Study on the Low-Temperature Deformation Mechanisms of Dual-Phase Titanium Alloys under Nanoindentation

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Abstract. To investigate the influence of temperature on dual-phase titanium alloys' deformation behavior and mechanisms during nanoscale indentation, molecular dynamics simulations are conducted. The atomic strains, deformation behavior, dislocation types, and lengths of the dual-phase titanium alloy are systematically analyzed during low-temperature nanoscale indentation. The results show that within the temperature range of 0.01 K to 70 K, the decreases in critical load of the dual-phase titanium alloy with increasing temperature indicates that plastic deformation is most likely to occur at 70 K. Near the indentation region, the distribution of atoms with high stress and strain becomes more concentrated. At 20 K, {10-11} twinning is observed in the dual-phase titanium alloy structures, suggesting that twinning is more easily activated at low temperatures. Furthermore, the dual-phase titanium alloys are dominated by 1/3<1-100> partial dislocations and mixed dislocations, and the total dislocation length increased with temperature, indicating that slip deformation is the predominant deformation mechanism at 70 K.

Keywords: Titanium alloys, Molecular dynamics, ultra-low temperature, plastic deformation

1 Introduction

Titanium and its alloys are widely used in fields such as automotive and aerospace due to their high specific strength, relatively low density, good fracture toughness, and corrosion resistance [1]. It is well known that different deformation mechanisms occur in metals at different temperatures [2]. Generally, as temperature decreases, alloys tend to exhibit increased strength but decreased ductility. The α+β dual-phase titanium alloy Ti6Al4V has been widely used in low-temperature environments [3]. To ensure that titanium alloys can be used at low temperatures, effective control of multiple deformation mechanisms to simultaneously enhance low-temperature strength and plasticity becomes crucial.

He and Zheng [4] employed molecular dynamics (MD) simulation to analyze the influence of the γ/α2 interface on the deformation behavior of TiAl alloys during nanoindentation. The results revealed that the interface acted as a barrier to dislocation motion, enhancing the strength of TiAl alloys. Chen et al. [5] utilized MD simulation to investigate the influence of temperature on the deformation mechanisms of

TiAl/Ti3Al composite materials and discovered that the phase interfaces can promote phase formation. Song and Liu [6], through MD simulations, analyzed the wear mechanisms of high-Nb TiAl alloys under different displacements and loads. The results indicated that the gradient twin-like layer interfaces hindered twin deformation and dislocation motion, thereby improving the ability of the alloy to resist wear.

Atomic-level computational simulations are capable of observing atomic arrangements and are extensively employed to investigate the development of microstructures. Molecular dynamics computational methods are important tools for studying the deformation mechanisms of titanium alloys. Molecular dynamics simulations can precisely monitor the dynamic migration and phase transformation processes of materials, along with the nucleation and progression of internal dislocations. To address the issue of plastic instability in titanium alloys at extremely low temperatures, this study utilizes molecular dynamics simulations to investigate the behavior of plastic deformation and mechanisms of titanium alloys at ultra-low temperatures.

2 Methodology

The molecular dynamics analytical method involves integrating motion equations to track the trajectories of individual atoms in a multiparticle system and study its physical properties. Given the equations of motion, numerical integration is performed with an appropriate time step until a specified mechanical convergence criterion is reached, resulting in final position coordinates. Then, using statistical mechanics methods, the simulated particle positions, velocities, and accelerations are used to calculate and obtain thermodynamic and dynamic properties.

Molecular dynamics simulations were conducted utilizing the LAMMPS [7] software package and the atomic data acquired from the simulations were subsequently analyzed using the OVITO visualization software [8]. A dual-phase titanium alloy model, depicted in Figure 1, was established for nanoindentation calculations using the lattice constants of a = 2.9525 Å and c = 4.6944 Å for the hexagonal close-packed (hcp) structure, and a lattice constant of 3.32 Å for the bcc structure. The model was developed based on a hybrid potential function. The red atoms correspond to the hcp structure, while the blue atoms correspond to the bcc structure, and the green atoms represent the faced-centered cubic (fcc) structure.

