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Atomistic simulation analysis of the effects of void interaction on void growth and coalescence in a metallic system

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ABSTRACT

Material deformation caused by the interaction between defects is a significant factor of material fracture failure. The present study employs molecular dynamics simulations of single-void and double-void crystalline Ni atomic systems to investigate inter-void interactions. Furthermore, simulations showing the evolution of dislocations for three different crystallographic orientations are conducted to study the void growth and coalescence. The simulations also consider the effect of the radius of the secondary void on dislocation evolution. The results show that double-void systems are more prone to yield than single-void systems. Further microstructural analysis indicates that the interaction between voids is realized by dislocation reactions. The simulation results of the dislocation evolution of the three orientations reveal that a relationship exists between the evolution of the dislocation density and the stress-strain curve. At the initial stage of dislocation, the dislocation grows slowly, and consists of Shockley partial dislocation. The dislocation growth rate then increases significantly in the sharply declining stage of the stress-strain curve, where most of dislocations are Shockley partial dislocation. Analysis of the dislocation length during the overall simulation indicates that the dislocation length of the [110] orientation is the longest, followed by that of the [111] orientation and the [100] orientation, which has the shortest dislocation length.

1Introduction

It is well known that the fracture failure of metallic materials is caused by casting defects such as voids and inclusions, and that deformation is prone to occur initially near such defects under mechanical loading. This deformation is well described by the growth of voids and the nucleation of microcracks around inclusions. With further loading, the existing and developing defects begin to interact. This results in void coalescence, crack merging, and void-crack interference effects, which are the primary causes to accelerate material deformation at this stage [1–5]. These micro-scale deformation behaviors in materials will eventually lead to the occurrence of macroscopic cracks, and further lead to fracture failure. Therefore, the investigation of the fracture behavior of materials is inseparable from microstructural analyses. Numerous studies have focused on the effect of microstructural evolution on fracture failure using both simulations and experiments.

Most previous investigations of ductile fracture processes based on void growth and microcrack nucleation occurring in the initial stages of deformation have employed various methods, such as the crystal plasticity finite element method [6–11], and dislocation dynamics and molecular dynamics [12–23]. Relatively few of these studies have focused on void growth behavior. Moreover, the modeling of void coalescence owing to the interaction of neighboring voids in the later stages of deformation has received far less attention than void growth. In terms of the interaction of defects, void coalescence has the most evident effect on material deformation [6,22].

Currently, the main factors that have been considered in computational studies of void coalescence are crystallographic orientation, stress triaxiality, and the spatial configuration of voids [2]. However, attempt have been done to model void coalescence in terms of a spatial configuration of voids either the geometric void size/spacing ratio between a pair of neighboring voids [8] or the plastic load limiting behavior of a non-hardening material containing regular array of voids [9–11]. The influence of various issues were addressed by Horstemeyer and Ramaswamy [1] and Pardoen and Hutchinson [24], such as void spacing, void shape, and strain hardening coefficient. In particular, Pardoen and Hutchinson divided void coalescence into either tensile void coalescence or shear void coalescence depending on the orientation of the ligament between the two coalescing voids. Any void coalescence model must introduce some microstructure information, such as the void/joint length and geometry. In addition, the evolution of internal microstructures should be considered. We noted that MD

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simulation have been used to reproduce the structural evolution at an atomic scale, including, dislocation motion and atomic diffusion [25,26]. Therefore, the MD simulation of void coalescence offers essential advantages unobtainable at larger scales of modeling.

Owing to the above considerations, the present study employs MD simulations of crystalline Ni atomic systems under uniaxial tension to investigate void growth and coalescence behaviors for different crystallographic orientations.

2. MD simulation methodology

In the present study, the embedded-atom method (EAM) potential developed by Mishin et al. [27] for Nickel is employed to simulate the uniaxial tensile behaviors of single crystal Ni with nanoscale voids. This potential has demonstrated a good ability for representing bonding in metallic systems and accounting for the dependence of the strength of individual bonds on the local environment, including features such as surfaces and defects. Therefore, this potential is expected to provide reasonable MD simulations of fracture and damage. Furthermore, this EAM potential is based on first principle calculations, and can reproduce many essential material properties such as the vacancy migration energy and the energies of both unstable and stable stacking faults. Several studies [28–31] have investigated material deformation behaviors using this EAM potential, which have verified the accuracy and reliability of the interatomic potential.

The present study employed the atomic system model shown in Fig. 1 to investigate the coalescence behavior of voids R1 and R2 under different crystallographic orientations listed in Table 1. The size in the Z direction is 20.064 nm, which is greater than the potential cut-off radius of 0.58 nm. The different arrangements of atoms under the different crystallographic orientations makes the difference in the number of atoms unavoidable in each case even though the size of the simulation box remains constant. The number of atoms in the [111] orientation model is the most, and is the least in the [110] orientation model. The lattice spacing is 3.52 Å × 3.52 Å × 3.52 Å for the [100] orientation, 4.97803 Å × 4.97803 Å × 3.52 Å for the [110] orientation, and 6.09683 Å × 5.74814 Å × 4.97803 Å for the [111] orientation.

