Computational Materials Science 132 (2017) 116–124

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Orientation effects on the tensile properties of single crystal nickel with nanovoid: Atomistic simulation

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ARTICLE INFO

Article history:
Received 16 May 2016
Received in revised form 19 February 2017
Accepted 20 February 2017
Available online 6 March 2017

Keywords:
Molecular Dynamics (MD) simulation
Lattice orientation
Nanovoid
Dislocation nucleation

ABSTRACT

The tensile behavior of monocrystalline nickel with nano-void was studied via molecular dynamics simulation (MD) considering different lattice orientations. A series of simulations were performed to analyze the effect of system size, void volume fraction and lattice orientation on mechanical properties and microstructure evolution. The influence of size of sample on the incipient yield stress is discussed. The results show that void volume fractions have significant effects on Young's modulus, incipient yield stress and incipient yield strain. Dislocation structure begins to nucleate in the stress concentration area. The critical stress of [1 0 0], [1 1 0] and [1 1 1] orientation is 6.97 GPa, 6.77 GPa and 7.31 GPa, respectively. The results of dislocation propagation and stress-strain responses reveal the elastic-plastic properties of different orientations. The fracture strain is the elongation of the specimen. The elongation of the sample along [1 1 1] orientation is greatest, which illustrate that the sample has good ductility performance along [1 1 1] orientation in the same initial damage. The reaction between the dislocations and the boundary leads to the rearrangement of the boundary atoms, which proves that the dislocation can not be stopped inside the crystal, or closed or terminated at the crystal surface or grain boundary. The difference of the rearrangement of the boundary atoms is due to the difference of the sliding systems of different orientations.

1. Introduction

The failure modes of materials have significant influence on the design of material properties in materials science. Rapture failure at the macroscopic scale can be attributed to nucleation, growth and propagation of cracks, but at the microscopic scale cracks are initially easily formed at defects in the casting process, such as voids and inclusions [1]. These defects are known to play a fundamental role in the deformation of the material. Nucleation, growth and coalescence of voids are deemed as the primary mechanism of ductile material fracture, in which void growth is particularly important. Therefore, it is necessary to study the deformation response of porous materials with the consideration of microstructure evolution.

Most previous work on void growth studies, both experimental and simulation approaches, have been used to better describe ductile fracture processes. Furthermore, some numerical methods, such as crystal plasticity finite element method [2–7], dislocation dynamics and molecular dynamics [8–19], have been used to reveal the mechanism of void growth.

Molecular dynamics (MD) is an effective tool for studying the fracture mechanism of micro-scale materials. It can directly observe the motion of atoms and obtain the details of atomic deformation. MD simulations in monocrystalline and bicrystalline copper were carried out with LAMMPS (large-scale atomic/Molecular Massively Parallel Simulator) to reveal void growth mechanisms. The results confirm that the emission of dislocation shear loops is the primary mechanism of void growth [20–24], consistent with the analytical results of [21] and [25–28]. Tang and his colleagues simulated the growth behavior of spherical nanovoids in γ-TiAl single crystal [17]. They found that the emission of dislocation loop is the main reason for the growth of void, and the continuous dislocation nucleation and the increase of the shear loop prompt the growth of voids. In addition, extensive work has been performed on other factors affecting void growth, such as size effect [13,14,16,26], initial void volume fraction [2,5,8,9,20,24,26] And strain rate [16,26,28]. The initial stage of the growth of nanocrystalline voids in monocrystalline aluminum was studied by MD simulation. The simulation results showed that the dependence of the critical negative pressure on void radius, system size and temperature was obtained at high rate tension [24]. The decrease in the ratio of the radius of the void to the system size leads to an increase in the tensile strength of the system. Tang

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http://dx.doi.org/10.1016/j.commatsci.2017.02.024
0927-0256/

et al. [29] based on a new analytical method for the emission energy of the dislocation loop, the reduction of stress with increasing void size is analyzed. Bhatia et al. [26] investigated nanovoid growth using MD and revealed its dependence on void size, strain rate, crystallographic loading orientation, initial nanovoid volume fraction, and simulation cell size. Dislocations and shear loops nucleate on different slip systems with different loading orientations, which include orientation that favors single slip and multiple slip. It is well known that the mechanical properties of monocrystalline metallic materials have a strong correlation with their crystal orientation. The mechanisms of void growth and failure modes are significantly different in different lattice orientations. Therefore, it is significant to study the void growth behavior of single crystal metallic materials with different orientations. A number of studies have been carried out in this area [3,7,9,10,13,15,30,31]. Potirniche et al. [15] interpreted that plasticity anisotropy caused by initial lattice orientation has only a minor effect on void growth in the microscale regions. Stress triaxiality is the main factor controlling the growth and coalescence of voids. The numerical results of Sangyul Ha and KiTae Kim [3] showed that the stress triaxiality and the deformation pattern specified by the crystal orientation have competitive effects on the evolution of voids. For low-level stress triaxiality, the deformation mode is mainly determined by the crystal orientation. Eduardo et al. [13] investigated the effect of loading orientation on void initiation in FCC metals. The results showed that there is a significant effect of the loading orientation on the sequence where the loops form and interact.

