Features of plasticity nucleation in deformed vanadium crystallite under irradiation

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Abstract. Molecular dynamics simulation of the defect structure nucleation in deformed vanadium crystallites under irradiation was carried out taking into account their internal structure. The crystallites studied contained grain boundaries of different types. The behavior of crystallites deformed to values close to the limit of elasticity under irradiation was simulated by the generation of atomic displacement cascades. The energy of the primary knock-on atoms which generated atomic displacement cascades was 5 keV. It was found that atomic displacement cascades in elastically deformed crystallites can lead not only to the formation of radiation defects, but also cause plasticity. It is shown that the nucleation of plasticity in crystallite is associated with elastic waves. These waves are formed in the region of atomic displacement cascade development. Their generation is due to the high-speed thermal expansion of the region in which atomic displacement cascade develops.

1. Introduction

Nanostructured metals and alloys are promising materials in many practical applications [1-4]. They have high strength, hardness and wear resistance due to the increased role of nanoscale and interface effects in their behavior [5, 6]. The high fraction of grain boundaries in the volume significantly changes the features of generation and accumulation of damage in such materials under radiation exposure and mechanical loading.

The main physical reason for this difference was that the mechanisms of plasticity due to the nucleation and propagation of dislocations do not act in nanoscale grains. It should be noted that grain boundaries are barriers that prevent the propagation of atomic displacement cascades from one grain to another under radiation [7, 8]. During operation materials may be under the influence of both mechanical loading and radiation exposure [7, 8].

It should be expected that mechanical loading of nanocrystalline materials in the elastic interval will have a significant impact on their behavior when irradiated with high-energy particle flows. Thus, in the works of [9] it was shown that the atomic displacement cascades in an elastically deformed iron crystal can generate not only point defects and their clusters of different sizes and configurations, but also lead to the nucleation and development of twins. Nucleation of twins is associated with accelerated expansion of the radiation-damaged region. High-speed thermal expansion of the cascade region leads to the generation of numerous elastic waves in the irradiated material [10]. These waves have a significant impact on the mobility of existing and formed defects.
In connection with the above in this paper the features of the generation and evolution of radiation damage in nanostructured vanadium under elastic deformation and radiation exposure are studied.

2. Formalism
The studies were carried out for a nanocrystalline vanadium sample consisting of four grains of approximately the same size. The simulated crystallite had the shape of a parallelepiped, in which the grains were formed on the basis of the construction of a Voronoi tessellation. The size of the sample was 300x200x200 Å. Periodic boundary conditions were set in two directions of the simulated sample. Hard boundary conditions were used in the third direction. A shear load was applied to the crystallite. The thickness of the shifted regions (punches) was 15 Å. The capture atoms were given a constant velocity in the shear direction, in the other two directions their position was fixed. The speed of the punches was 5 m/s. The initial structure of the simulated crystallite of vanadium and the shear loading scheme are shown in figure 1. Calculations were carried out at room temperature. For the generation of atomic displacement cascades, which simulated the radiation exposure, a momentum corresponding to the energy of 5 keV was set to one of the atoms. As in [11-15] calculations were carried out on the basis of molecular dynamics method using computational package LAMMPS [16]. Interatomic interaction was described by manybody potentials obtained in the Finis-Sinclair approximation [17]. The structure of the nearest environment of atoms was identified using Common Neighbor Analysis (CNA) [18]. To visualize the crystallite structure, the OVITO graphic package was used [19].

![Figure 1. Structure of vanadium nanocrystallite and loading scheme. Red regions are the punches. Arrows indicate the direction of punch displacements.](image)

3. Simulation results
The behavior of nanocrystalline vanadium was studied by analyzing the structural changes during shear loading. To do this, the $S_{yy}$ stress and the fraction of atoms which nearest environment changed the relative positions were calculated depending on the magnitude of the shear. The results of the calculations for the direct shear loading shown in figure 1, and in the reverse direction are presented in figure 2ab, respectively. The figure clearly shows the correlation between the stress curves and the fraction of atoms which nearest environment has been changed (hereinafter we will call them non-BCC atoms). For direct shear loading the elastic displacement interval of the capture is about 8 Å, and for the reverse – 10 Å. Anisotropy of elastic behavior is associated with a small number of grains in the simulated crystallite, which leads to a significant asymmetry of the structure relative to the direction of loading.

