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Molecular dynamics simulation-based cohesive zone representation of fatigue crack growth in a single crystal nickel

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ABSTRACT

Nanoscale fatigue crack growth was investigated by introducing a cohesive zone model based on molecular dynamics simulations. The evolutions of the microstructure and stress in fatigue crack growth over two different cyclic loading regimes were investigated using pre-existing centre crack specimens. Under increasing strain amplitude cyclic loading, dislocations emitted and persistent slip bands formed around the fatigue crack tip, which retarded crack propagation and changed the stress distributions; under constant amplitude cyclic loading, crack opening and closing was accompanied by void formation in the crack plane. Different fatigue loading regimes resulted in different crack propagation mechanisms and stress distributions; the peak stress was accompanied by microstructure evolution ahead of the crack tip, which induced the variation in fatigue crack growth rates and crack opening displacements.

1. Introduction

Fatigue is one of the most damaging mechanisms for structural components. With the development of nanomaterials and nanostructures, fatigue damage within single crystals at the nanoscale has become a pressing issue for researchers and designers.

Molecular dynamics (MD) simulation can model atomic scale evolution processes for studying the failure mechanisms of materials. Cyclic loading behaviour and related plastic deformation of fatigue crack growth in single crystals has been investigated by MD simulations. Nishimura and Miyazaki [1] revealed that the fatigue-crack growth mechanism of α-Fe is due to coalescence of the crack and the vacancies caused by the emission and absorption of dislocations at the crack tip by MD simulation. Potirniche et al. [2–4] analyzed fatigue damage in nickel and copper single crystals under four loading orientations [1 1 1], [1 0 0], [1 1 0], and [1 0 1], to reveal different crack propagation mechanisms for different orientations under constant and variable amplitude loadings. Farkas et al. [5] investigated the mechanisms of fatigue behaviour in nanocrystalline metals and showed that the main atomistic mechanism of fatigue crack propagation was the formation of nanovoids ahead of the main crack and found that the stress intensity amplitude was consistent with experimental studies and a Paris law. Tang et al. [6] and Ma et al. [7] analysed the fatigue behaviour of an hcp magnesium single crystal and bcc iron under cyclic loading, respectively, and revealed microstructures (such as dislocation emissions, twin bands, slip bands, and vacancies) occurring at the crack tips played major roles in the fatigue crack growth. Uhnakova et al. [8,9] investigated the dislocation emission and plastic growth of ductile cracks in bcc iron under cyclic loading and monotonic tensile loading by using 3-D atomistic simulation. The results showed that twinning and dislocation emission in oblique slip systems $\langle 1\bar{1}1\rangle\{0\,1\,1\}$ and $\langle 1\bar{1}1\rangle\{1\,2\,1\}$ occurred under cyclic loading but not under monotonic tensile loading. Furthermore, Machova et al. [10] and Uhnakova et al. [11,12] investigated the fatigue behaviour of ductile cracks in bcc iron in modes I, II, and III, and pointed out different fatigue crack behaviours and microstructures at the crack front under different, or mixed, modes. These studies based on MD simulations revealed microstructure evolutions and fatigue fracture mechanisms, but did not analyse the relationship between the stress and microstructure evolution during fatigue crack growth. Due to the microstructure evolution of atoms around the crack tip resulting in a change of stress field around the crack tip severely affecting crack growth rates and material fracture properties [13–17], it was essential to understand crack tip plasticity-induced non-linear behaviour and stress fields during fatigue crack growth based on the analysis of the microstructure and stress evolution near the crack tip.

Considering that strength theory predicts a non-physical stress singularity at the crack tip, it is inappropriate to investigate crack

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propagation by analyzing the stress state near the crack tip. The cohesive zone model (CZM) describes non-linear crack behaviour by means of cohesive forces in an infinitely thin strip. This simplified the plastic zone, removed the unrealistic stress singularity at the crack tip, and regarded crack growth as a progressive process of material degeneration [18]. In particular, the CZM can adequately track crack propagation dynamics and obtain the relationships between the crack tip stress and microstructure evolution, crack opening displacement and normal stress as the crack propagates. Recently, MD simulations based on the CZM were successfully used to investigate the microstructure and stress evolution around a crack tip and the associated fracture mechanisms of materials under monotonic tensile or shear loading [19,20]. In our previous work, the crack-tip stress and microstructure evolution of single crystal nickel during the crack and void growth under monotonic tensile loading also have been investigated by introducing a CZM based on MD simulation [21]. Here, we will further study fatigue crack growth mechanisms and stress distribution characteristics under cyclic loading.

