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Dislocation mechanism of void growth at twin boundary of nanotwinned nickel based on molecular dynamics simulation

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ABSTRACT

Molecular dynamics simulation was performed to investigate dislocation mechanism of void growth at twin boundary (TB) of nanotwinned nickel. Simulation results show that the deformation of nanotwinned nickel containing a void at TB is dominated by the slip involving both leading and trailing partials, where the trailing partials are the dissociation products of stair-rod dislocations formed by the leading partials. The growth of a void at TB is attributed to the successive emission of the leading partials followed by trailing partials as well as the escape of these partial dislocations from the void surface.

1. Introduction

Fracture of ductile metals is often induced by nucleation, growth and coalescence of voids, where void growth plays the most important role. Over the last decades, a number of continuum models have been proposed to study the behavior of void growth [1–3]. Furthermore, several numerical methods, such as crystal plasticity finite element method (CPFEM) [4], discrete dislocation dynamics (DDD) [5] and molecular dynamics (MD) [6], have been used to reveal the mechanism of void growth. Of the three methods, MD simulation has been proved to be a powerful candidate for observing the atomic details of fracture behaviors. Therefore, more and more researchers have devoted themselves to investigating the void growth by means of MD simulation. Traiviratana et al. [7] revealed mechanisms of void growth in both monocrystalline and bicrystalline coppers subjected to uniaxial tensile strains, and they confirmed that the emission of shear loops is responsible for the primary mechanism of void growth. Tang et al. [8] investigated growth and coalescence of voids in magnesium single crystals at the nanoscale, and they found that loading strain rate and temperature have an apparent influence on the twin or dislocation pattern, the evolution of void shape and the uniaxial stress–strain response. Mi et al. [9] studied mechanisms of void growth and coalescence in aluminum single crystal with pre-existing voids, where dislocation propagation was demonstrated and the effects of length scale on the effective stress–strain response, the stress triaxiality and the void fraction evolution were investigated. Tang et al. [10] studied the growth of spherical nanovoids and the fracture properties of γ-TiAl single crystal, and they also found that the emission of shear loops is responsible for the primary mechanism of the void growth. Their results agree with those obtained by Traiviratana et al. [7]. Chiang et al. [11] analyzed the interaction between voids and grain boundary (GB) in UO_2, and they found that grain boundary (GB) is able to migrate toward the void from a very large distance and GB has the ability to pin and dissolve the void.

However, all the studies reported in the current literatures, which deal with void growth, focus on the voids nucleating at GB or in grain interior. No literatures, which are related to the voids nucleated at twin boundary (TB), have been found. So far, the investigations on the effects of TB during the deformation have focused on crack propagation and conventional deformation [12–16]. Therefore, in the present study, dislocation mechanism of void growth at TB of nanotwinned nickel was investigated by means of MD simulation.

2. Modeling and methods

Fig. 1 shows the computational configuration of the nanotwinned nickel used in the present study. In the simulation, [111], $[\bar{1}\bar{1}2]$ and $[1\bar{1}0]$ directions were set as x-axis, y-axis and z-axis of the Cartesian reference frame, respectively. The size of the nanotwinned nickel model was $30 \times 30 \times 24$ unit cells and a spherical

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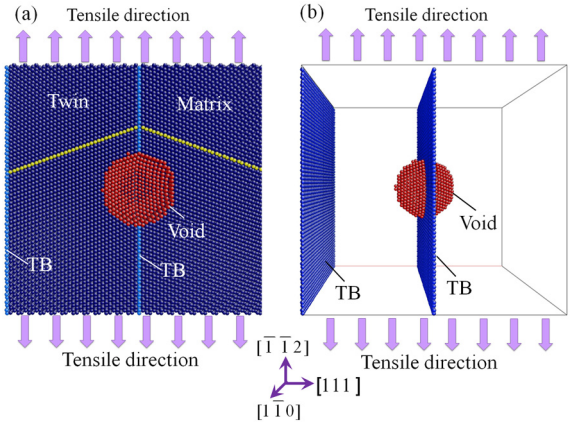

Fig. 1. Computational configuration of the nanotwinned nickel: (a) Cross section; (b) Model with only void and TB highlighted.

void with the radius of 3 unit cells was preset at the TB, where the crystal lattice constant a is 0.352 nm for nickel. Periodic boundary conditions were used in all the three directions. The initial configuration was first relaxed at 0.01 K so that the energy is minimized. Subsequently, a uniaxial tensile loading with a strain rate of 2×10^8 s^{-1} was applied on the model along the direction shown in Fig. 1. All the simulations were conducted at the temperature of 0.01 K so that thermal effects could be eliminated.

