Molecular dynamics simulation of a nonequilibrium grain boundary in titanium under the ultrasonic action

A.A. Mukhametgalina and A.A. Nazarov

Institute for Metals Superplasticity Problems, Russian Academy of Sciences, 39 Khalturin st., 450001 Ufa, Russia

E-mail: a.mukhametgalina@mail.ru

Abstract. Effect of oscillating tension-compression stresses on a nonequilibrium grain boundary containing a disclination dipole in titanium is studied by means of molecular dynamics simulations. The system with nonequilibrium boundary was constructed by joining two bicrystals with tilt boundaries $\Theta = 36.87^\circ$ and $\Theta = 28.07^\circ$, thus the disclination dipole had a strength $\omega = 8.8^\circ$. The system was relaxed and equilibrated at temperature $T=300$ K for 200 ps. Then a sinusoidal stress $\sigma = \sigma_0 \times \sin (2\pi t / \tau)$ with a period $\tau = 160$ ps was applied along $x$ axis at the same temperature and its effect on the structure of the bicrystal was studied. It is shown that under the action of oscillating stresses the nonequilibrium boundary emits lattice dislocations that sink at appropriate surfaces. This process is irreversible and leads to relaxation of the nonequilibrium structure of the boundary. There is an optimal amplitude at which the nonequilibrium boundary emits a sufficient number of dislocations to relieve internal stresses.

1. Introduction

Ultrafine-grained (UFG) materials processed by severe plastic deformation methods have an imperfect structure characterized by long-range internal stresses, the sources of which are nonequilibrium grain boundaries (GB) [1]. Ultrasonic treatment (UST) is one of the promising methods for processing ultrafine-grained metals. Experimental studies show that UST leads to changes in the microstructure and properties of UFG materials. It affects the defect structure of the material and contributes to the reduction of internal stresses, the relaxation of nonequilibrium grain boundaries and the increase in the fraction of high-angle boundaries under certain conditions [2]. Changes in the defect structure affect the mechanical properties of UFG materials. It was shown that preliminary UST led to an increase in the ductility of UFG nickel at room temperature without a decrease in the strength [3]. High-frequency oscillating stresses resulted in the reduction of the flow stress, the increase in elongation and the strain rate sensitivity coefficient during tensile tests of titanium alloy Ti-6Al-4V in the conditions of superplasticity [4].

Computer simulation methods are an important tool for understanding the mechanisms of the effect of ultrasound on the structure of materials. Evolution of disordered dislocation structures in a model two-dimensional grain under ultrasonic influence was studied in [5, 6]. Ultrasonic vibrations cause the movement, interaction and annihilation of dislocations. By molecular dynamics simulations it has been shown in [7] that ultrasonic stresses lead to the generation of lattice dislocations by a nonequilibrium boundary of nickel bicrystal, which results in the compensation of the stress fields of a disclination dipole and the recovery of the equilibrium structure and energy of the boundary. The effect of
ultrasonic vibrations on columnar nickel nanocrystals with nonequilibrium GBs was studied in [8, 9]. It was shown that under oscillating stresses the GBs generated lattice dislocations, which traveled across the grains and were absorbed by opposite GBs thus resulting in a relaxation of the structure.

Most of the theoretical and experimental studies on the effect of ultrasonic treatment have been carried out for cubic metals. However, the effect of ultrasonic treatment on hexagonal metals can be significantly different.

In this study the effect of oscillating tension-compression stresses on a nonequilibrium GB in titanium is simulated by molecular dynamics method following the methods used in [7].

2. Atomistic model and simulation procedure
To study the influence of oscillating tension-compression stresses on the atomic structure of the nonequilibrium GB, an initial structure of hexagonal α-titanium bicrystal containing a tilt boundary with the misorientation axis [0001] was constructed.

The choice of the misorientation axis was based on the fact that in pure α-titanium at room temperature the preferred slip plane is \{1010\} with the direction [1120] [10]. The nonequilibrium boundary was constructed by joining two bicrystals with tilt boundaries having misorientation angles $\Theta = 36.87^\circ$ and $\Theta = 28.07^\circ$, respectively, thus the disclinations located at the joint lines had strengths $\omega = \pm 8.8^\circ$ (figure 1). Bicrystals were fitted with each other by their crystallographic planes \{1010\} in such a way that their tilt boundaries continued one another along the $x$ axis, so that material overlaps at one end of the second bicrystal, while voids at the other end form. These overlaps and voids were eliminated by elastic deformations of the second bicrystal. The as-constructed structure contained 113126 atoms and had periodic boundary conditions along the $x$ and $z$ axes. Along $y$ axis the computational cell had finite dimensions and open surfaces in order to provide a sink for grain-boundary dislocations and exclude the existence of other boundaries. The dimensions of the computational cell in three directions were equal to $H_x=15h_1+13h_2=449.39$ Å, $H_y=360$ Å, and $H_z=14.5$ Å, where $h_1$ and $h_2$ are the periods of bicrystals with tilt boundaries $\Theta = 36.87^\circ$ and $\Theta = 28.07^\circ$, respectively.

