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Fracture in a thin film of nanotwinned copper

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ABSTRACT

Nanotwinned Cu exhibits an unusual combination of ultra-high strength and high tensile ductility. However, its fracture behavior and associated microscopic mechanisms remain largely unexplored. Here we study the fracture in a free-standing thin film of nanotwinned Cu using molecular dynamics (MD) simulations. For a pre-crack inclined to the twin boundary, MD simulations show a characteristic fracture mode of zigzag cracking, which arises due to periodic deflections of the crack path by twin boundaries. The mechanism of fracture involves the screw dislocation-mediated local thinning ahead of the crack, instead of cleavage fracture. Importantly, MD simulations show a unique fracture footprint of $\langle 1\,1\,0\rangle$-oriented crack edges, consistent with the previous experimental observation from in situ transmission electron microscopy. Our results reveal the toughening mechanisms by nanotwins and also have broader implications for understanding the mechanical failure of metallic thin films.

1. Introduction

Ultrafine grained copper with embedded nanoscale twin lamellas (hereafter referred to as nanotwinned Cu) exhibits an unusual combination of ultra-high strength (~1 GPa) and high tensile ductility (~14% elongation to failure) [1–4]. However, most engineering applications would require the materials to have high fracture resistances as well [5]. Unlike the strength and tensile ductility that have been extensively studied [6–14], the fracture behavior and associated microscopic mechanisms in nanotwinned metals are much less known.

Several recent studies have investigated the fracture in nanotwinned metals. Qin et al. [15] processed bulk coarse-grained Cu samples by dynamic plastic deformation and obtained a composite microstructure of nanoscale grains with embedded nanoscale twin bundles. They measured an enhanced fracture toughness relative to samples without nanotwins, and found that twin bundles caused the elongated deep dimples on fracture surfaces that contributed to an increase of fracture energy. Singh et al. [16] measured the fracture toughness and fatigue crack growth in nanotwinned Cu processed by electrodeposition, and showed that the presence of nanotwins enhanced both monotonic and cyclic crack growth resistances. Shan et al. [17] and Kim et al. [18] used the in situ transmission electron microscopy (TEM) to directly observe crack growth in nanotwinned Cu. Fig. 1 shows the representative in situ TEM results of crack growth across twin groups in a thin foil of nanotwinned Cu [17]. It is seen from Fig. 1(a) that a characteristic zigzag crack path formed during tensile loading. Fig. 1(b) presents magnified images of region 1 in Fig. 1(a) showing the $\langle 1\,1\,0\rangle_M$ and $\langle 1\,1\,0\rangle_T$ crack edges in the adjoining matrix (M) and twin (T) crystals. Kim et al. [18] and Zhou and Qu [19] performed molecular dynamics (MD) simulations of fracture in thick nanotwinned samples. They observed the damage and fracture processes, including crack blunting through dislocation emission, crack bridging by twin lamella, crack deflection by grain boundaries, and nanovoid formation at the intersections between grain boundaries and twin boundaries.

The experimental and modeling studies discussed above suggest that the crack-twin boundary interactions can be beneficial to enhance fracture toughness. But the toughening mechanism associated with nanotwins are still little understood. Particularly, the following questions have hitherto not been well addressed: What are the intrinsic fracture mechanisms in nanotwinned metals? How do twin boundaries affect crack propagation? The present work is motivated by previous in situ TEM observations [17,18] and aims to address the above questions by studying the growth of a pre-crack in a free-standing thin film of nanotwinned Cu using MD simulations. Furthermore, MD simulations can directly reveal the underlying atomic-level processes of deformation and fracture, thereby shedding light onto the failure mechanisms of nanotwinned metals.