The boundary conditions in the X and Y directions were free boundaries, and the periodic boundary condition (PBC) was applied to the Z direction. Therefore, the thickness effect was not considered in this research.

Microcanonical ensemble was employed during the simulation process, and the temperature of the thermostat atom was controlled by rescaling the mobile atomic velocity over a period of 40 ps in 1 fs time steps. Therefore, the model relaxes to an equilibrium state before stretching the simulation. As shown in Fig. 1, the left boundary of the atomic system was then held fixed while a uniaxially load was applied at the right boundary at a constant strain rate of 5×10^8 s^{-1}. All simulations were performed by LAMMPS at a temperature of 300 K.

The atomic stress tensor is calculated using the virial definition,

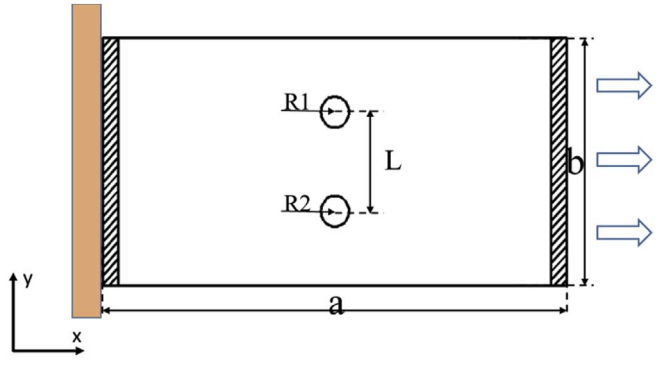

Fig. 1. Simulation model (a = 100 nm, b = 50 nm, R1 = R2 = 2 nm, L = 19.2 nm).

Table 1
Parameters for atomic systems with different crystallographic orientations.

Crystallographic orientation	X	Y	Z	Number of atoms
[100]	[100]	[010]	[001]	9,197,121
[110]	[110]	[$\bar{1}$10]	[001]	9,164,859
[111]	[111]	[11$\bar{2}$]	[$\bar{1}$10]	9,218,124

which can be expressed as

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

where f_α is the interatomic force acting between atoms i and j in the α direction (α = x, y, and z), r_β is the distance in the β direction, and N is the total number of atoms. The average of σ_t over a volume around atom i within the cut-off distance consisting of n atoms is given as

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

The open visualization tool (Ovito) developed by Stukowski [32] is employed to observe and analyze the atomic configuration throughout the stretching process. The centrosymmetry parameter defined by Kelchner et al. [33] was applied for highlighting defective atoms, and for observing the evolution centrosymmetry of slip bands, partial dislocations, and stacking faults during MD simulation. The slip system can be observed by controlling the centrosymmetry parameter. Dislocation analyses were conducted using the dislocation extraction algorithm (DXA) integrated in the Ovito software.

3. Results and discussion

Void growth and coalescence behavior was analyzed and discussed from the following two aspects: crystallographic orientation and the void radius.

Numerous studies have shown that the addition of a second void significantly affects void growth [19,34]. To study the effect of a second void on void growth and coalescence, the mechanical properties obtained from MD simulations for single void models and double-void models with different crystallographic orientations were compared. The stress-strain curves are summarized in Fig. 2, and the extracted mechanical properties are listed in Table 2.

Obvious differences are observed from the stress-strain curves of the single void and the double-void models in Fig. 2. Double-void systems are more prone to yield than single-void systems, and the critical yield

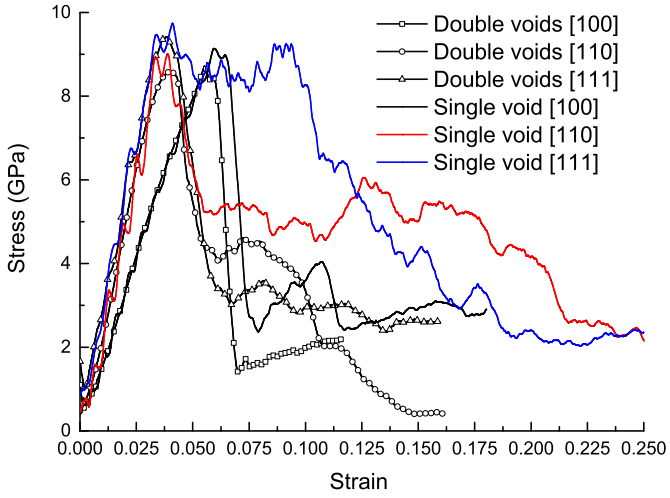

Fig. 2. Stress-strain curves of single-void and double-void models.