Computational Materials Science 113 (2016) 203–210

Contents lists available at ScienceDirect

Computational Materials Science

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

Molecular dynamics-based cohesive zone representation of microstructure and stress evolutions of nickel intergranular fracture process: Effects of temperature

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

[a] Department of Engineering Mechanics, School of Civil Engineering, Wuhan University, Wuhan 430072, China
[b] State Key Laboratory of Water Resources & Hydropower Engineering Science, Wuhan University, Wuhan 430072, China

ARTICLE INFO

Article history:
Received 29 July 2015
Received in revised form 10 October 2015
Accepted 1 December 2015

Keywords:
Deformation twinning
Intergranular fracture
Crack-tip stress
Molecular dynamics simulations
Cohesive zone model

ABSTRACT

In this study, we find microstructure mechanisms and stress distributions around the crack-tip of an intergranular fracture process in bicrystal nickel are strongly dependent on temperature by using a molecular dynamics (MD)-based cohesive zone model (CZM). At a lower temperature, deformation twinning occurs in the two opposite directions along the grain boundary, and the crack propagation eventually forms an intergranular fracture. As the temperature increasing, deformation twinning is becoming increasingly hard to occur around the crack-tip along the grain boundary but more readily to generate the slip bands, and the crack propagation will not form intergranular fracture along the grain boundary. Moreover, based on the calculation of CZM, the slip bands are stronger to prevent intergranular crack growth than deformation twinning around the crack-tip, and a high stress is found in the region of microstructure evolution near the crack-tip. The present results may provide useful information for understanding intergranular fracture mechanisms and stress distributions at the atomic-scale.

1. Introduction

Intergranular fractures are the cracks that occur along the grain boundary (GB) of a material. Thus, the GB is weakened or embrittled by impurity segregation. The atomic arrangement at GB becomes disordered with many defects such as microcracks, vacancies, dislocations, and bond deformations. GB is the preferred place of crack initiation, where microcracks easily grow and coalesce at GB perpendicular to the loading axis, thus leading to intergranular fractures [1,2].

However, intergranular fracture behavior at the nanometer scale is less understood and being investigated currently. At this small scale, the intergranular fracture behavior is strongly dependent on the local atomic environment such as the GB [3–7], lattice orientation [7,8], loading conditions [9–12], local atomic structure, and plastic deformation [12,13]. Furthermore, the temperature also significantly affects the interfacial fracture strength and microplastic deformation of nanocomposites [14,15]. It is well known that at a low temperature, the two major mechanisms responsible for the plasticity of materials are ordinary dislocation plasticity and deformation twinning [16,17]. The responses of fractures in crystalline metals to the temperature are complex phenomena, involving many microplastic deformations such as deformation twinning [16–19], stacking fault [19], dislocation motions [20,21], void growth and colasence [22,23], and slip bands [24,25].

The occurrence of plastic deformation is closely related to the crack-tip stress field, and it may play an important role in crack propagation [19,25,26]. Abraham's research [27] pointed out the atomic stress near the crack-tip controls the stability of brittle crack propagation. Recently, many atomistic simulations of crack propagation and fracture behaviors by Xu and Deng [26], Krull and Yuan [28], and Wu and Yao [25,29] also illustrated that the calculation of the atomic stress field around the crack-tip was very important in understanding the nanoscale fracture events. However, as we know, it is inappropriate to calculate directly the stress state near the crack-tip because of the stress singularity at the crack-tip. The cohesive zone model (CZM), as a method for calculation of local properties in the field of fracture mechanics, has been extensively used because it can avoid the stress singularity at the crack-tip and represent the physics of the fracture process at the atomic scale [30,31]. In our previous work, a molecular dynamics (MD)-based CZM was applied to track crack propagation dynamics of a pre-cracked single crystal nickel and obtain the crack-tip stress

* Corresponding author at: Department of Engineering mechanics, School of Civil Engineering, Wuhan University, Wuhan 430072, China. Tel./fax: +86 27 68775496.
E-mail address: wpwu@whu.edu.cn (W.-P. Wu).

http://dx.doi.org/10.1016/j.commatsci.2015.12.001
0927-0256/

distribution and microstructure mechanism as well as local mechanical properties under monotonic and cyclic loading [32,33], however, these studies mainly focused on crack propagation of a single crystal nickel at constant temperature, the intergranular crack propagation and the effect of temperature on the intergranular fracture behavior were not involved in the previous work.

Here, we continue to apply a MD-based CZM for analyzing the intergranular crack propagation process, crack-tip stress distribution and microstructure evolution of a bicrystalline nickel at different temperatures. The effect of temperature on the intergranular crack propagation is investigated, and the temperature dependence of deformation mechanism and stress distribution for a pre-cracked bicrystalline nickel are obtained. The simulation helps to understand the temperature dependence of intergranular fracture behavior and microstructure evolution during the intergranular crack propagation.

