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FEATURES OF NUCLEATION AND EVOLUTION OF DEFECT STRUCTURE IN VANADIUM UNDER CONSTRAINED DEFORMATION

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Abstract. Atomic mechanisms of structural transformations leading to fragmentation in vanadium under deformation in constrained conditions without changing its volume are investigated on the basis of the molecular dynamics method. The process of formation of a fragmented structure in a deformed specimen can be divided into two stages. At the first stage, twins nucleate and grow in the crystallite. In the second stage, the orientation of lattice in twins may change due to the intersection of twins leading to their anisotropic deformation. In this case, the directions of stretching and compression of the crystal lattice in the deformed twin quite closely lie in the directions of stretching and compression of the whole crystallite.

1 INTRODUCTION

The mechanical load when large deformations are reached can lead to a fragmentation of the microstructure of the metallic materials. For this purpose, various methods of severe plastic deformation (SPD) are most frequently used, for example rolling, equal-channel angular pressing and torsion under high pressure [1,2]. It is believed that the main mechanism determining deformation-induced fragmentation of grains is dislocation activity such as multiplication and interaction of dislocations, as well as the formation of various configurations of dislocation boundaries. The formation of these dislocation boundaries is due to the fact that dislocation sliding is the prevailing deformation regime in majority of metals when loaded by SPD methods at room temperature with ordinary deformation rates ($<1\ s^{-1}$).

Deformation twinning also plays an important role in deformation of metals [3,4]. It becomes the main regime of plastic deformation at low temperatures and/or at high deformation rates [5,6]. It is due to the fact that the critical shear stress for twinning becomes lower than stress required for dislocation glide. In this case plastic deformation results in the generation of numerous deformation twins in the grains and the spacing between neigboring twin boundaries may reach an order of nanometers. Further deformation leads to the formation of equiaxed grains from twin lamellae. Thus, deformation twinning can be considered as a process preceding the nanoscale fragmentation of material.

The onset and evolution of plastic deformation on a microscopic level determines the deformation behavior of materials at higher scale levels. In view of the smallness of the spatial and temporal scales of the processes computer simulation is a powerful tool for

studying the dynamics of structural transformations at the micro level [7-9]. It should be noted that some of the grains in the bulk can be in the constrained conditions during the deformation of polycrystalline materials that affect their mechanical response under load. In this work, we study the atomic mechanisms of fragmentation of vanadium crystallite under deformation in constrained conditions.

2 SIMULATION DETAILS

The calculations were based on the molecular dynamics method [10,11]. The interatomic interaction in vanadium was described by the Finnis-Sinclair potential [12]. The initial crystallite had a parallelepiped shape and was heated to the room temperature. Periodic boundary conditions were applied in all directions. To simulate the constrained deformation the crystallite was uniformly stretched in one direction and compressed in other two directions without changing its volume. The crystallite was stretched along one of following crystallographic directions: X - $[11\bar{2}]$, Y - [111] and Z - $[1\bar{1}0]$. An analysis of the simulated crystallite structure of was carried out using Common Neighbor Analysis (CNA) [13] and the Dislocation Extraction Algorithm (DXA) [14]. Visualization of obtained structures was performed in the OVITO software [15].

3 RESULTS AND DISCUSSION

It is shown that structural defects begin to nucleate in the material when the threshold value of tensile strain is reached. This value depends on the crystallographic direction of loading. It is minimal when stretching the specimen along the Y direction and maximum for the Z direction. When the threshold value of tensile strain is reached, the potential energy of the simulated crystallite decreases abruptly (Fig. 1).

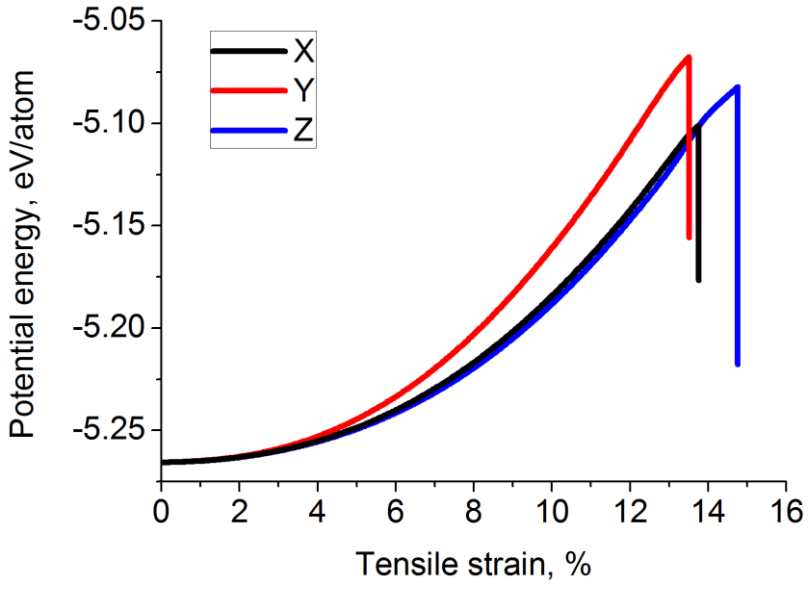

Figure 1: Dependence of the specimen potential energy per atom on the tensile strain along different crystallographic directions