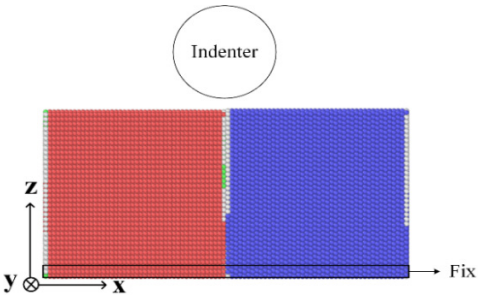

Fig. 1. The dual-phase titanium alloy nanoindentation model.

The crystal orientations of the α-phase in the x, y, and z axes are [0001], [1-100], and [11-20], while the crystal orientations of the β-phase in the x, y, and z axes are [110], [-112], and [1-11]. The dimensions of the dual-phase model are 206 Å in length, 219 Å in width, and 103 Å in height. In the α phase, random additions of Al atoms comprising a weight percentage of 0.1 and V atoms comprising a weight percentage of 0.02 were incorporated based on hcp-Ti. In the β phase, random additions of Al atoms with a mass fraction of 0.03 and V atoms with a mass fraction of 0.25 were incorporated based on bcc-Ti. The final dual-phase model had an Al mass fraction of 0.06 and a V mass fraction of 0.04. A spherical virtual indenter with a radius of 25 Å was located 5 Å away from the model. To prevent rigid body motion during the nanoindentation process, the atoms at the bottom were fixed as the boundary layer with a thickness of three atomic layers, equivalent to 8.85 Å.

Initially, the NPT relaxation technique was employed to stabilize the model over 20 picoseconds to attain system equilibrium. During the nanoindentation process, periodic boundary conditions were imposed along the x and y axes, whereas open boundary conditions were employed along the z-axis. A spherical indenter moved downward at a consistent speed of 40 m/s, applying compression in the z-direction. The step size for the nanoindentation process was set to 60 ps, with a maximum indentation depth of 19 Å.

The function responsible for defining the interaction among atoms is referred to as a potential function. According to the principle of superposition, the collective potential energy of a system can be formulated as a function of the particle coordinates [9]:

$$U(R) = \sum_{k=1}^{N} U_1(R_k) + \sum_{k<l}^{N} U_2(R_k, R_l) + \sum_{k<l<m}^{N} U_3(R_k, R_l, R_m) + \cdots \quad (1)$$

In the equation, U(R) represents the total potential energy, which can be decomposed into multiple contributions. The material studied in this paper is titanium alloy, where both the Embedded Atom Method (EAM) potential and the Modified Embedded Atom Method (MEAM) potential are employed to describe the interactions between titanium elements and alloying elements [10].

3 Results and Discussions

3.1 The Deformation Behavior of Dual-Phase Titanium Alloys

The load-depth curves of dual-phase titanium alloys under varying temperatures are shown in Figure 2(a). The dual-phase titanium alloy structure experiences a maximum load of 391 nN at a temperature of 0.01 K. Within the temperature interval from 20 K to 70 K, the load on the dual-phase titanium alloy structure decreases with increasing temperature, reaching a minimum load of 200 nN at 70 K.

The critical load of dual-phase titanium alloys at different temperatures is shown in Figure 2(b), and it diminishes as the temperature rises. At a temperature of 0.01 K, the dual-phase titanium alloy exhibits the maximum critical load of 19.91 nN, while at 70 K, the lowest critical load of 5.81 nN is observed, indicating the highest susceptibility to plastic deformation.

