Computational Materials Science 104 (2015) 212–218

Contents lists available at ScienceDirect

Computational Materials Science

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

Cohesive zone representation of crack and void growth in single crystal nickel via molecular dynamics simulation

Yun-Li Li [a], Wen-Ping Wu [a,b,*], Nan-Lin Li [a], Yuan Qi [a]

[a] School of Civil Engineering, Wuhan University, Wuhan, China
[b] State Key Laboratory of Water Resources & Hydropower Engineering Science, Wuhan University, Wuhan, China

ARTICLE INFO

Article history:
Received 17 December 2014
Received in revised form 8 April 2015
Accepted 11 April 2015
Available online 25 April 2015

Keywords:
Molecular dynamics simulation
Stress distribution
Microstructural evolution
Cohesive zone model
Single crystal nickel

ABSTRACT

Pre-existing center crack and void growth in single crystal nickel under Mode I loading are investigated by introducing a cohesive zone model (CZM) based on molecular dynamics (MD) simulation. The microstructural evolution and stress distribution during crack and void growth are analyzed as are the associated mechanical properties. The results indicate that the crack and void have different fracture mechanisms. Crack-tip blunting occurs due to the [1 1 0] super-dislocations emission during crack growth, while for void growth the primary micro-mechanism is the formation of stacking faults, which result in the different growth rates, opening displacements, and stress states. Based on the calculation of the CZM, the crack has a greater growth speed and opening displacement, but a lower tensile stress and fracture strain than the void under the same loading conditions, and the high stress is accompanied by microstructural evolution during crack and void growth.

1. Introduction

Fracture behavior at the atomic scale is strongly dependent on the atomistic structure, lattice orientation, and the discrete nature of matter distribution. Most experimental evidence [1,2] and phase field simulations [3] have shown that the internal microstructures have a strong influence on fracture behavior at the nanoscale. Recent molecular dynamics (MD) simulations have already demonstrated the occurrence of microstructural evolution during crack and void growth and its influence on the fracture behavior. MD has also provided an understanding of the failure mechanisms on the atomic scale. For example, Matsumoto et al. [4] performed a MD simulation to investigate the internal structure change around the crack tip of an amorphous metal and its influence on the crack extension behavior and deformation state. Traiviratana et al. [5] investigated the void growth mechanisms in monocrystalline and bicrystalline copper by MD simulations, and revealed that the emission of shear loops was the primary mechanism of void growth. Potirniche et al. [6] performed a molecular dynamics simulation to analyze how the material length scale influences the damage progression of single crystal nickel by void growth and coalescence. Mi et al. [7] investigated the mechanism of void growth and coalescence in aluminum based by conducting dislocation analysis with MD simulations and observed the influence of the length scale on the stress–strain response, stress triaxiality and void fraction evolution. Zhao et al. [8] investigated nano-void growth in face-centered cubic (FCC) single crystal copper by MD simulation and revealed the effects of the cell size, crystalline orientation, and initial void volume fraction on the effective Young's modulus and yield strength. Tang et al. [9] used MD simulation to investigate nano-void growth and the fracture properties of single crystal γ-TiAl, and found that the production of dislocation cores and the propagation of shear loops make the void grow. These studies indicate that the micro-structural defects and their evolution have an important effect on the fracture properties of materials.

Because the internal microstructural evolution is closely related to the atomic stress field around the crack tip and material failure can be determined by the stresses and strains of strength theory, it is essential to consider the stress state during crack and void growth. Abraham's results [10,11] indicated that the atomic stress near the crack tip controlled the stability of brittle crack propagation. Xu and Deng [12] reported that atomic stress played a controlling role in nano-scale fracture. Nishimura and Miyazaki [13] calculated the tensile stress at the crack tip during the crack propagation process, and pointed out when the stress at the crack tip exceeded the ideal strength, the crack will propagate brittlely and without plastic deformation. Tang et al. [14] revealed that

* Corresponding author at: School of Civil Engineering, Wuhan University, Wuhan, China. Tel./fax: +86 27 68775496.
E-mail address: wpwu@whu.edu.cn (W.-P. Wu).

http://dx.doi.org/10.1016/j.commatsci.2015.04.011
0927-0256/

the von Mises stress or normal stress around the crack tip controlled the fatigue crack growth behavior. Zhou et al. [15] analyzed the stress distributions along grain boundary crack propagation and explored the relationship between crack propagation and the microstructural evolution at the crack tip. Previously, we investigated [16,17] the stress distributions and microstructural evolution characteristics near the crack tip during crack propagation by MD simulations.

However, considering that strength theory predicts a non-physical stress singularity at the crack tip, it is inappropriate to investigate crack propagation by analyzing the stress state near the crack tip. The cohesive zone model (CZM) removes this unrealistic stress singularity at the crack tip and regards crack growth as a progressive process of material degeneration. Currently, the CZM has been extensively used because it avoids the stress singularity at the crack-tip and represents the physics of the fracture process at the atomic scale [18–20]. Especially, the CZM can adequately track crack propagation dynamics and obtain the tensile stress and opening displacement relationship (traction–displacement relationship) [21]. This relationship gives the constitutive behavior of the fracture, which is not obtained only by MD simulation. Therefore, an analysis of the stress field and microstructural evolution by introducing a CZM based on MD simulation is important and of interest for the study of the fracture properties of materials from an atomistic perspective.

