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Nanostructurally small cracks (NSC): A review on atomistic modeling of fatigue

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ABSTRACT

Fatigue is one of the most damaging mechanisms in structural components. With the development of structural nanomaterials, it is imperative to investigate the fatigue damage phenomena at the atomic scale. To study fatigue behavior at the nanoscale, one must apply non-continuum modeling frameworks, such as molecular statics (MS), molecular dynamics (MD), and Monte Carlo (MC) methods. To date, only MD and MS simulations using embedded atom method (EAM) and modified embedded atom method (MEAM) potentials have been conducted, and this paper reviews these simulations of the nanoscale fatigue-crack growth in nickel and copper including single crystals, bicrystals, and polycrystals. A nanoscale size middle tension (MT) specimen with the lateral side applied periodic boundary conditions was used to investigate the fatigue behavior in nickel and copper single crystals. Simulation results revealed that the cyclic plastic deformation at the crack tip was the main influencing factor for fatigue-crack growth. Two main nanoscale mechanisms of crack propagation were observed: (1) the main cracks linked with the voids nucleated in front of crack tip due to high dislocation density generated by the cyclic loading; and (2) the main cracks broke the atomic bonds in the crack plane without much plasticity. For the bicrystals and polycrystals, the grain boundaries exerted resistance to the crack propagation. To study the interactions between cracks and grain boundaries, four cases of grain boundary interfaces for copper and two cases of grain boundaries for nickel were simulated. In copper bicrystals, the crack path deviated and moved from one grain to another for high misorientations, while there were voids nucleating at grain boundaries in front of the crack tip that linked back with the main crack. Similar to macroscale fatigue, dislocation substructures were observed to develop in the atomic lattice during cyclic loading. In nickel bicrystals, for large misorientations, the cracks were stopped by grain boundaries. For small misorientations, the crack propagated through the grain boundary, but the growth rate was reduced due to the resistance of the grain boundary. Fatigue-crack growth rates for nanocracks were computed and compared with growth rates published in the literature for microstructurally small cracks (micron range) and long cracks (millimeter range). A nanostructurally small crack (NSC) was introduced in terms of the CTOD. The quantified NSC growth rates in copper single crystals were very similar with those experimentally measured for small cracks (micron range) and with those at stress-intensity-factor ranges lower than the threshold for long cracks (millimeter range). The atomistic simulations indicated that reversible plastic slip along the active crystallographic directions at the crack tip was responsible for advancing the crack during applied cycling. In the case of single or double plastic slip localization at the crack tip, a typical Mode I fatigue crack arose along a slip band and then grew into a mixed Mode I + II crack growth mechanism. For crystal orientations characterized by multiple slip systems concomitantly active at the crack tip, the crack advance mechanism was characterized by nanovoid nucleation in the high density nucleation region ahead of the crack tip and by linkage with the main crack leading to crack extension. To facilitate observations of fatigue-crack growth, the simulation of a copper polycrystal was performed at low temperature 20 K as well. The crack propagated along persistent slip bands within the grain. The crack propagated along grain boundaries when the angle between the direction of crack propagation and the grain boundary was small, while it was impeded by the grain boundary when the angle was large. The results obtained for the crack advance as a function of stress intensity amplitude are consistent with experimental studies and a Paris law exponent of approximately two.

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1. Introduction

Fatigue in metallic materials subject to repeated cyclic loading has been an active research area since last century and continues to be a focus of structural materials study. Most investigations of fatigue have been performed at the microscale and/or macroscale. Hence, the mechanism of fatigue failure is fairly well understood with the crack lengths ranging from a few microns to millimeters/centimeters. The classic continuum approaches are very powerful tool to solve the problems at the macro- or microscale. However, several reasons exist for performing atomic scale simulations. First, due to the development of nanomaterials and nanostructures, fatigue will become, at some point, an issue for the designers. Without the knowledge base for nanoscale fatigue, the designs will not be as robust. Second, macroscale fatigue models, particularly ones with microstructural sensitivities do not cover the length scale in the atomic region. To garner nanoscale crack growth rules in order to get more accurate macroscale predictive tools, atomistic simulations are warranted to provide mechanism understanding of grain boundary effects, crystal orientation effects, and driving force versus material resistance effects. Finally, nanoscale fatigue simulations such as those provided in this review can give insight into the fidelity of higher scale mathematical models and micromechanical finite element simulations by either providing the pertinent equations or at least the parameters for already developed equations.

