Peculiarities of grain boundary migration in vanadium crystal under shear loading

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Abstract. The atomic mechanisms of migration of the symmetric tilt grain boundaries in V crystallites under shear loading are studied. The calculations were carried out on the basis of molecular-dynamics method using many-body potentials of interatomic interaction. It is shown that the migration rate of the grain boundaries depends on the misorientation angle and the rate of shear loading. The movement of the grain boundaries has jump-like character, due to jump-like growth and decrease of stresses initiated by shear loading. It is revealed that migration of grain boundaries is realized by a certain sequence of rearrangement of grain atomic planes adjacent to the grain boundary. These planes are by turns rearranged into the structure of the atomic planes of the grain boundary until they are adjusted to the lattice of another grain.

1. Introduction
The properties of materials largely depend not only on the chemical composition, but also on the characteristics of the internal structure, for example, on the density of grain boundaries (GB). The behavior of GB with different types at external actions determines most properties of polycrystalline materials. One of the most important properties of GB is their ability to migrate, which underlies the process of low-temperature recrystallization. The ability to manage this process allows obtaining materials with pre-required properties.

The identification of mechanisms responsible for the GB migration is important both in terms of obtaining new scientific knowledge and in terms of developing new approaches to stabilize the internal structure. New knowledge and practical approaches can be used to inhibit processes of grain consolidation, because this is in many cases an undesirable phenomenon. For a realistic description of the GB migration in a polycrystalline material, it is necessary to take into account a number of parameters, such as 5 macroscopic degrees of GB freedom, the presence of triple and more grain junctions, metastability of the intergranular structure, etc [1]. In addition, it is necessary to take into account the fact that the real materials are crystalline and the crystallinity imposes restrictions on the movement of GB. Experimental techniques that make it possible to reliably monitor the GB behavior in materials are not yet available. Note that molecular dynamics simulation naturally takes into account all these features and parameters in the study of GB migration.

In [2], it was shown on the basis of molecular dynamics simulation that the GB movement along the normal is often associated with the tangential translation of the grains, which leads to a deformation shift of the lattice crossed by the GB. In turn, the shear stresses applied to the
GB can cause its displacement along the normal. The local velocity of GB can be positive or negative with respect to the normal to the GB plane. During the GB migration, one grain grows by reducing another. In this case, GB plays the role of the front on which growth and dissolution processes take place [3]. The behavior of the GB under mechanical loading can also be connected with grain-boundary slip, when one grain as a whole is displaced along the GB plane relative to another grain. Mechanical loading can also lead to rotations of one grain relative to the other. Such rotations are always accompanied by relative displacements of grains by GB [3].

In many cases, the migration has the GB dislocation character. At the same time, high-speed shear loading of a crystallite can lead to the formation of vortex motion of atoms in some region of the tilt GB [4,5]. The diameter of vortex consists of few lattice parameters, and vortex motion is characterized by considerable atomic displacements not only in the direction of loading, but in the plane of the GB. This process is dynamic in nature and accommodation of the material is based on the abnormally high rate of displacement of GB. Migration of GB is realized through coordinated and collective atomic displacements. Despite the fact that the displacement of each atom in the GB region is small, as a result of consistent atomic displacements of the vortex the large region one grain is adjusted under the structure of the neighboring grain.

The aim of this work is to study atomic mechanisms of migration of tilt GBs in vanadium initiated by high rate shear loading.

2. Formalism of simulation
To solve the problem, the molecular dynamics method was used [6–8]. Simulations were carried out with the use of the LAMMPS software package [9]. The interatomic interaction was described by the many-particle potential calculated in the framework of the embedded atom method in the Finis-Sinclair approximation [10]. These potentials allow calculating with good accuracy energy and structure of free surfaces and GBs, energies of point defect formation and migration, elastic characteristics and other properties that are necessary for a correct simulation of crystallite behavior under mechanical loading. The simulated sample was set in the form of a parallelepiped with edge lengths \(9.0 \times 9.0 \times 6.5\) nm\(^3\) and contained about 40000 atoms. In the \(X\) and \(Z\) directions, periodic boundary conditions were used, in the third direction shear loading was applied to sample faces. The sample temperature was 300 K. Simulation was carried out for two samples, one of them had the \(\langle310\rangle(001)\) symmetrical tilt GB, another one had the \(\langle210\rangle(001)\) symmetrical tilt GB. The rate of shear loading along the \(X\) direction in different calculations varied from 1 to 100 m/s. Visualization of the calculation results was carried out using the graphical package OVITO [11]. To construct the grain boundary, we used the gamma-surface minimization algorithm [12]. Simulated sample and scheme of loading is presented in figure 1.

3. Results and discussion
The calculated results showed that the shear loading of the crystallites leads to a displacement of the simulated GBs. The position of the \(\langle310\rangle(001)\) GB at different time instants is shown in figure 2. The velocity of GB displacement is determined by the angle of its misorientation and the rate of the applied shear displacements. The average displacement velocity of the \(\langle210\rangle(001)\) GB for the investigated shear rates lies in the interval from 3 to 280 m/s, increasing with the applied shear rate. In the case of \(\langle310\rangle(001)\) GB, the displacement velocity also increases from 2 to 180 m/s with increasing of the shear rate.

