Acta Materialia 99 (2015) 77–86

Contents lists available at ScienceDirect

Acta Materialia

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

Atomistic mechanisms of fatigue in nanotwinned metals

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ARTICLE INFO

Article history:
Received 7 March 2015
Revised 29 June 2015
Accepted 18 July 2015

Keywords:
Fatigue crack
Nanoscale twins
Dislocation
Detwinning
Atomistic simulation

ABSTRACT

We investigate the fatigue behavior of nanotwinned Cu using a combination of molecular statics and molecular dynamics simulations. The presence of nanoscale twins is found to enhance fatigue crack growth resistance. For the twin-free nanocrystalline samples, the fatigue crack propagates by linking the nanovoids that are formed ahead of the crack tip. In the case of the nanotwinned samples, however, it advances as the crack tip alternately blunts and re-sharpens due to dislocation emission and slip. Both detwinning and crack closure are observed in the path of the fatigue crack in nanotwinned samples with a high density of twin boundaries. As the twin number per grain (quantified by the ratio of the mean grain size to the twin boundary spacing d/λ) increases, detwinning increases the dissipated energy of fatigue cracking, leading to enhanced fatigue resistance. The atomistic simulations show that fatigue crack growth in nanotwinned Cu conforms to Paris' law. In conjunction with the experimental results, we obtain a quantitative estimation of the Paris' law exponent (~4.0), which is in agreement with the theoretical predictions from the damage accumulation model.

1. Introduction

Fatigue is one of the most common failure modes in metallic materials. Investigating the fatigue behaviors and the associated deformation mechanisms of metals/alloys under cyclic loading is of scientific and technological interest. Nanocrystalline (NC) metals possess good fatigue resistance because a large number of internal grain boundaries (GBs) can substantially impede fatigue crack propagation [1]. Early studies on the fatigue behaviors of NC metals have revealed a nanoscale mechanism [2,3], i.e., vacancies coalesce into nanovoids at the GBs in front of a crack tip, and then, the main crack advances by linking with these nanovoids. Over the past few years, nanotwinned (NT) metals, a new type of hierarchical nanostructured material, have attracted enormous research attention [4–21]. In such materials, high-density nanoscale twins are introduced into the sub-micron-sized grains and act as sub-structures that can not only confine the dislocation segment length but also store the mobile dislocations during deformation [7]. Consequently, NT metals exhibit an unusual combination of ultra-high strength, good ductility, elevated strain hardening, and high fracture toughness [4–7,14–19]. So far, there have been only limited studies on the fatigue of NT metals, and the underlying mechanism currently remains mysterious and sometimes even controversial. For example, the experiments conducted by Singh et al. [17] revealed that NT Cu has a noticeably improved resistance to the fatigue crack growth compared to its twin-free ultrafine-grained (UFG) counterpart and that the NT samples with higher twin densities show stronger resistance than those with lower twin densities. However, Shute et al. [20] recently reported that the S–N curves (a characteristic curve to predict fatigue life of materials) of NT Cu are similar to those of UFG counterparts, implying that the nanoscale twins might have negligible effects on the fatigue properties of UFG or NC metals. Most recently, it was found from the fatigue tests on coarse-grained Cu and its alloys with annealing twins [22] that the coherent twin boundaries (TBs) surrounding twin lamellae reduce the fatigue properties. The origin is that the TBs can serve as the nucleation sites and propagation paths of fatigue cracks due to the complicated interactions between TBs and dislocations. The most recent experimental studies [23,24] on the fatigue of bicrystalline Cu with a coherent TB have shown that when a TB is inclined to the loading direction, the fatigue crack initiates along the TB.