In this paper, we investigate the microstructural evolutions and stress distributions during crack and void growth using a MD-based CZM in a pre-cracked single crystal of nickel. The objective of the present work is to determine the relationships between the crack tip stress field and the microstructural evolution, tensile stress and opening displacement as the crack and void propagate. Meanwhile, the different mechanisms of crack and void growth under Mode I loading and their associated mechanical properties are obtained.

2. Atomistic models and stress calculations

In this work, we carry out a MD simulations based on the CZM to investigate the internal microstructural and stress evolutions during crack and void growth. The geometries of the models containing a central crack or a central void are shown in Fig. 1. Both models are in the cubic orientation (i.e., *X*-[100], *Y*-[010], and *Z*-[001]). The size of the blocks ($X \times Y \times Z$) are $100a \times 60a \times 4a$ (352 Å × 211.2 Å × 14.08 Å), where $a = 3.52$ Å is the lattice constant of nickel. In these two models, a central crack or void is inserted in the center of the crystal by removing atoms. The length of the initial crack is equal to $10a$ (35.2 Å) and its width is $2a$ (7.04 Å), as shown in Fig. 1(a); the diameter of the central hole is equal to $10a$ (35.2 Å), as seen in Fig. 1(b). In order to calculate the stress field and its distribution during crack and void growth under Mode I loading and to study the local properties and microstructural evolution from atomistic simulations, The initial configuration is divided into $n = 100$ cells (where the width of one cell is the lattice constant of nickel) along the *X* direction, and a cohesive zone height of $n = 12$ cells along the *Y* direction, as shown in Fig. 1(c). These cohesive surface cells (elements) in Fig. 1(c) are introduced to describe material separation and determine the relationships between local stress distribution and microstructural evolution, tensile stress and opening displacement as the crack and void propagate under Mode I loading.

In the present MD-based CZM simulations, the embedded-atom-method (EAM) potential provided by Mishin et al. [22] was used, which has previously been successfully applied to simulate the failure process of FCC single crystal nickel [16,17,23]. The atoms in the top and bottom two layers are fixed, and the two layers of atoms on right side of the models are fixed for motion along the *X*-direction to limit boundary effects. Periodic boundary conditions are formulated in the *Z* direction, and non-periodic boundary conditions are applied in the *X* and *Y* directions. At the start of the

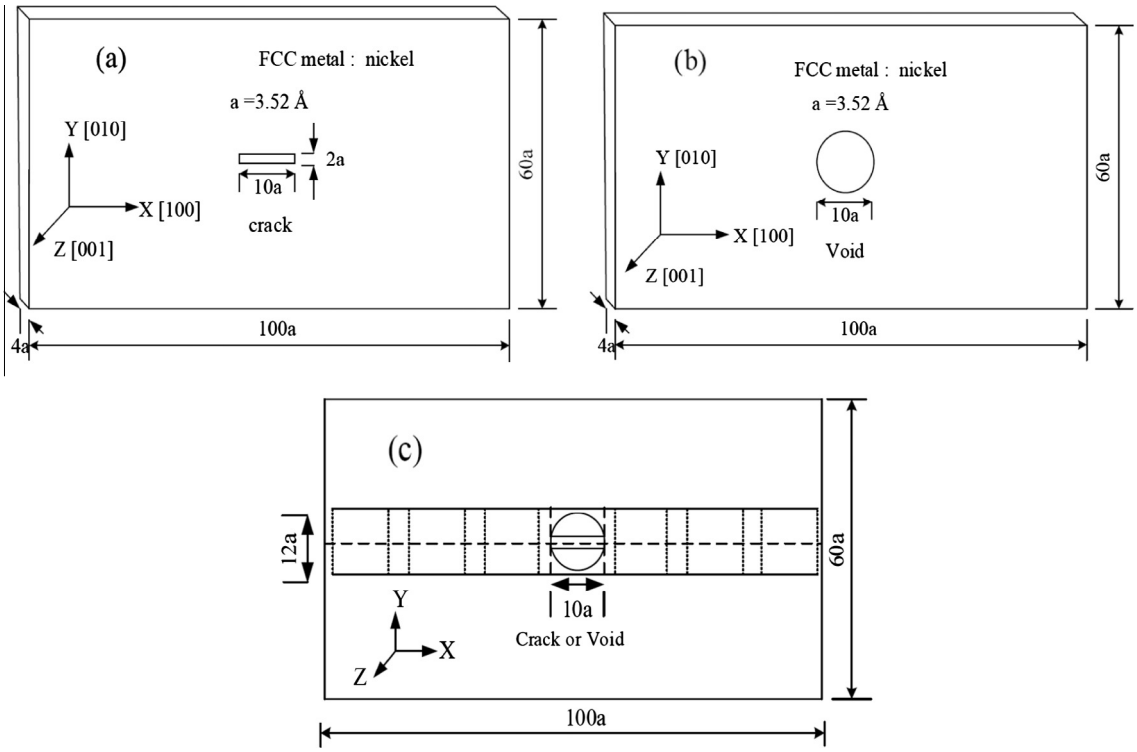

Fig. 1. The specimen geometry of a FCC nickel single crystal for a (a) specimen with a central crack, and (b) specimen with a central void. (c) A schematic of the regions used to calculate the local properties for the CZM.