To describe atomic interactions, the potential based on the embedded atom method (EAM) was used, which is fitted to the lattice parameters $a = 2.965$ Å, $c = 4.721$ Å and cohesive energy $E_0 = -4.85$ eV [11]. The simulation of all processes was carried out using the molecular dynamics code XMD [12]. Visualization of the structure was done using the code OVITO [13].

The constructed structure was subjected to relaxation at zero absolute temperature by running 30000 energy minimization steps. After reaching a local energy minimum in the bicrystal, high energy regions are preserved near the disclination nuclei. Then the structure was kept at a temperature of $T = 300$ K for 70000 steps until thermodynamic equilibrium was reached. The total relaxation time of the structure was 200 ps.

The potential energy of the system increases and redistributes during heating, at that long-range stress fields characteristic of the nonequilibrium grain boundary are preserved. Fields of long-range elastic stresses cause significant distortions of the crystal lattice, which is manifested in the growth of elastic micro-distortions and atomic displacements from crystal lattice sites. The Moiré pattern formed due to the superposition of the images of atomic structure with the perfect periodic structure of pixels on the monitor screen serves as an evidence of distortions of the crystal lattice due to the nonequilibrium grain boundary (figure 2).

To simulate the effect of ultrasonic vibrations at a constant room temperature, a sinusoidal uniaxial stress $\sigma = \sigma_0 \times \sin \left( \frac{2\pi}{\tau} \right)$ with a period $\tau = 160$ ps along $x$ axis at $T = 300$ K was applied. The amplitudes of stress varied in the range from 10 to 50 MPa.
Figure 1. Schematics of the construction of a computational cell.

Figure 2. Moiré pattern indicating the distortions of crystal lattice in the grains.

3. Computation results

Figure 3 shows the maps of energy distribution of the system before and after the action of 10 cycles of the stress with an amplitude of 30 MPa. In the initial structure regions of increased energy caused by long-range stress fields of the nonequilibrium grain boundary are observed (figure 3a). As can be seen from the figure 3b, the oscillating stresses resulted in the reduction of atomic energies within the grains. However, not a complete relaxation of the grain boundary occurred. Local areas of increased energy are preserved near the cores of disclinations.

Figure 3. Energy maps of the bicrystal before (a) and after 10 cycles of UST 30 MPa.

Under the action of cyclic stresses the nonequilibrium grain boundary starts to generate lattice dislocations. These dislocations glide along prismatic planes to sinks to the appropriate surfaces of the bicrystal and do not return to the boundary when the direction of the applied stress changes (figure 4). This process leads to the relaxation of the nonequilibrium structure of the boundary.

The glide of the emitted dislocations leads to plastic deformation of the bicrystal in the y direction. This deformation can be seen from the neck-like shape of the system after the ten cycles of straining (figure 3b).
Figure 4. Generation (a) and slip of a dislocation (b) with a Burgers vector $\mathbf{b} = 1/3[1\overline{2}0]$.

Graphs of changes in the excess energy of the computational cell as functions of the number of stress cycles are shown in figure 5. The excess energy has been calculated with respect to the defect-free crystal consisting of the same number of atoms. As can be seen from the graphs, the excess energy of the titanium bicrystal decreases after 10 cycles of straining with all amplitudes studied. At the same time, the sharpest decrease in the energy is observed after the first cycle. Under the further action of oscillating stresses, the change in energy occurs less intensively or nonmonotonously (in the case of the amplitude of 50 MPa).

Figure 5. Changes of the excess energy of the simulation cell as functions of the number of cycles of straining with different amplitudes of oscillating stresses.

At the stress amplitudes up to 20 MPa, the main decrease of the excess energy occurs after the first cycle of straining. After this, applied stress is no longer enough for the grain boundary to generate new dislocations during the subsequent cycles of deformation and the further gradual decrease in energy occurs due to the local rearrangements of atoms.

The further increase in the amplitude of the applied stress does not result in a larger reduction in the excess energy. At stress amplitude of 30 MPa, in addition to the nonequilibrium grain boundary, the open surfaces of the bicrystal begin to participate in the generation of dislocations. Thus, the grain boundary becomes not only a source of lattice dislocations, but also a sink, and the relaxation effect is partially leveled. Furthermore, in the constructed system several prismatic planes of the hexagonal crystal lattice are advantageously oriented relative to the direction of the acting stress. Dislocations of
non-coplanar systems under the influence of oscillating stresses can interact with each other and at the same time leave a chain of vacancies along the z direction (black points in figure 3b).