To clarify the above controversies and provide a fundamental understanding of fatigue mechanisms in the NT metals, we

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http://dx.doi.org/10.1016/j.actamat.2015.07.045
1359-6454/

investigate the cyclic deformation of the NT Cu using atomistic simulations. Here, a combined scheme of molecular statics (MS) and molecular dynamics (MD) is used to overcome the timescale limitation of the MD method [2]. The underlying deformation mechanisms that are responsible for the fatigue crack growth in the NT metals are captured at the nanoscale because of the inherent atomistic resolution of MS/MD simulations.

2. Atomistic simulations

2.1. Simulation details

The simulated samples are generated via the Voronoi construction. Each sample contains 25 grains and is [1 1 0]-textured in the out-of-plane direction. The samples have an average grain size d of 10 nm, 15 nm and 20 nm, with dimensions of $50 \times 50 \times 2.05$ nm^3, $75 \times 75 \times 2.05$ nm^3 and $100 \times 100 \times 2.0\ 5$ nm^3, respectively. The maximum simulated sample contains 1.71 million atoms. A crack is created by removing several layers of atoms, with the crack tip located near the sample center to reduce the boundary effect on the fatigue crack propagation. Three types of samples with different microstructures are constructed to elucidate the influence of twin density on the fatigue behaviors. The first type of sample is free of twins. The second is a large spacing nanotwinned (LSNT) sample with a TB spacing λ of 1.88 nm and 2.71 nm for d = 10 nm and 15 nm, respectively. The third is a small spacing nanotwinned (SSNT) sample with a λ of 0.83 nm and 1.04 nm for d = 10 nm and 15 nm, respectively. For these three types of simulated samples, the grain shape and the crystallographic orientations of all of the grains are retained as the TB spacing and/or the grain size change. Notably, d/λ for the LSNT and SSNT samples used in our simulations are close to those of the experimental samples [17] with d = 450 nm, λ = 85 nm and 32 nm. For the LSNT and SSNT samples, d/λ is approximately 5 and 12, respectively. To further explore the effects of the mean grain size d and the TB spacing λ on the fatigue cracking resistance, we also investigate the fatigue behaviors of samples with different d/λ ratios (see Table 1). The dimensionless parameter d/λ means the twin number per grain and essentially reflects the density of the nanoscale twins.

We perform both MD and MS simulations to study the fatigue crack growth using LAMMPS [25]. The interatomic interaction is described by the embedded atom method potential for Cu [26]. This potential was developed based on the data from a large number of experiments and ab initio calculations [23] and has been widely recognized to be one of the best potentials to mimic the mechanical properties of Cu. In MD simulations, we use the NVT ensemble with a Nose-Hover thermostat to keep the temperature at 300 K and the velocity-Verlet algorithm with a time step of 10^{-15} s. All of the simulated samples are initially equilibrated by the conjugate gradient method and the free dynamics relaxation and then loaded to a minimum stress intensity factor $K_{\min}$ of 0.08 MPa m$^{1/2}$ to make the crack tip atomically sharp. Fig. 1 shows the atomic configurations of three typical samples with d = 10 nm after equilibration. In MD simulations, the crack is loaded/unloaded by successive increments/decrements in the stress intensity factor of 0.01 MPa m$^{1/2}$ (i.e., dK in Fig. 2), each followed by a system relaxation for 10^{-12} s. In MS simulations, the system relaxation after every loading increment or unloading decrement is realized by the conjugate gradient method. Specifically, the MS method provides the equilibrium structures near the crack tip, while the MD technique reflects the dynamic response of the crack tip at high loading rates. The loading in the MS/MD simulations is achieved by applying a mode I crack-tip displacement to the outer boundary of the simulated samples. The relevant details of cyclic loading are given in the following section. All of the stress intensity ranges, ΔK, imposed on the samples in the MS simulations are summarized in Table 1. In both MD and MS simulations, each sample is loaded for 30 cycles with an identical $K_{\min}$. Accordingly, a typical MD case with ΔK = 3.2 MPa m$^{1/2}$ lasts for 19.2 ns over 30 cycles. To identify various defects during deformation, we paint atoms with different local crystalline orders in colors via the common neighbor analysis [27]. Gray refers to perfect fcc atoms, red denotes hcp atoms, and other atoms are in green. Therefore, a single red line represents a coherent TB, two adjacent red lines stand for an intrinsic stacking fault, while two red lines separated by one gray line mean an extrinsic stacking fault.