In the present study, the MD simulation was performed by means of LAMMPS [17]. Since only the global mechanical behaviors of the nanoscale nickel crystal are studied, the virial stress for a system of atoms was used. It has been proved that Lagrangian virial stress is the most accurate candidate for evaluating the stress values in dynamical simulations [17]. The embedded-atom-method (EAM) potential developed by Foiles et al. [18] was used to describe the interaction among nickel atoms. For the purpose of visualizing defects in the nanotwinned nickel, colors were assigned to the atoms according to a local crystalline classification by using common neighbor analysis (CNA) [19], which is capable of detecting whether an atom is in a hexagonal close-packed (HCP) environment or in a face-centered cubic (FCC) environment. The visual software AtomEye [20] was used to identify various deformation mechanisms during simulation by analyzing and classifying the environment around each atom. In the present study, the HCP atoms were colored in blue, and the distorted structure atoms were colored in red. However, the FCC atoms were concealed so as to highlight the defects. Dislocations were extracted from the CNA results by means of dislocation extraction algorithm (DXA) [21].

3. Results

Fig. 2 shows the dislocation evolution of the nanotwinned nickel containing a spherical void at TB. It can be seen that the void at TB acts as the source of dislocation during deformation of the nanotwinned nickel. The yielding of the nanotwinned nickel results from nucleation of a pair of shear loops on the matrix side, where the shear loops are composed of dislocations and stacking faults. With the increase in the strain, these shear loops expand outwards from the void surface on the close-packed planes. When the shear loops encounter the TB, the propagation of them along $[\bar{1}\bar{1}\bar{1}]$ direction are impeded by the TB. Subsequently, another pair of shear loops, which is nucleated at the corners between the shear loops in the matrix and the void surface, is induced on the twin side. The new shear loops expand on a plane which is symmetrical to the one on the matrix side. As a consequence, these shear loops symmetrically expand outwards from the void surface on both sides of TB, as illustrated in Fig. 3. Meanwhile, further increase of strain also results in nucleation of a pair of shear loops in the matrix interior and the twin interior, respectively. Similar to those aforementioned dislocations nucleated in the twin, these shear loops initiate at the corners between the void surface and the shear loops induced previously. All of the shear loops expand with the progression of deformation and intersect at the junction of the slip planes.

In order to index the Burgers vectors and slip planes in the simulation, a double Thompson tetrahedron is used, as shown in Fig. 4. In the double Thompson tetrahedron, α, β, γ and δ are the centers of planes BCD, ACD, ABD and ABC, respectively, and they are used to express the four slip planes in the matrix. α', β', and γ' are the centers of planes BCD′, ACD′ and ABD′, respectively, and they are symmetrical to α, β, γ with respect to plane δ and are used to express the slip planes in the twin. The double Thompson tetrahedron is orientated in such a way that the direction $\boldsymbol{\delta A}$ coincides with tensile axis and the plane ABC is perpendicular to the

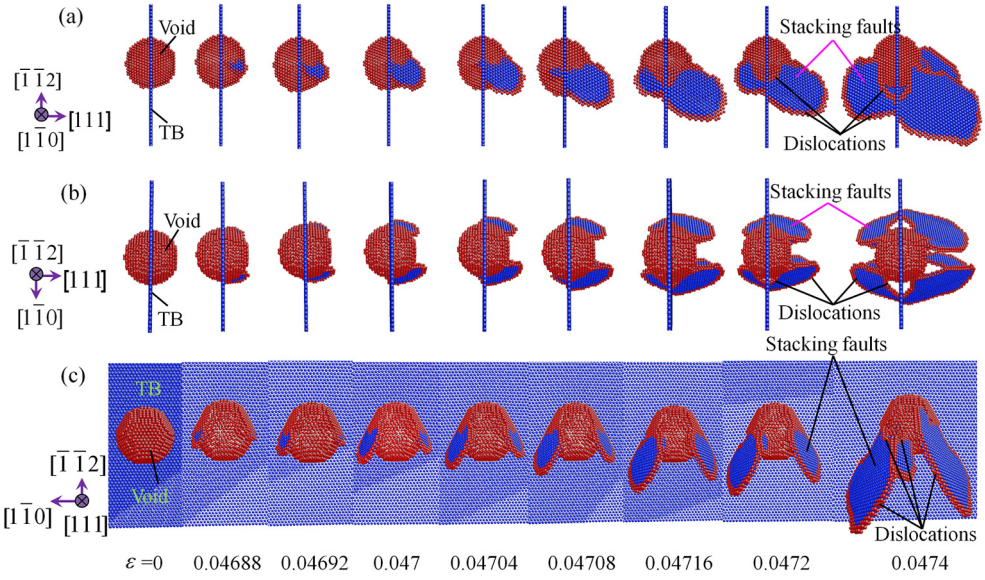

Fig. 2. Dislocation evolution of the nanotwinned nickel containing a spherical void at TB: (a) Viewing from $[1\bar{1}0]$ direction; (b) Viewing from $[\bar{1}\bar{1}2]$ direction; (c) Viewing from [111] direction.