Based on the above studies, it has been found that dislocation nucleation and morphology of different crystal orientations have not been systematically studied in detail. In this study, uniaxially stretched MD simulation was used to analyze the effect of lattice orientation on tensile fracture in thin nickel specimens with infinite cylindrical voids. Nickel is a typical FCC material. In addition, its alloys, such as B2-type NiAl, LI2-type Ni3Al, are used in the aerospace industry due to their excellent high temperature performance. The study will examine the microstructural evolution and the mechanism of void growth through stress-strain responses and morphological changes of voids in different crystal orientations. At the same time, size effects and void volume fraction effects are taken into account.

2. MD simulation presentation

2.1. Atomistic model and simulation conditions

In this simulation, a system of size $64.416 \times 27.0336 \times 5.28$ nm^3 was chosed to investigate the orientation effect, as shown in Fig. 1. Considering that the size of the model must be a multiple of the lattice spacing, the lattice spacing in the [1 1 1]-oriented z is different from that of [1 0 0] and [1 1 0]. A [1 1 1]-oriented simulation system of size $64.416 \times 27.0336 \times 5.4758$ nm^3 is used herein. The radius of the cylindrical nano-voids was 5.28 nm. The size in z direction is greater than the potential cut-off radius 0.58 nm. Model with three different orientations was used to simulate the uniaxial tensile behavior of single crystal nickel and nano-voids. The parameters are shown in Table 1.

Periodic boundary conditions (PBC) was applied to the z-direction, x and y were the shrink-wrapped boundary. Micro-canonical ensemble was taken during the simulation process, and the temperature of the thermostat atom is controlled by rescaling the atomic velocity by 40 picoseconds in 1 fs time step. Therefore, the model relaxes to the equilibrium state at the beginning of the simulation. These models hold the left boundary and are uniaxially loaded at a constant strain rate of 5×10^8 s^{-1} at the right boundary, as shown in Fig. 1. All simulations were performed by LAMMPS at an invariable temperature of 300 K.

The atomic stress tensor is calculated using the virial definition, which can be expressed as:

$$\sigma_t(i) = -\sum_{j \neq (i)}^{N} f_\alpha(i,j) r_\beta(i,j) \tag{1}$$

$$\sigma_e(i) = \sum_{t=1}^{n} \sigma_t(i)/n \tag{2}$$

where f_α is the interatomic force between atom i and j in the direction α, r_β is the distance in direction β. Considering average over the volume around atom i within the cut-off distance, σ_e is the average atomic stress tensor obtained by function (2).

2.2. EAM potential

In recent years, the embedded atomic method [32,33] (EAM) interatomic potential has been widely used for crack propagation in metal materials and many other simulations. Compared with the F-S and L/J potentials, it can calculate the elastic properties of materials, energy changes, and the position of atoms in the whole simulation process of metal materials. Many examples have shown that EAM is an accurate representation of the interatomic forces in a metal lattice.

In this study, the embedded atom method of Ni developed by Mishin et al. [34] was used to simulate the uniaxial tensile beha vior of single-crystal nickel with nanovoid.

A reasonable simulation of fracture and damage can be obtained considering that the potential energy can well describe the bonding capacity in a metal system and the dependence of the strength of a single bond on the local environment (e.g., surface and defects). In addition, this EAM potential, based on the first principles, can reproduce many of the fundamental properties such as vacancy migration energy, unstable and stable stacking fault energy. Many studies [35–38] have used this EAM potential to investigate the deformation behavior of materials, which further validates the accuracy and reliability of this interatomic potential.

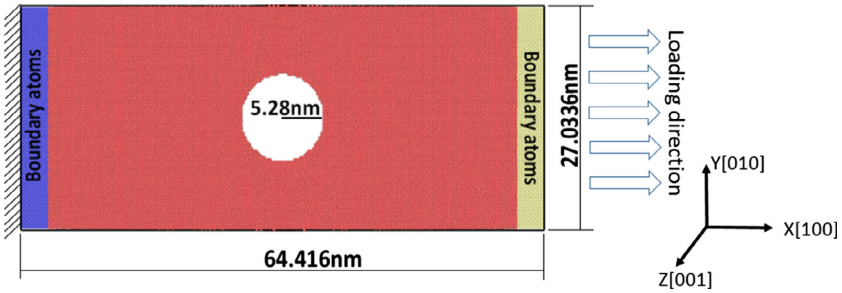

Fig. 1. Simulation Model (left boundary is fixed, right is loading at a constant strain rate).