Table 1
Applied stress intensity amplitudes in unit of MPa m$^{1/2}$ for all of simulated samples.

Samples	ΔK_1	ΔK_2	ΔK_3	ΔK_4	ΔK_5	ΔK_6	ΔK_7
Twin-free, d = 10 nm	2.40	2.72	2.88	3.04	3.20	–	–
LSNT, d = 10 nm, λ = 0.83 nm	2.40	2.72	3.04	3.20	3.36	3.60	–
SSNT, d = 10 nm, λ = 1.88 nm	3.04	3.20	3.36	3.60	3.84	4.08	4.32
LSNT, d = 15 nm, λ = 1.04 nm	3.00	3.20	3.40	3.60	–	–	–
SSNT, d = 15 nm, λ = 2.71 nm	3.20	3.40	3.60	4.00	–	–	–
d = 10 nm, λ = 5.01 nm	2.40	2.72	3.20	–	–	–	–
d = 10 nm, λ = 9.39 nm	2.40	2.72	3.20	–	–	–	–
d = 15 nm, λ = 0.83 nm	3.40	3.60	4.00	–	–	–	–
d = 20 nm, λ = 1.88 nm	3.60	–	–	–	–	–	–
d = 20 nm, λ = 5.01 nm	3.20	–	–	–	–	–	–

2.2. Cyclic loading method

In the MS and MD simulations, external loading is achieved by applying displacements on the outer boundary of the entire simulated sample according to the linear elastic fracture model of the mode I crack with the a stress intensity factor K_{I}. The periodic boundary condition is imposed in the out-of-plane direction to maintain a plane-strain state. The corresponding plane-strain displacement field of a mode I crack is expressed as,

$$\begin{cases} u_x = \frac{K_{\mathrm{I}}}{2\mu}\sqrt{\frac{r}{2\pi}}\cos\frac{\theta}{2}\left(2-4\nu+2\sin^2\frac{\theta}{2}\right) \\ u_y = \frac{K_{\mathrm{I}}}{2\mu}\sqrt{\frac{r}{2\pi}}\sin\frac{\theta}{2}\left(4-4\nu-2\cos^2\frac{\theta}{2}\right) \end{cases} \quad (1)$$

where r and θ are the polar coordinates centered at the initial crack tip and μ and ν are the shear modulus and the Poisson's ratio of materials, respectively. During simulations, every loading cycle includes loading and unloading steps, as illustrated in Fig. 2. In each loading/unloading step, the analytical displacement (Eq. (1)) is imposed on the boundary atoms within 1 nm from the periphery of the samples. These boundary atoms are fixed during the system relaxation after each loading/unloading step. A schematic illustration of the applied cyclic loading is shown in Fig. 2. In the MS simulations, each loading/unloading step has dK = 0.03–0.08 MPa m$^{1/2}$, while for the MD simulation, dK = 0.01 MPa m$^{1/2}$. The loading increments in the MS and MD simulations are optimized to simultaneously ensure the stability and efficiency of the calculations.

The loading method that we adopted has been broadly used in atomistic simulations, e.g., fatigue crack propagation of NC Ni [2], fracture of NT Ni [16], and hydrogen embrittlement of Fe [28]. However, this method has an intrinsic limitation in modeling dynamic crack propagation in ductile materials. The displacement field in Eq. (1) is actually an approximate elastic solution for a semi-infinite sharp crack under remote tensile loading. When this field is imposed on the outer boundary of a finite sample, it to some extent, constrains the K-dominant zone and further confines the plastic zone. Especially for ductile materials, when the crack