2. Modeling and simulation

2.1. MD Model geometry and simulation process

To simulate an intergranular fracture, a bicrystal simulation cell is used, and the geometry of the crack propagation system is shown in Fig. 1. The size of nickel ($X \times Y \times Z$) is $150a \times 100a \times 6a$ (528 Å × 352 Å × 21.12 Å). The crystal dimension in the X-axis is long enough for steady-state crack propagation during MD simulations. Periodic boundary conditions are applied in all the directions. The model has two broad layers, marked as "Crystal I" and "Crystal II", forming a bicrystalline system with a flat GB in the middle. The crystallographic orientations of Crystals I and II are shown in Fig. 1a. In the imposed coordinate system of the model, the orientation of Crystal I is: (X: [100], Y: [02$\bar{1}$], and Z: [01$\bar{2}$]), and the orientation of Crystal II is: (X: [100], Y: [021], and Z: [0$\bar{1}$2]). In this manner, Crystal II is a mirror image of Crystal I relative to the crystallographic plane (100), and the initial crack fronts at the left and right sides are along the [$\bar{1}$00] and [100] directions, respectively. The system thickness h in the z-direction equals to 6 (012) crystallographic planes, more than four times larger than the range of the interatomic potential. This prevents interference of the atoms with their periodic images and preserves the local three-dimensional (3D) physics in the system, because the macroscale values of strength and toughness do not represent the unique response of a particular interface at which a local fracture event may occur. In the model, the initial center crack is inserted in the middle of a bicrystalline system with a flat GB by removing atoms. The length of the initial crack is equal to $10a$ (35.2 Å), and its width is 3.52 Å, where a = 3.52 Å is the lattice constant of nickel.

In this study, the EAM potential obtained by Mishin et al. [34] is used to simulate the failure process of a precracked bicrystalline nickel, because this potential can provide a reasonable simulation of fracture and damage and has been successfully applied to simulate the fracture process of nickel [25,29,32,33,35]. To simulate the intergranular fracture process under uniaxial tensile loading in the y-direction, at the start of simulation, this atomic system is relaxed using the conjugate gradient method to reach the minimum energy state. Then the relaxed system is stretched in the y-direction by an incremental displacement loading every 20 ps, by maintaining the top and bottom boundaries parallel to each other, and the simulation is carried out by integrating Newton's equations of motion for all the atoms using a time step of 1×10^{-15} s, this result in the global strain rate is 2.0×10^{8} s^{-1}. In the next step, the same displacement increment is applied again, and the process is repeated. Finally, the deformed configuration of the system is computed by

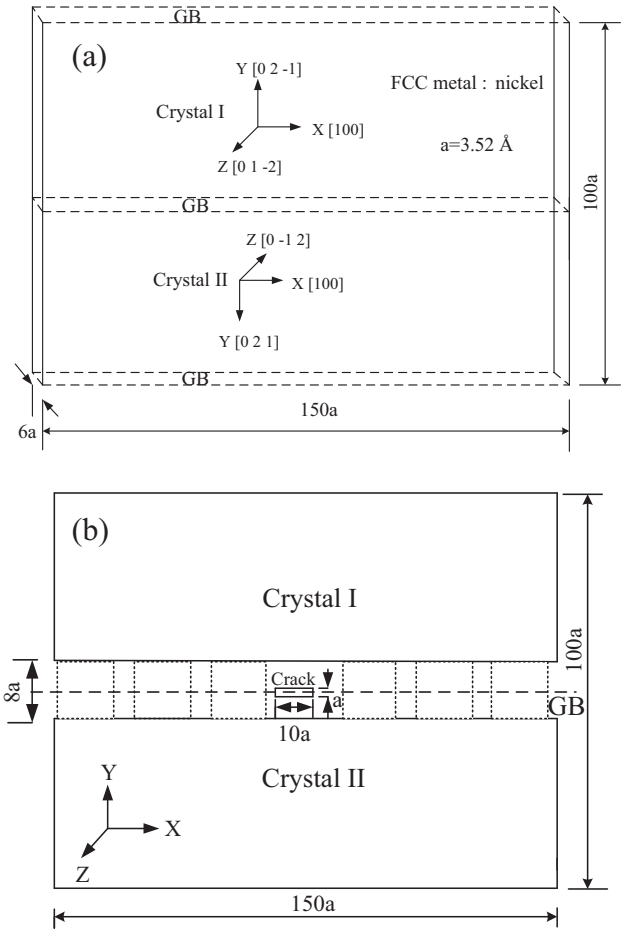

Fig. 1. Simulation model. (a) Sample geometry of a bicrystalline nickel with a flat GB in the middle and (b) schematic of regions used to calculate the local properties and initial crack geometry.

MD simulation combined with the CZM. To study the temperature effect, the simulations are conducted at four different temperatures: 30, 100, 300, and 500 K. The open-source MD code LAMMPS [36] and the visualization tools AtomEye [37] are used in the atomistic simulations. The atomic configurations and their evolutions are analyzed by Centro-symmetry parameter (CSP) proposed by Kelchner et al. [38], which provides details of the evolutions of the crack growth. The calculation of the atomic stress is similar to our previous work [32,33], which is defined based on a strength measurement of the inter-atomic interactions of the atom with its neighboring atoms proposed by Born and Huang [39] and Horstemeyer et al. [40].

2.2. Cohesive zone model

In order to calculate the stress field and its distribution during intergranular crack growth and to study the local properties and crack-tip microstructure evolution from MD simulations, a schematic of cohesive zone is used to analyze facture properties [31–33]. The initial configuration is divided into n = 150 cells (where the width of one cell is the lattice constant of nickel) along the X direction, and a cohesive zone height of n = 8 cells (eight times the lattice constant of nickel) along the Y direction, as shown in Fig. 1b. This model homogenizes the discrete damage processes as a smeared continuum to ascertain the relationship governing its cohesive behavior from MD simulations. Meanwhile, these cohesive surface cells in Fig. 1b are introduced to describe material