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Influence of loading directions on dislocation slip mechanism of nanotwinned Ni with void defect at the twin boundary

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ABSTRACT

In this study, a molecular dynamics model is used to simulate the compressive loading process along different crystal orientations of nano-twinned Ni with void defect at the twin boundaries. The loading angle is defined as the angle between the loading direction and the twin boundary, loading angles of 0, 15, 30, 45, 60, 75, and 90° were investigated in this study. The effects of different loading directions on the mechanical properties and the dislocation glide mechanisms were investigated. The dislocation glide process during the initial stage of plastic deformation for different loading directions was also studied. The results show that the dislocation glide mainly occurs along the {1 1 1} plane that is inclined to the twin boundaries when the loading direction is 0°. The dislocation glide process is constrained by the twin boundaries and, therefore, slips along the twin layers. As the loading angle increases from 0° to 45°, the dislocation gradually shifts and slips along the (1 1 1) slip plane that is parallel to the twin boundaries and twin migration and twinning occur. As the loading angle continues to increase to 90°, the dislocation slips along the {1 1 1} plane again during the loading process. In addition, the dislocation slips toward the adjacent twin layers because they are strongly hindered by the twin boundaries.

1. Introduction

In the past ten years, the strengthening of metal materials has been a research focus in material science. By introducing more impediments to prevent the movement of dislocations [1–3], the refinement of the material at the nanoscale is an effective method that increases the strength of many nanomaterials. Many strengthening methods result in a loss of ductility compared to its coarse-grained material and this inevitably limits the actual application value of the material. One strengthening method is the creation of nanoscale coherent twin boundaries (TBs) [4], which effectively impede the movement of dislocations and have the same effect as the traditional grain boundary strengthening method. In addition, this method significantly improves the toughness of the material because the TBs near the dislocation provide sufficient storage space and structural stability [4,5]. This approach has a broad application potential [6], therefore, nano-twinned materials have attracted broad attention worldwide.

The excellent comprehensive properties of nano-twinned materials are closely related to their unique plastic deformation mechanisms [7–12]. Song et al. [10] studied the effect of different TB densities on the mechanical properties of nano-twinned copper using a molecular dynamics method. It was found that the initial yield stress and the TB spacing exhibited Hall-Petch effects when the spacing was less than 10.23 nm and the dislocation slip was hindered by the TBs. On the contrary, when the spacing between the TBs was larger than 10.23 nm, the initial yield stress and the TBs exhibited inverse Hall-Petch effects. The different interactions between the dislocations and between the dislocation and the TBs were the main reason for the phenomenon. Zhou et al. [11] used the molecular dynamics method to simulate the uniaxial tensile deformation of graded nanocrystals of Cu. When the twin layers were thick, a large number of partial dislocations occurred and the interaction of these dislocation slides dominated the plastic deformation mechanism and improved the material toughness. On the contrary, when the twin layers were thin, the plastic deformation mechanism was dominated by full dislocation and the dislocation slide was impeded by the TB, this resulted in improved material strength. The simulation results of the graded nanocrystals were in good agreement with the experimental results of Lu [12]. Bai et al. [13] conducted rolling and deformation tests on preferentially oriented Cu nanocrystals at room temperature. It was found that the Shockley partial dislocations at the TBs and the slip along the TBs resulted in reverse twinning in the direction of the maximum shearing stress. The local reverse twinning

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mechanism dominated the process of plastic deformation when the strain was small.

Defects such as cracks and voids are unavoidable during the process of material preparation. Extensive research has been conducted on the effects of defects on the properties of twinned nanocrystals. Xu et al. [14] developed a uniaxial compressive simulation of γ-TiAl alloy. The results showed that the shrinking of the void was caused by the symmetric expansion of the dislocation around the void defect. With the increase in the strain, the interaction of the adjacent stacking faults (SFs) is the result of the hardening behavior of the material, the continuous expansion of the dislocation caused further shrinking of the void. Zhao et al. [15] studied the effect of the void's volume fraction to void growth mechanism of single crystal Cu. The results showed that the void growth was mainly caused by the expansion of the dislocation from the void surface and the interaction of the dislocations from the {1 1 1} slip plane. The results also indicated the void growth mechanism was not affected by the void volume fraction. Zhang et al. [16] studied the void growth mechanism of nano-twinned Ni under uniaxial tensile stress. The results indicated the existence of TBs can suppress the dislocation expansion and reduce the overall stiffness of the material, in addition, the expansion of the leading partial and trailing partial from {1 1 1} caused a loss of the surface atoms of the void. As the strain increased, the void grew gradually. Wang et al. [17] created a uniaxial tensile simulation of nano-twinned Ni_3Al with cracks inside the grain boundaries. The results showed that the crack was usually the origin of the dislocation during the initial stage of plastic deformation and dislocation nucleation occurred at the cracks' tipping points. With increasing strain, the Lomer-Cottrell lock occurred in the model due to the partial dislocation slip, the dislocation pile-up, and the penetration appearing at the TBs.