With a subsequent increase in the amplitude of stress oscillations, the applied stresses begin to exceed the mechanical stresses required for the relaxation of the nonequilibrium boundary. The number of generated defects in bicrystal grains increases. This process prevents complete relaxation of the system.

In the case of oscillating tension-compression stresses with a maximum amplitude of 50 MPa, the energy change as a function of number of cycles occurs non-monotonously (figure 5). In this case, the appearance of a twin with stacking fault was observed, which contributed to a sharp increase in the excess energy of the system after the second cycle in addition to other defects.

Thus, the largest relaxation effect in this simulation of the cyclic stress effect on the nonequilibrium boundary of the titanium bicrystal was obtained under the influence of oscillating stresses with an amplitude of 20 MPa. Since complete relaxation of the nonequilibrium boundary has not been achieved, the optimal stress amplitude is probably in the range of 20–30 MPa.

4. Conclusions
Preliminary results obtained by molecular dynamics simulation show that under the influence of oscillating tension-compression stresses a nonequilibrium grain boundary containing a disclination dipole emits lattice dislocations that sink at open surfaces. This process is irreversible and leads to the relaxation of the nonequilibrium structure of the boundary. Moreover, the effect of the cyclic straining depends on the amplitude of the applied stresses. There is an optimum value of amplitude at which the nonequilibrium boundary emits a sufficient number of dislocations to relieve internal stresses. With increasing amplitude of oscillating stresses the number of defects increases, which prevents the relaxation process. In the bicrystal model considered, the main energy decrease was observed after the first cycles of cyclic straining.

Acknowledgments
The present work was carried out as part of the state task of the Institute for Metals Superplasticity Problems of the Russian Academy of Sciences.

References
[1] Valiev R Z, Zhilyaev A P and Langdon T G 2013 Bulk Nanostructured Materials: Fundamentals and Applications, Hoboken, Wiley.
[2] Samigullina A A, Mukhametgalina A A, Sergeyev S N, Zhilyaev A P, Nazarov A A, Zagidullina Yu R, Parkhimovich N Yu, Rubanik V V and Tsarenko Yu V 2018 Microstructure changes in ultrafine-grained nickel processed by high pressure torsion under ultrasonic treatment Ultrasonics, Vol.82 313-321.
[3] Samigullina A A, Nazarov A A, Mulyukov R R, Tsarenko Yu V and Rubanik V V 2014 Effect of ultrasonic treatment on the strength and ductility of bulk nanostructured nickel processed by equal-channel angular pressing Rev. Adv. Mater. Sci. V. 39 48-53.
[4] Samigullina A A, Murzinova M A, Mukhametgalina A A, Zhilyaev A P and Nazarov A A 2018 Effect of Ultrasonic Treatment on the Characteristics of Superplasticity of Titanium Alloy Ti-6Al-4V Def. Diff. Forum 385 53-58.
[5] Bachurin D V, Murzaev R T, Baimova J A, Samigullina A A and Krylova K A 2016 Ultrasound influence on behavior of disordered dislocation systems in a crystal with non-equilibrium grain boundaries Letters on materials 6 183-188.
[6] Bachurin D V, Murzaev R T and Nazarov A A 2017 Ultrasonic influence on evolution of disordered dislocation structures Modelling Simul. Mater. Sci. Eng. 25, 085010.
[7] Nazarov A A 2016 Molecular dynamics simulation of the relaxation of a grain boundary disclination dipole under ultrasonic stresses Letters on materials 6 179-182.
[8] Nazarov A A, Murzaev R T 2018 Nonequilibrium grain boundaries and their relaxation under
oscillating stresses in columnar nickel nanocrystals studied by molecular dynamics
Computational Materials Science 151. 204-213. 10.1016.

[9] Nazarov A A, Murzaev R T 2018 A method for the construction of initial structures for molecular dynamics simulations of nanocrystals with nonequilibrium grain boundaries containing extrinsic dislocations Letters on materials 8(1) 5-10.

[10] Hirth J P, Lothe J 1982 Theory of dislocations, 2ed., Wiley.

[11] Hammerschmidt T, Kersch A and Vogl P 2005 Embedded atom simulations of titanium systems with grain boundaries Physical Review B 71 (20), 205409.

[12] http://xmd.sourceforge.net/about.html.

[13] Stukowski A 2010 Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool Modell. Simul. Mater. Sci. Eng. 18, 015012.