With respect to multiscale fatigue models, several have recently been developed [1–5] precious few have focused on the nanoscale. Since atomistic modeling is a useful tool to help understand and model the motion of each atom in the material, molecular dynamics and statics simulations can provide understanding into the dislocation nucleation, motion, and interaction with cracks. As opposed to continuum theories, atomistic modeling is capable of providing insight into solving fatigue problems based more on first principles. As long as the interatomic potential is reliable, it can disclose the fundamental physical mechanisms of fatigue. As such, some questions that have driven the research in atomistic fatigue are the following: can the equations that represent the microstructurally small crack growth regimes be used for nanocrack growth since material resistance is present at both length scales? Can long crack growth models be used to capture the nanocrack growth rates? Does the crystallographic orientation effect change our paradigm of small crack growth? Do we see the same mechanisms at the nanoscale as we do at the microscale and macroscale?

To provide context for the nanoscale fatigue study presented here, it is worth mentioning that extensive studies on single crystal, bicrystal, and polycrystalline under monotonic loads have been accomplished by several researchers. Daw et al. [49] provided a nice summary of using embedded atom method (EAM) potentials for understanding dislocation nucleation and propagation, application to hydrogen environments, and issues with free surfaces like cracks. Holian et al. [81] and Abraham et al. [82] were probably the first to examine large scale parallel computing simulations of cracks growing via molecular dynamics simulations. Baskes et al., [57] studied biomaterials interfaces under monotonic loads. Gall et al. [58] conducted molecular dynamics simulations to study the crack growth of aluminum–silicon biomaterial interfaces. Fang et al. [59] performed Bauchinger effect studies by examining single and bicrystal nickel specimens to associate the type of dislocations with reverse yielding effects. Clearly, a whole review is warranted just to discuss the plasticity and fracture related to atomistic simulations, but a few seminal papers were mentioned here to provide context for the nanoscale fatigue discussions ahead.

The fatigue behavior of materials has not been studied extensively at atomic level. The basic reason is relate to the difficulties arising from the associated length and time scales. To the best of our knowledge, only several researchers conducted the computational study on fatigue-crack growth of face-centered cubic metal, namely, copper and nickel at atomic scale [6–9]. The results of atomistic simulation by Farkas et al. [9] are consistent with the experimental results of fracture and fatigue in a bulk nanocrystalline Ni–Fe alloy carried out by Yang et al. [10] who revealed that the fatigue crack in the nc Ni–Fe alloy initiated by nanovoid coalescence ahead of the dominant crack tip. Nishimura and Miyazaki [11] performed the molecular dynamics simulation of α-Fe to examine the mechanical behaviors around a crack tip for a system containing both a crack and two tilt grain boundaries under cyclic loading. They proposed that the fatigue-crack growth mechanism is due to the coalescence of the crack and the vacancies caused by the emission and absorption of the dislocations at the crack tip. Chang and Fang [12] analyzed the tensile and fatigue behavior of nanoscale copper at various temperature using molecular dynamics simulation. They concluded that the effect of increasing temperature is an increase in fatigue stress and the ductile fracture configuration occurred under lower applied stress.

In light of the aforementioned comments, the focus of this paper is to present a review on the atomistic modeling of fatigue-crack growth in single crystals, bicrystals, and polycrystals of copper and nickel reported in [6–9]. We try to sum up the works performed in this field so far. The survey of the literature is included in Sections 2–4. We also added some new atomistic fatigue-crack growth results in nickel bicrystals and copper polycrystals, which had not been published in the literature. The summary is presented in the final section with thoughts regarding new areas of research regarding atomistic modeling of fatigue.

2. Simulation method

2.1. Interatomic potentials

In atomistic modeling, the properties of materials can be defined by the interatomic potential (to a continuum mechanics person, this is the constitutive relationship), which is the basic input of molecular simulation besides the structural information such as the initial configuration of atoms, type of atoms and their velocities, etc. The choice of interatomic potential is vital to the simulation results. The embedded atom method (EAM) potential was devised to solve practical problems in metals with many-body bonding properties [13,14] and were used the fatigue studies of [6–9]. EAM treats each individual atom as an embedded particle in a host aggregate composed of all the other atoms. The embedding energy contributes to the total energy of the system through the local electron density where an individual atom is located. The EAM theory is based on local-density functional principles and its central idea is that the cohesive energy of a system can be described as the energy provided by an atomic system during the embedding process of each constituent atom in that particular system, as given in the equation

$$E = \sum_i G_i\left(\sum_{j\neq i}\rho_j^a(R_{ij})\right) + 1/2\sum_{i,j(i\neq j)} U_{ij}(R_{ij}) \quad (1)$$

where G is the embedding energy, ρ^a is the average electron density, R_{ij} is the distance between the atoms i and j and U is the energy due to the electrostatic interaction between two atoms [14]. As shown Eq. (1), an important assumption is that the embedding energy of any atom (which can be viewed as an impurity) is a function of the electron density of the host before the atom is added. The functions G_i and U_{ij} are calculated from experimental curve fitting of the lattice parameter, elastic constants, and sublimation and vacancy formation energies [13]. An improvement to the EAM is the modified embedded atom method (MEAM) potential [15,16]. In