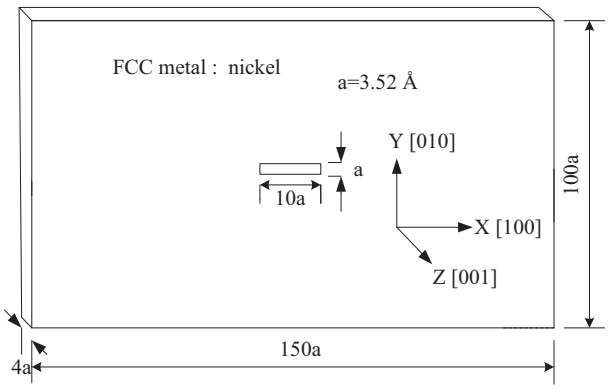
In the present work, MD simulations based on CZM were used to examine the crack-tip stress and microstructure evolution during fatigue crack growth. The objective of the present study was to characterise the fatigue damage caused by the crack-tip stress and microstructure evolution during fatigue crack growth in a middle-tension (MT) specimen of nickel, as well as to determine the relationship between changes in the stress field near the crack tip and the microstructure evolution. Meanwhile, the fatigue crack growth length, crack opening displacement and their associated physical mechanisms were obtained under increasing strain amplitude cyclic loading and constant amplitude cyclic loading.

2. Modelling and simulations

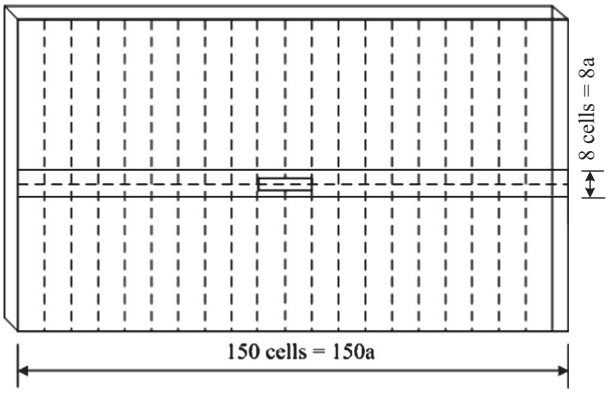
2.1. Molecular dynamics and cohesive zone models

In this work, a constrained three-dimensional MD model was used for the study of fatigue failure in a face-centred cubic (FCC) single nickel crystal under cyclic loading: the initial configuration of this single crystal with its pre-existing central crack was as shown in Fig. 1a. The crystal lay in its cubic orientation (*i.e.* *X*-[100], *Y*-[010], and *Z*-[001]), the size of the sample ($X \times Y \times Z$): $150a \times 100a \times 4a$ (528 Å × 352 Å × 14.08 Å). In the model, a central crack was formed in the crystal by removing atoms, the initial length of the crack was $10a$ (35.2 Å) and its width a (3.52 Å), where a was 3.52 Å (the lattice constant of nickel). The atoms in the top and bottom layer, which have a thickness (4.80 Å) equal to the potential cut-off distance, were fixed by freezing on their perfect lattice sites. Periodic boundary conditions were formulated in the *X* and *Z* directions, and non-periodic boundary conditions were applied in the *Y* direction.

In order to calculate the stress field and its distribution during fatigue crack growth under cyclic loading and to study the local properties and crack-tip microstructure evolution from MD simulations, a schematic of cohesive zone was used to calculate fatigue facture properties. The initial configuration was divided into

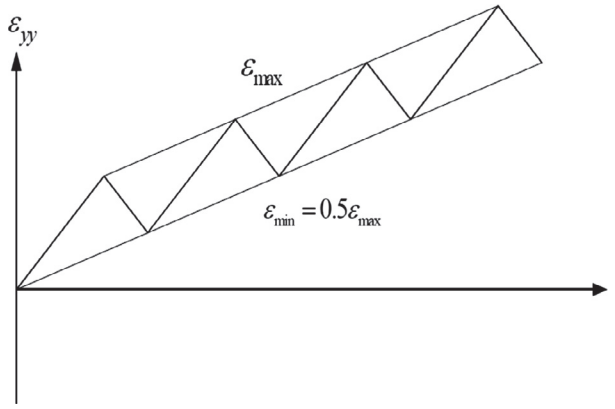


(a) Molecular dynamics model geometry

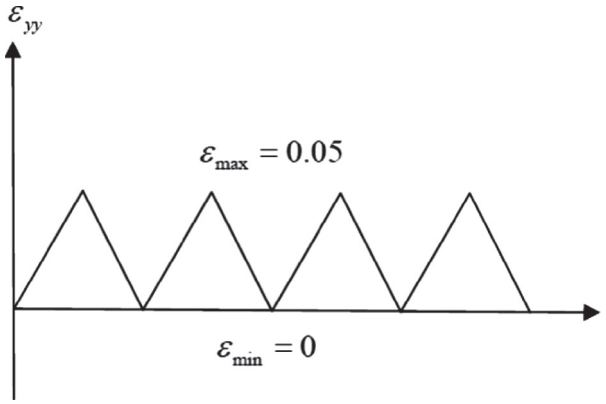


(b) Schematic of cohesive zone model used to calculate facture properties.

Fig. 1. (a) Sample geometry of an FCC single crystal nickel containing a single centre crack and (b) Schematic of region used to calculate facture properties and obtain the cohesive behaviour mechanism from molecular dynamics simulation.



(a) Cyclic loading I: increasing strain amplitude fatigue loading



(b) Cyclic loading II: constant strain amplitude fatigue loading

Fig. 2. Cyclic loading Regimes I and II: (a) increasing strain amplitude fatigue loading and (b) constant strain amplitude fatigue loading.