It should be noted that the displacement of the grain boundaries is jump-like in nature, as is clearly seen in figure 3(a). As the shear loading of the crystallite increases, elastic stresses rise. Decrease of stresses is realized by a jump-like displacement of atomic planes parallel to the direction of shear, which are adjusted to the new position of the captures. The correlation of the jumps of atomic displacements and the stresses arising in the sample is clearly seen in figure 3(a, b). At the same time, the highest displacements occur for atoms in the GB region.
Figure 1. Initial structure of a sample, which contains the \(\langle 210\rangle(001)\) GB, and the scheme of loading. Orange indicates the fixed shear regions; blue corresponds to GB region; the arrows indicate the shear loading direction.

Figure 2. Position of the \(\langle 310\rangle(001)\) GB in the simulated crystallite at different time instants after the onset of shear loading: 0 (a), 14.9 (b), 33.2 ps (c). Blue color—the initial position of the GB; green—the current one.

Calculations have shown that the atomic rearrangements in the \(\langle 310\rangle(001)\) and GB \(\langle 210\rangle(001)\) GB regions, which are responsible for the migration of GB, differ significantly.

An analysis of simulation results showed that the displacement of the \(\langle 210\rangle(001)\) GB occurs as a result of atomic rearrangements in three atomic planes: two planes belong to GB region and one plane of the donor grain adjacent to them. In figure 4 the blue color shows the atomic planes belonging to the GB, and the green color shows the plane of the upper grain, which, due to shear loading, will be adjusted to the structure of the lower grain, as shown in figure 4(b).

The integral displacements of atoms in the plane, which are necessary for such a rearrangement, are shown in figure 4(c). It is seen in figure 4(c, d) that the displacements in the \(X-Z\) plane are the same and synchronous. The value of the resulting displacements is about 0.08 nm, and the necessary time for this is 110 ps.

The adjustment of the atomic plane of the upper grain [marked green in figure 4(a)] to the structure of the lower grain occurs as a result of three consecutive displacements in different directions. The duration of each displacement is about 20 ps. The magnitudes of displacements are approximately 0.07, 0.03 and 0.06 nm. As a result of such displacements the green plane
Figure 3. Displacement velocities $V_d$ of the atomic planes from the $\langle 210 \rangle (001)$ GB region, causing its migration (a), and the stresses $S_{xy}$ (b) versus the capture displacement value ($l$). The colors denote the displacements of the three atomic planes. The shear loading rate was 1 m/s.

Figure 4. Structure of the sample with the $\langle 310 \rangle (001)$ GB (a) before loading and (b) after shear the GB to three planes, as well as the projection of the displacements on (c) the $Y$–$Z$ and (d) $X$–$Z$ planes. For clarity, the displacements are increased 3 times. Blue and green indicate the current position of the GB and the plane that has passed from the upper grain to the lower one, respectively. The shear loading rate was 1 m/s.

It should be noted that pronounced displacements are also observed for the atoms belonging to atomic planes located far from the GB during the sample is rearranging. This is due to the fact that a continuous accumulation of stresses occurs in the system as a result of the movement consistently changes to fit the structure of the upper and next the lower planes of the GB, and finally adapts to the lattice of the lower grain.
Figure 5. The sample structure with the \(\langle 210\rangle (001)\) GB (a) before loading and (b) after the GB shifting on six planes. The GB planes are marked by blue color. The plane that has shifted after the displacement of the GB from the upper grain to the lower one is marked by green color. Parts (c) and (d) show the projections of the displacements of atoms on the corresponding planes \(Y-Z\) and \(X-Z\) during the transition of the green plane. The shear loading rate was 1 m/s.

of the captures. The relaxation of these stresses is due to the movement of the GB when the adjustment of the atomic planes of the upper grain to the structure of the lower grain occurs.

The results of the calculations showed that 6 atomic planes simultaneously participate in the displacement of the \(\langle 210\rangle (001)\) GB. The five planes [marked blue in figure 5(a)] constitute the GB and the sixth plane (marked green) belongs to the upper grain. As a result of a more complex sequence of displacements compared to the \(\langle 310\rangle (001)\) GB the green plane is successively changed into the structures of the blue planes and at the last displacement it is adjusted to the structure of the lower grain, as shown in figure 5(b).

4. Conclusions

Based on the molecular dynamics simulation, it has been shown that a high-speed migration of symmetric tilt GB occurs in vanadium crystallites as a result of shear loading. The rate of GB migration as a function of the GB misorientation angle and the shear rate can vary over a wide range and can reach several hundred meters per second. It is shown that the GB movement has jump-like character. A jump in the GB movement occurs when threshold stresses in the loaded sample are reached and leads to their jump-like decrease. Due to the crystallinity of the structure and the symmetry of the tilt GB this process is repeated. It is found that the GB migration is realized due to a certain sequence of displacements of atomic planes of the grain adjacent to GB. These planes by turns are reconstructed into the structure of the atomic planes of the GB until they are adjusted to the structure of another grain. It should be noted that under such a loading scheme for samples with symmetric GB, the formation of traditional structural defects (dislocations and twins) does not occur, despite the high values of the shear displacements.

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