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Molecular-Dynamics Simulation of the α-Ti Plastic Deformation Under Conditions of High-Energy Effects

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Abstract. Modeling of high-speed deformation of α-Ti at a pressure of 20 GPa and a temperature of 700 K simulating the conditions of high-energy effects is carried out. The mechanisms of plastic deformation, including sliding along prismatic planes and the α-ω transition, are established. A feature of the deformation process of titanium in the considered conditions, which leads to the formation of disperse inclusions of the α-phase in the ω-phase matrix, is revealed.

INTRODUCTION

Titanium and its alloys have high strength, biocompatibility and corrosion resistance. In combination with light weight, these properties place them among the main materials for aerospace and medical applications. The high strength of these materials is often achieved by the formation of a fine-grained structure by the methods of plastic deformation. To date, the mechanisms of plastic deformation of titanium with an hcp structure (α-Ti) under atmospheric pressure and low strain rates have been well studied [1]. The specific features of the deformation mechanisms of α-Ti at elevated pressures and temperatures under conditions of high-energy effects remain undefined. The deformation of titanium under pressure from 2 GPa to 20 GPa is accompanied by an α-ω transition [2,3,4], as a rule, in the presence of shear stresses [5].

Features of the deformation process at the atomic level are studied using computer simulation by molecular dynamics (MD), which makes it possible to obtain information at the level of detail not available to experimental methods of research. Recent studies of the α-Ti deformation under uniaxial stress conditions along the [0001] direction by the MD method revealed details of the twinning mechanism and the realization of slip planes, although the specific characteristics of this process proved to be essentially dependent on the interatomic potentials used [6]. The information obtained on the details of the deformation process serves as a basis for the prediction of plastic deformation of metallic materials and structures made from them in terms of continual approaches [6]. At the same time, there remains the problem of existing interatomic potentials in a significant underestimation of the energy of formation of the stacking fault I_2 in the hcp lattice of titanium [6], whose magnitude largely determines the development of the plastic deformation process in α-Ti.

In this paper, we present the results of MD simulations of high-speed deformation of α-Ti at elevated temperatures and pressures simulating the conditions of high-energy effects. A modified interatomic potential is used to model the ω, α and β phases of titanium [7] constructed in the framework of approach for systems with metallic and covalent types of chemical bonds [8]. This potential gives good agreement with the experimental data,

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including the energy of formation of the stacking fault I_2, the calculated value of which (293 mJ/m^2) is close to the experimental value of 300 mJ/m^2 [9].

RESULTS AND DISCUSSION

To study α-Ti under high-pressure conditions and its high-speed deformation process, two series of model experiments were carried out using the MD method. A model Ti sample with an hcp lattice was specified as a rectangular parallelepiped; it contained 53760 atoms in the computational cell. The Cartesian coordinate axes were oriented along the crystallographic directions of the hcp lattice in such a way that the x-axis//[10 $\bar{1}$ 0], the y-axis//[$\bar{1}$ 2 $\bar{1}$ 0] and the z-axis//[0001]. Periodic boundary conditions were used.

The first series was the MD simulation of hcp titanium at a constant pressure P in the range from 0 GPa to 20 GPa, using a Berendsen barostat [10] and the constant temperature T = 700 K, using a Nose-Hoover thermostat [11] (NPT-ensemble) under isotropic deformation conditions. MD simulation was carried out for 500000 MD steps with a step size of 2 fs. In all the model experiments of the first series, the hcp lattice of titanium was retained and the transition to the omega phase was not observed, despite the reach of pressures in the region of the equilibrium omega phase at 700 K [12]. This result correlates with the experimental data [13], where the difficulty of the α-ω transition was noted under conditions of hydrostatic pressure without initiation by additional action, e.g. pulsed laser irradiation. This can be attributed to the small thermodynamic force of this transition due to a small difference in the enthalpy of hcp and C32 of titanium lattices, of the order of 5 meV [7].