The literature review shows that the interaction between the dislocations and the TBs dominates the plastic deformation process and is also the main factor affecting the macro-mechanical properties of nano-twinned materials. The slipping system follows Schmid's law for face-centered-cubic (FCC) crystalline materials [18]. The loading direction changes the dislocations along different directions and affects the interaction between dislocations and TBs. Although some experiments on the failure behavior of materials under different crystal orientations have been reported [19], there are few published studies on the mechanism of the interaction between dislocations in different loading directions for nano-twinned materials. In this study, the molecular dynamics method was used to simulate the compressive loading process of nano-twinned Ni with void defect in the grain boundaries for different crystal directions. The dislocation slide and dislocation interaction mechanism were investigated as well.

2. Modeling and methods

Fig. 1 shows a nano-twinned crystal model in which the atom has a common {1 1 1} plane in the twin region and the parent region. The specific arrangement details of the atoms in the twin plane are also clearly indicated in the figure. All Ni atoms in the structure are mirrored along the twin planes. The model was rotated clockwise (0, 15, 30, 45, 60, 75 and 90°) along the Y-axis [1–10] to obtain the specific crystal orientations. The model has a dimension of 18.1 × 18.1 × 18.1 nm with 540,000 atoms. In the molecular dynamics simulations, the selection of potential functions can significantly affect the accuracy of the simulation results. In this study, the embedded atomic method developed by Mishin [20] is used to describe the interaction between the atoms. The potential function is obtained by the first-principles calculation and experimental data fitting, which has shown good results in the literature. In addition, it accurately reproduces the development of defects such as voids, cracks, and dislocations in the metal Ni model. The potential energy of the system can be expressed as:

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\alpha(\gamma_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(\gamma_{ij}) \tag{1}$$

where the subscripts i, j represents the ith and jth atom respectively; the first term of the equation is the embedded energy that represents the energy of the atom in the electron cloud with density ρ. The second term represents the interaction between the two atoms, where:

$$\rho_\alpha(\gamma_{ij}) = \sum_{k=1}^{2} A_k(r_k - r_{ij})^3 H(r_k - r_{ij}) \tag{2}$$

$$\phi_{\alpha\beta}(\gamma_{ij}) = \sum_{k=1}^{6} a_k(r_k - r_{ij})^3 H(r_k - r_{ij}) \tag{3}$$

where

$$\mathrm{H(x)}\begin{cases}0, & x>0\\ 1, & x<0\end{cases} \tag{4}$$

A_k, R_k, a_k, r_k are constants and $R_1 > R_2$, $r_1 > r_2 > \ldots > r_6$.

In this study, the large-scale atomic/molecular massively parallel simulator (LAMMPS) program [21] was used to study the effect of the loading direction on the growth mechanism of the dislocation at the TB with void defect and the mechanical properties of the materials. In the model, the time step is initially set to 1 fs. The temperature and pressure settings during the simulation are the same as those used by Nose-Hoover [22] and Parrinello-Rahman [23] respectively. The periodicity boundary condition is applied in the XYZ directions to eliminate the surface effect. Energy minimization is achieved using the conjugate gradient method and then a 300 ps full relaxation is performed at a temperature of 1 K. The compression tests with different crystal orientations were carried out in the NPT system with an applied strain rate of $5 \times 10^8\,s^{-1}$ and a simulated temperature of 1 K. The data for the atomic coordinates, temperature, potential energy, and kinetic energy were output every 100 steps.

The central symmetry parameter (CSP) method in the AtomEye software package [24] is used to analyze the microstructural evolution of the model. The method is expressed as:

$$CSP = \sum_{i=1}^{N/2} |R_i + R_{i+N/2}| \tag{5}$$

where N is the number of atoms around the central atom and $R_i + R_{i+N/2}$ is the vector from the central atom to the nearest atom. A CSP value of zero indicates that the atoms are at the perfect lattice position. A non-zero CSP indicates that there is a defect near the central atom. Therefore, this technique recognizes voids, dislocations, and SFs generated in the model during the loading process. The dislocation extraction algorithm (DXA) [25] in OVITO [26] software was used to identify the development of the dislocations during loading. The dislocation slide process in the model can be more clearly observed by deleting the perfect FCC structural atoms in the initial plastic deformation mode. The Burgers vector for each dislocation is represented by a double Thompson tetrahedron [27] and the reaction between the dislocations can be expressed in conjunction with the Burgers vector equation. As shown in Fig. 1, α, β, γ, δ is the midpoint of the plane BCD, ACD, ABD, and ABC (twin plane) respectively, which represents the four slip planes in the parent region. α', β', γ' is the midpoint of the plane *BCD′*, *ACD′*, and *ABD′* respectively, which represents the twin plane of each slip plane. The slip systems and Burgers vectors of the nano-twinned Ni are listed in Table 1. There are three types of slip patterns associated with the double Thompson tetrahedron: (1) the dislocation slip on the coherent twin plane (ABC plane) such as AB, AC, and BC. **b1, b2, b3** are Burgers vectors corresponding to the full dislocation; (2) the dislocation slide on the slip plane inclined to the twin planes; the Burgers vectors of the dislocations are parallel to the twin planes (e.g. AB, AC, and BC) and are also denoted by **b1,b2,b3**