In both directions the nucleation of plasticity in crystallite is connected with motion of dislocations from grain volume to the grain boundary regions (figure 3ab). This motion is reflected by the first break of the stress curves $S_{yy}$ in figure 2ab. The experimental observations show that this behavior is the
same as dislocation behavior during annealing of nanocrystalline materials [3]. In particular, dislocations from the grain volume move in the direction of the grain boundary regions. Although the total density of dislocations decreases during low-temperature annealing, their density increases in the grain boundary regions, which in turn increases the degree of non-equilibrium of grain boundaries. This leads to the activation of grain boundary processes such as grain boundary sliding, diffusion and interaction with lattice dislocations [20].

Figure 2. Dependence of the fraction of non-bcc atoms (gray curve) and stresses (black curve) on the displacement value of the capture for the direct (a) and reverse (b) shear loading.

Figure 3. Fragment of the grain boundary structure of the crystallite under direct (a) and reverse (b) shear loading. The arrows indicate dislocations. Regions of grains with bcc structure are invisible.

Shear loading leads not only to an increase in the fraction of non-bcc atoms, but also to the formation of strong tensile stresses in certain grain boundary regions. Some adjacent grains may shift in opposite directions during the shear loading, which leads to the appearance of tensile stresses on their boundary. As a result, in the region of this boundary, the atomic volume first increases, and then pores can be formed. In the simulated crystallite, the pore size in diameter was about 15 Å. The results of the calculation showed that grain boundary sliding was the main mechanism for the development of the plasticity of the crystallite.

Calculations showed that the radiation damage of elastically deformed nanocrystalline vanadium can lead not only to the generation of radiation defects, but also to the nucleation and development of plasticity far beyond the radiation-damaged zone. The dynamics of changes in Frenkel pairs during the evolution of the atomic displacement cascade for the crystallites under study is shown in figure 4. It can be seen that the change in the number of point defects on the ballistic and in most of the recombination stages is approximately the same for both samples. Analysis of calculation results showed that an increase in the number of point defects (atomic displacement from the initial lattice sites) at the
recombination stage in the deformed crystallite is associated with the nucleation and development of plasticity, but not the formation of vacancies or interstitials. It is known [9] that the atomic displacement cascade causes the generation of elastic waves, which can initiate nucleation and motion of structure defects, in particular, dislocations. The structural changes of the crystallites during irradiation are shown in figure 5. As seen in the figure, the shear deformation of the crystallite led to the formation of a dislocation in one of the grains (figure 5c). Upon irradiation of this crystallite, elastic waves formed by an atomic displacement cascade caused the movement of this dislocation (figure 5d), which led to an increase in the blue curve at the recombination stage (figure 4).

**Figure 4.** Dependence of the number of Frenkel pairs on time for an undeformed sample (red curve) and with a shift of 9 Å (blue curve). Roman numerals indicate the stages of development of the atomic displacement cascade: I – ballistic, II – recombination, III – primary damage state.

**Figure 5.** Structures of undeformed crystallite (a, b) and with 9 Å punch displacement (c, d) on the ballistic (left column) and recombination (right column) stages of the development of the atomic displacement cascade. The arrow indicates a dislocation, point defects formed by the cascade are green. Atoms with the bcc symmetry of the nearest environment are invisible.
4. Conclusion
The simulation results showed that the shear loading of nanocrystalline vanadium leads to the propagation of grain dislocations to the grain boundary region. As a result, the degree of non-equilibrium of the grain boundaries increases, which facilitates grain boundary sliding and increases the plasticity of the material. Irradiation of a deformed nanocrystalline vanadium leads to the generation not only of radiation damage, but also can initiate nucleation and development of plastic deformation. The nucleation of plasticity is due to the fact that atomic displacement cascades form elastic waves that propagate over long distances and can lead to nucleation and movement of structure defects in a deformed lattice.

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