The second series of model experiments included the MD simulation of the initial sample of hcp titanium at 700 K and 20 GPa pressure under conditions of nonisotropic deformation according to the known transition path from the hcp to C32 structure [14]. This pathway has the smallest barrier among the known hcp-C32 transition pathways and involves a simultaneous decrease in the relative size of the sample along the [10 $\bar{1}$ 0] direction to 0.913, an increase in size along the [$\bar{1}$ 2 $\bar{1}$ 0] direction to 1.118, and a decrease in size along the [0001] direction to 0.979. To analyze the effect of the rate of high-speed deformation, simulations were performed at strain rates of 10^8, $5*10^7$, and 10^7, calculated from the change in the sample size along the x-axis. Model experiments were implemented for $6*10^5$, $1.2*10^6$ and $6*10^6$ MD steps with a step of 2 fs for each noted strain rate, respectively. For comparison, the recent simulation of uniaxial deformation of hcp titanium [6] was carried out at strain rates of 10^8 and 10^9. As a result of the simulation, a sample with the dimensions 123.5×83.2×94.0 Å passed into a sample with the dimensions 111.4×88.4×85.3 Å. It should be noted here that the chosen path of the hcp-C32 transition was studied earlier within the framework of the density functional theory as a coherent change in translation periods and the displacement of atoms in a unit cell of 6 atoms [14]. The approach reported in [14] does not take into account the real deformation mechanism, which can include the formation of defects realizing plastic deformation.

An indication of the formation of defects in the process of high-speed deformation of a model sample can be seen from the analysis of the dependence of the stress on the magnitude of the deformation. Figure 1 shows a change in the σ_{xx} component, which we use to visualize the stresses in the process of high-speed deformation. As can be seen from Fig. 1, there are two sharp jumps in the σ_{xx} change in the range of the relative deformation values between 0.035 and 0.08. To analyze the change in the structure of the deformed sample in the marked regions, we performed an atomic structure study by the visualization method using the Ovito package [15]. With deformations from 0 to 0.035, the sample retains a defect-free hcp structure. After reaching a strain of 0.035, a fluctuation nucleation of defects realizing plastic deformation is observed. Figure 2a illustrates the atomic structure of the sample under deformation of 0.04. There are defects in the form of plates located in planes perpendicular to the plane of the figure.

Figure 2a illustrates the results of our analysis using the visualization method. High-speed plastic deformation of α-Ti begins with the fluctuation initiation of plane defects lying in the (1 $\bar{1}$ 00) plane and moving with deformation in the [11 $\bar{2}$ 0] direction, the displacement of atoms in the ends of plane defects occurs in the (10 $\bar{1}$ 0) plane. This defect agrees with the known prismatic slip plane (10 $\bar{1}$ 0) with the Burgers vector of dislocations in the [11 $\bar{2}$ 0] direction, which is the main slip plane for Ti [16]. The noted mechanism realizes the plastic deformation of α-Ti from 0.035 to 0.08 in Fig. 1.

When the range of deformation values reaches 0.08, the mechanism of high-speed deformation changes. The formed planar defects serve as sources of nucleation of the ω phase, the fast transformation into which realizes the plastic deformation mechanism of α-Ti in the next stage.

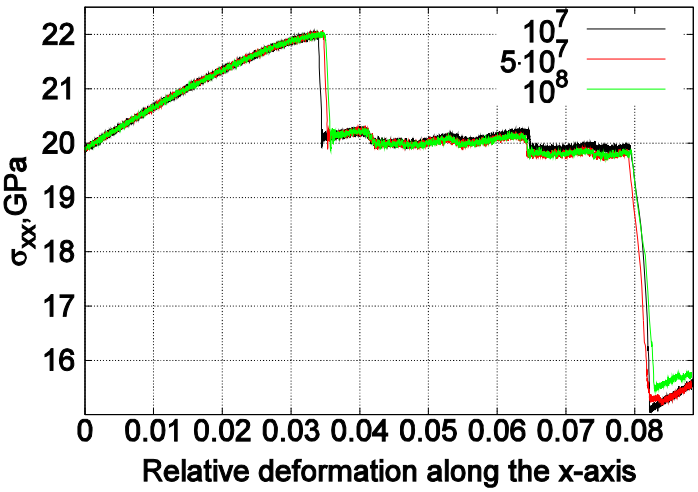
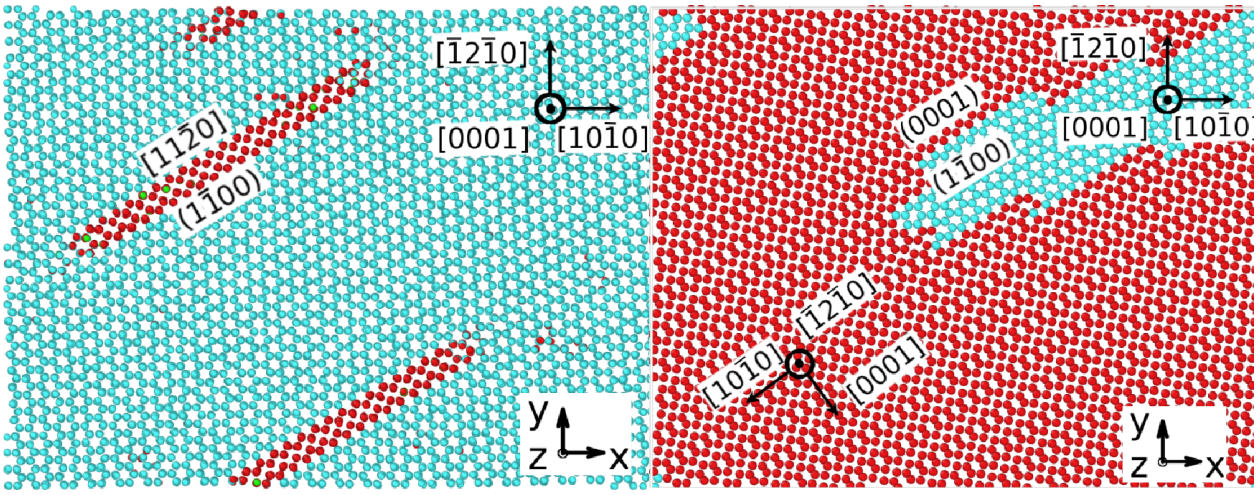