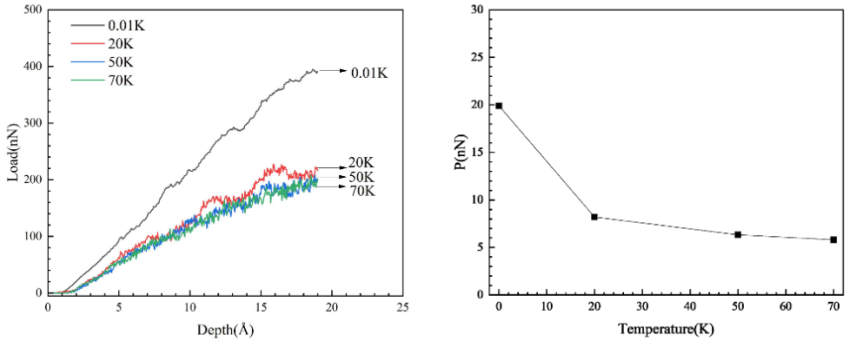

Fig. 2. The deformative characteristics of dual-phase titanium alloys at different temperatures.

Different temperature-dependent atomic strain distributions in dual-phase titanium alloys after nanoindentation are illustrated in Figure 3. The findings indicate that the high-strain regions of the α phase remain near the indentation zone, while the high-strain regions of the β phase start to spread towards the peripheral regions as the temperature increases. The area of diffusion expands gradually with rising temperature.

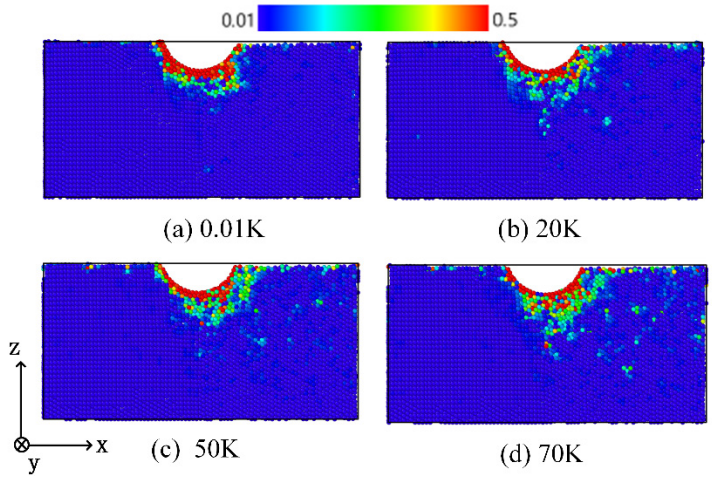

Fig. 3. The atomic strains of the dual-phase titanium alloy at different temperatures.

3.2 The Deformation Mechanisms of Dual-Phase Titanium Alloys

Figure 4 illustrates the defect evolution in dual-phase titanium alloys at different temperatures. At 0.01 K, intrinsic stacking faults are observed in the α phase of the dual-phase titanium alloy structure, while a small number of atoms of unidentified species are present in the β phase.

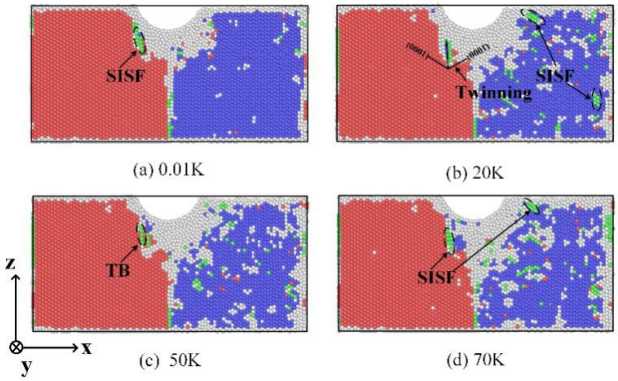

Fig. 4. The defect evolution in the dual-phase titanium alloy at different temperatures.