The process of structural rearrangements in the deformed specimens can be divided into two stages. In the first stage, twins nucleate in the specimen, the growth of which is accompanied by the generation of the 1/2 <111> and <100> dislocations. The density of the 1/2<111> dislocations formed is much larger. Dislocations are nucleated at twin boundaries and propagate into the volume of matrix. The dislocation density inside the twins is much lower than in the surrounding volume. Formed twins grow until they intersect with other counterparts. In the second stage, a redistribution of the stresses occurs in the vicinity of intersected twins. This can lead to a reorientation of the crystal lattice in the region of twins and/or a decrease in their dimensions, until they disappear completely. The typical structure of the specimens stretched to a threshold value along different directions is shown in Fig. 2. It is seen in the figure that a large twin is formed when tension is applied along the X direction (Fig. 2a). Stretching along Y and Z directions leads to the formation of a large number of fragments. Moreover, when stretching along the Z direction, the largest number of fragments with the smallest average size is formed (Fig. 2c). The results of calculations showed that the total volume of fragments for specimens stretched along Y and Z directions is practically the same and they occupy approximately 4% of the simulated crystallite volume. The twin formed in the specimen stretched along the X direction occupies 10% of crystallite volume.

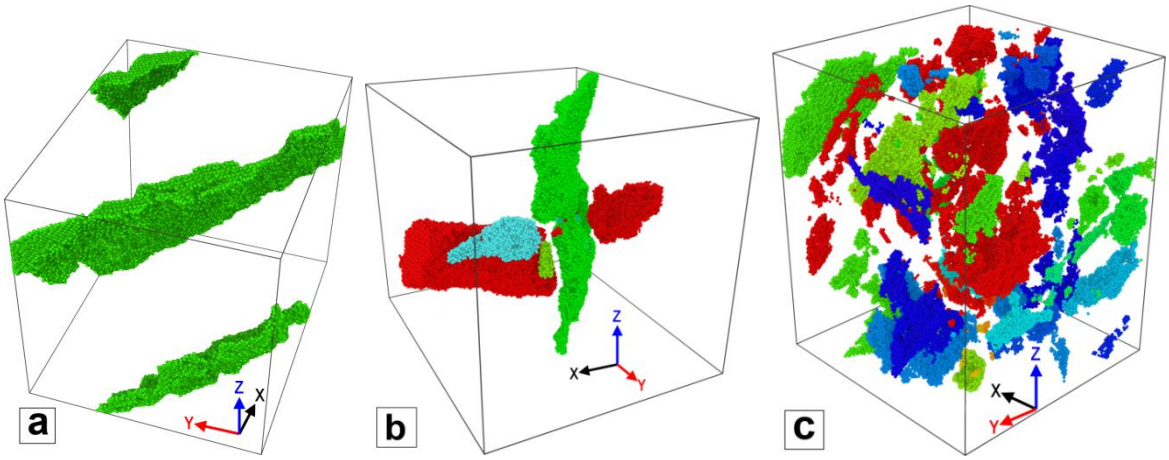

Figure 2: The defect structure of specimens stretched to a threshold value along the X $[11\bar{2}]$ (a), Y [111] (b) and Z $[1\bar{1}0]$ (c) directions. Specimen fragments reoriented relative to the initial lattice are shown. Each fragment has its own color

We have carried out a comparative analysis of the fragment size distribution in specimens stretched along different directions. For this purpose, 10 calculations for each direction were performed and the results were summed. On the basis of these data, two intervals can be distinguished in which the number of fragments differs significantly for various streching directions. Calculations showed that small fragments that contain less than 10 thousand atoms are formed in a larger amount in a specimen stretched along the Z direction than along the Y one. There are no small fragments in a specimen stretched along the X direction (Fig. 3a). For large fragments containing more than 10 thousand atoms, the size distribution is directly opposite: the largest fragments are typical for specimens stretched along the X direction. Their dimensions are 2-3 times larger than the size of fragments for specimens stretched along

X and Y directions (Fig. 3b). The number of such fragments is larger in specimens stretched along the Y direction.