FIGURE 1. The magnitude of the stress tensor component σ_{xx} as a function of the relative decrease in the size of the model sample Ti along the x-axis during the high-speed deformation at a pressure of 20 GPa and a temperature of 700 K for the deformation rates of 10^7, $5*10^7$ and 10^8



(a) (b)

FIGURE 2. (a) – three neighboring atomic layers in the (0001) planes of the hcp Ti model sample with a relative decrease in the sample size by 0.04 along the x-axis (crystallographic direction [10 $\bar{1}$ 0]). Atoms with a local hcp environment are highlighted by the blue color. Atoms with a violation of hcp packaging, located in the planes (1 $\bar{1}$ 00), are highlighted by the red color; (b) – three adjacent atomic layers in planes perpendicular to the z-axis of the Ti model sample after the modeling of plastic deformation is completed. Atoms with local environment hcp and C32 are highlighted by the blue and red colors, respectively. The crystallographic directions in the C32 lattice (ω phase) are shown. The planes hcp (1 $\bar{1}$ 00) and C32 (0001) at the interphase boundary α/ω are noted.

It should be noted here that the Ovito package [15] allows the hcp structure to be identified; however, it does not determine the local position of the atoms in the C32 structure. In order to identify this structure, projections of atomic planes with a thickness of 2-3 atomic layers in a region different from hcp of titanium were compared with known projections of the atomic planes of the C32 structure. The correspondence of all projections of the atomic planes to the C32 structure is established, and the crystallographic directions of the C32 lattice are determined in the simulated sample. Figure 2b illustrates the atomic structure of the sample after the simulation of the deformation is completed, which is characterized by the presence of two phases – α-Ti and ω-Ti.

The simulation of the process of high-speed deformation of titanium at 20 GPa resulted in a transition to the ω phase of the whole model sample, with the exception of small α-Ti inclusions. The residual inclusions are explained by the kinetic factor. On the one hand, at a pressure of 20 GPa and a temperature of 700 K, the ω phase of titanium is thermodynamically advantageous [12]. Besides, the chosen α-ω transition path [14] and the dimensions of the simulated sample formally allow the sample to be completely transformed into the ω phase under the condition of simultaneous coordinated displacement of all atoms according to the trajectories proposed in [14]. On the other hand, as shown by the simulation results, plastic deformation occurs non-uniformly in the bulk of the sample. In this case, the inclusion of hcp titanium inside the C32 lattice cannot be ideally transformed into the ω phase due to differences in the atomic volumes of these lattices.

CONCLUSION

The MD modeling of high-speed deformation of α-Ti at a pressure of 20 GPa and a temperature of 700 K, simulating deformation under high-energy conditions, has shown a consistent realization of two mechanisms. Plastic deformation of titanium begins according to the known mechanism of realization of prismatic slip planes of the type $(10\bar{1}0)$. Then, from the slip planes, nucleation and growth of the ω phase of titanium occur, and this realizes the second mechanism of plastic deformation. The process of high-speed deformation ends with the conversion of most of the simulated sample into the ω phase, in which the α-phase inclusions remain due to differences in the atomic volumes of the hcp and C32 titanium lattices. This result indicates a possible method for obtaining fine-grained α-Ti by means of exposure to laser radiation pulses or other high-energy effects through a temporary transfer of α-Ti to the ω phase. With such an effect, it can be expected that the remaining disperse inclusions of the α phase will serve as seeds for the growth of α-Ti crystallites and form a fine-grained structure during the return to normal pressure and temperature conditions.

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