At 20 K, minor intrinsic stacking faults are detected within the β phase of the dual-phase titanium alloy structure, and the α phase exhibits {10-11} twinning. At 50 K, grain boundaries appear within the α phase of the dual-phase titanium alloy structure. At 70 K, intrinsic stacking faults are observed in both the α and β phases of the dual-phase titanium alloy structure. With increasing temperature, the number of unidentified atoms at the interface between the two phases increases, and the quantity and area of atoms of unidentified species in the β phase also increase.

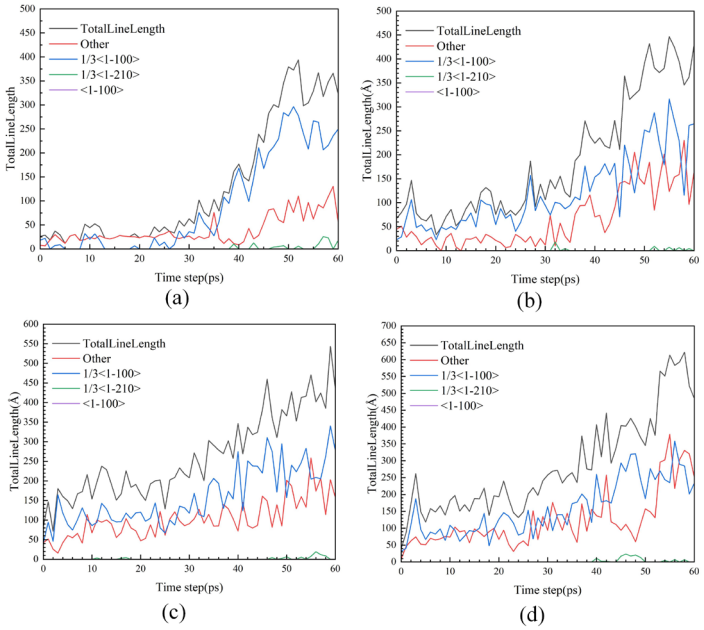

Fig. 5. The variation in dislocation types and lengths in the dual-phase titanium alloy at different temperatures.

The evolution of dislocation types and lengths during nanoindentation in dual-phase titanium alloys at varying temperatures is depicted in Figure 5. The results indicate that the overall length of dislocation lines grows with temperature. At 0.01 K, the cumulative length of dislocation lines is relatively short when the indenter penetrates to 0-30 ps. However, after 30 ps, there is a sharp increase in the length of 1/3<1-100> dislocation lines, indicating the dominance of partial dislocations of 1/3<1-100> type. At temperatures ranging from 20 K to 70 K, partial dislocations of 1/3<1-100> type and mixed dislocations are dominant, and with increasing temperature, the proportion of mixed dislocation line lengths gradually increases. At 70 K, the lengths of 1/3<1-100> dislocation lines and mixed dislocation lines are essentially the same.

4 Conclusions

This research utilized molecular dynamics simulations to explore the nanoscale indentation process of dual-phase titanium alloys at low temperatures. The behavior under deformation and mechanisms of dual-phase titanium alloys in the course of low-temperature nanoindentation were systematically examined. The results showed that the dual-phase titanium alloys exhibit a decrease in critical load with increasing temperature. This implies that plastic deformation is most likely to occur at 70 K, as it is the temperature at which the materials are most susceptible to undergo plastic deformation. As the region near the indentation area is approached, there is an increased density of atoms experiencing high stress and strain, and the area of the high-strain region in the dual-phase titanium alloy structure expands with increasing temperature. At a temperature of 20 K, the dual-phase titanium alloys exhibit the presence of {10-11} twinning, indicating that the mechanism of plastic deformation in the material is predominantly governed by twinning at lower temperatures. The dominant dislocation types are 1/3<1-100> partial dislocations and mixed dislocations. Moreover, the overall length of dislocations increases with the temperature rise. This indicates that at 70 K, the deformation mechanism of titanium alloys tends to favor slip deformation.

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