The difference in the number and size of the fragments is related to the orientation of the preferred slip systems with respect to the direction of stretching. As a consequence, at the stage of plastic deformation nucleation a different number of twin nuclei is formed in the crystallite for different load directions. When stretching along the X direction, a twin is formed in one of the {112} planes, which subsequently crosses the entire specimen. When loaded along the Y direction, one nucleus is formed, consisting of two twins oriented at an angle to each other. These twins subsequently become the largest fragments, such as the red and green fragments in Fig. 2b. When stretching along the Z direction, a large number of twins with a thickness of several atomic layers are formed in one region. Their growth is accompanied by the generation of new twins at the periphery of the defective area. Moreover, the rate of increase in their longitudinal dimensions (area) is much higher than the rate of increase in their transverse dimensions (thickness). As a result, the intersection of these twins leads to the formation of a structure consisting of small size fragments (Fig. 2c).

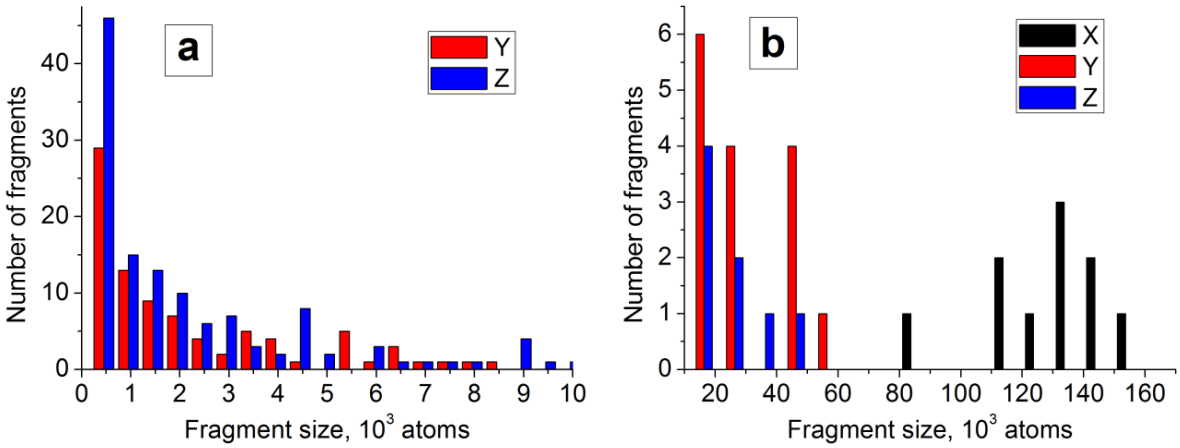

Figure 3: Distribution of fragments by their sizes (<10^4 atoms (a), >10^4 atoms (b)) in specimens for different directions of stretching

All reoriented fragments are formed due to the growth and interaction of twins. Some of them have orientations that differ from twinning ones. Fig. 4 shows such a fragment in a specimen stretched along the Z direction. Initially, when the specimen was loaded, a twin was formed (indicated by the arrow in Fig. 4a). As a result of the twin growth and its interaction with other defects, the orientation of the region in which the twin nucleated has changed. This region and its surroundings are highlighted with a red border in Fig. 4b and are shown in Fig. 4c. The orientation of this fragment does not correspond to the twin, which is clearly seen from comparing the structures in Fig. 4c and Fig. 4d. The latter shows a part of the twin considered, which retained its orientation. An analysis of the structure change in the central region in Fig. 4c showed that its crystal lattice is elastically deformed according to the scheme shown in the inset of Fig. 4a. In the insert, green and blue atoms from two {110} planes are shown, the lines indicate the cross section of the elementary bcc cell by the {110} plane. The arrows show that the lattice is compressed in the <110> direction and stretched in the <100>

direction. It should be noted that the directions of stretching and compression of the crystal lattice in the twin are sufficiently close to the directions of preliminary stretching and compression of the entire specimen. The resulting lattice structure in the reoriented fragment is shown in the inset of Fig. 4b, the cross section of the elementary bcc cell by the {100} plane is highlighted by lines. Thus, the reorientation of fragments of the specimen can occur due to deformation of the formed twins. This deformation is elastic and is realized by the compression and stretching in different directions by a different value. This leads to the formation of a new crystallographic orientation of the lattice without significant rotation of the fragment as a whole.

