to 15-20% of the total volume). It was difficult to determine the dominating phase for the structures obtained at the cooling velocity of $10^{13} \text{K/s}$. In one case, FCC dominated in the model, in the other case – F-C phase consisting of conjugated icosahedrons did. As it is seen from table 1, the percentage of this phase has the biggest spread for the velocity of $10^{13} \text{K/s}$.

The 16-top log F-C figures were not found at all. The total number of F-C figures with 14 and 15 vertexes appeared to be very small – less than 0,1% of the total number.

The number of FCC and HCP elementary cells and F-C figures was high enough in calculated blocks at the cooling velocities of $10^{14}$ and $10^{15} \text{K/s}$. But they were chaotically spread over the volume and did not form conjugated ordered structures. That meant the absence of the corresponding phase.

In the paper, the analysis of the number of tetrahedrons deformed variously in metals under study was made. The regularity was evaluated by two criteria: by the volume ($K_v$) and perimeter ($K_p$).

$$K_v = \left( \frac{V}{V_0} - 1 \right) \times 100\%,$$

$$K_p = \left( \frac{p_1p_2p_3}{p_0^3} - 1 \right) \times 100\%,$$

(1)

Here, $V$ - volume of the tetrahedron; $p_1$, $p_2$, $p_3$ – perimeters of the sides, adjacent to the atom under study; $V_0$ – volume of an ideal tetrahedron; $p_0$ – perimeter of the side of an ideal tetrahedron.

**Figure 3.** The distribution of tetrahedrons by two criteria of regularity in an ideal FCC crystal (a) and calculated blocks cooled using the velocities of $10^{13} \text{K/s}$ (b), $10^{14} \text{K/s}$ (c) and $10^{15} \text{K/s}$ (d).
From the figure 3 two distinct peaks corresponding to two types of tetrahedrons forming FCC lattice can be seen: ideal tetrahedrons and tetrahedrons having deviations in the perimeter. As expected for the metals cooled with velocity of $10^{13}$ K/s, the division of tetrahedrons by the criteria of regularity also had two peaks in the same positions as the case with an ideal crystal (see figure 3a, 3b). In case of metals cooled using velocities of $10^{14}$ and $10^{15}$ K/s, only one peak close to an ideal tetrahedron was noticed in the diagram (see figure 3c, 3d). The majority of tetrahedrons appeared to be insignificantly deformed. It was seen a distinct peak, which is shifted by 2-3% to the bigger perimeter and volume.

Studying the distribution of tetrahedrons in the volume of the calculated block, it was found that ideal tetrahedrons did not form Delon’s chains. The clusters consisting of ideal tetrahedrons, as a rule, contained only two or three conjugated tetrahedrons, but sometimes four ones. Similar result was obtained also in paper [7]. The clusters represented “nuclei of an ideal tetrahedral structure”. The structure around the nuclei also consisted of tetrahedrons, but they were deformed. The further tetrahedrons were from the “nucleus”, the more deformed they were. The average distance between the “nucleus” came up to nearly 10 Å.

4. Conclusion
It was found by molecular dynamics method that amorphous metals can have at least two variants of the structure. The structure of cooled Ni consists of conjugated and variously deformed tetrahedrons at the cooling velocity of $10^{14}$ and $10^{15}$ K/s. In this case “nuclei of an ideal tetrahedral structure” – clusters of two or three conjugated regular tetrahedrons – are noticed. Less ideal tetrahedrons are situated around the nuclei. The deformation of tetrahedrons increases with ranging from the “nucleus”. The average distance between “nuclei” is nearly 10 Å.

F-C phase consisting of conjugated and variously deformed icosahedrons form in metal at the cooling velocity of $10^{13}$ K/s. The formation of FCC and HCP nanocrystals competing with F-C phase takes place at the given cooling velocity. The concentration of 14 and 15 vertexes polyhedrons of F-C is negligible, it does not exceed 0,1%. 16-top log polyhedrons are not observed at all.

Two different methods of cooling were used in the paper: a linear decrease of temperature and a linear decrease of atoms’ velocity. The results obtained by two methods are very similar.

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