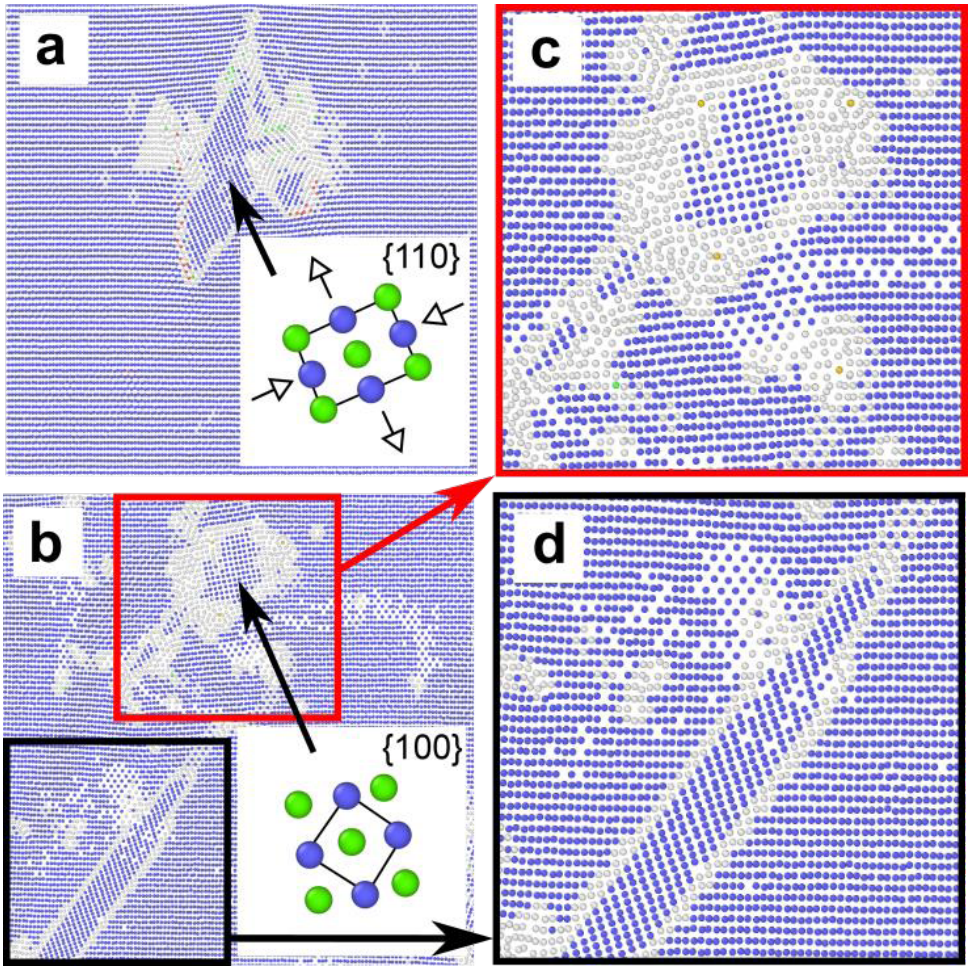

Figure 4: Structure of the two {110} atomic planes of the specimen, stretched along the Z [$1\,\bar{1}\,0$] direction by 14.75%, after stopping the loading in: a) 10 ps b) 70 ps. Figures c and d show enlarged areas in red and black frames in figure b, respectively

4 CONCLUSIONS

The vanadium crystallite behavior under constrained deformation without changing its volume was studied by means of molecular dynamics simulation. Loading of the crystallite leads to nucleation and growth of twins, which is accompanied by the generation of

dislocations. The formation and interaction of twins leads to the fragmentation of the crystallite.

The difference in the number and size of the fragments is related to the orientation of the preferred slip systems with respect to the direction of streching. The twin of maximum size is formed by stretching along the X direction. Stretching along Y and Z directions leads to the formation of a large number of fragments. The greatest number of fragments is formed in the specimen stretched along the Z direction. The volumes of fragmented parts of the specimens stretched along Y and Z directions are almost the same.

The process of fragmentation of the deformed specimens can be divided into two stages. In the first stage, twins nucleate in the specimen, the growth of which is accompanied by the generation of dislocations. Formed twins grow until they intersect with each other. In the second stage, a redistribution of the stresses occurs in the vicinity of intersected twins. This can lead to a reorientation of the crystal lattice in the region of twins and/or a decrease in their dimensions, until they disappear completely.

It is shown that the process of the lattice reorientation in fragments can be realized due to anisotropic deformation of the formed twins. The directions of stretching and compression of the crystal lattice in the deformed twin quite closely lie in the directions of stretching and compression of the whole crystallite.

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