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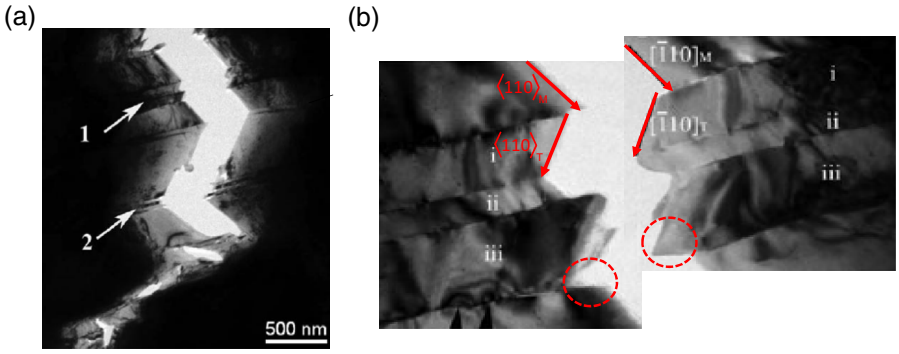

Fig. 1. In situ TEM images of crack growth across twin groups in a thin foil of nanotwinned Cu, from a previous study by Shan et al. [17]. (a) A zigzag crack formed during tensile loading. (b) Magnified images of region 1 in (a), showing the $\langle 1\,1\,0\rangle_M$ and $\langle 1\,1\,0\rangle_T$ crack edges in the adjoining matrix (M) and twin (T) crystals. Circles indicate the short crack edges on twin boundaries.

2. Method

Fig. 2 shows the setup of MD simulations containing a free-standing thin film of nanotwinned Cu with a pre-crack. The MD sample has an in-plane size of 22.1 nm × 43.6 nm and a thickness of 1.7 nm. The twin boundaries are equally separated by 8.6 nm. Each twin lamella consists of the perfect Face-Centered Cubic (FCC) lattice. A pre-crack with a length of ~7 nm is created at the sample edge by removing a single layer of atoms on the inclined $\{1\,1\,1\}$ plane. As a result, the pre-crack has its edge along the $\langle 1\,1\,2\rangle_M$ direction in the matrix (M) crystal. The total number of atoms in the system is 146,783. The periodic boundary condition is imposed only in the horizontal [1 1 2] direction. A uniaxial tensile load is applied in [1 1 2] direction at a constant strain rate $\dot{\varepsilon}$ of 2×10^9/s, while both the [1 1 0] and [1 1 1] directions are traction free. The system temperature is maintained at 5 K. We perform MD simulations with an embedded atom method (EAM) potential of Cu [20] using LAMMPS [21].

3. Results and discussion

Fig. 3 presents a sequence of MD snapshots showing the simulated zigzag mode of crack growth. As the applied load increases,

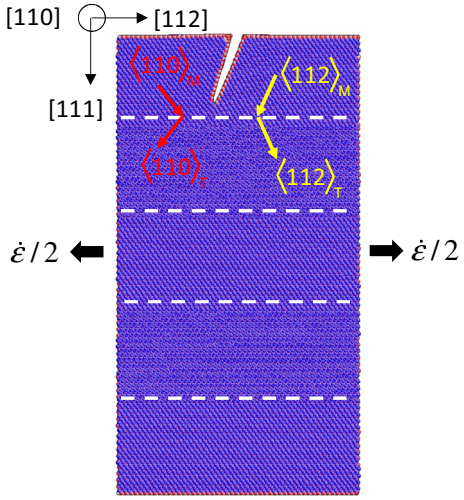

Fig. 2. The MD setup involving a nanotwinned Cu thin film with a pre-existing edge crack. The dashed lines indicate twin boundaries. A uniaxial tensile load with constant strain rate $\dot{\varepsilon}$ is applied parallel to the twin boundary. Atoms are colored by the coordination number (CN). Atoms in a perfect FCC lattice have CN = 12 (yellow), while defective atoms have CN = 10 (green), 9 (pink), 8 (white), or 7 (blue). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

dislocations on the $\{1\,1\,1\}_M$ slip plane in the matrix crystal emit from the crack tip and then pile up against the twin boundary that temporarily obstruct the movement of dislocations. As a result, a high local stress arises to act on the leading dislocation in the pileup array. As the applied load continues to increase, this local stress becomes so high that the leading dislocation transmits into the adjoining twin lamella and further glides on the conjugate $\{1\,1\,1\}_T$ slip plane in next twin lamella. Dislocations behind the leading one in the pileup array repeat this "stop-and-go" process. Meanwhile, transmitted dislocations in the adjoining twin lamella develop a pileup array, due to obstruction of the twin boundary further away from the crack tip. A similar "stop-and-go" process occurs at this twin boundary. Gliding of dislocations in each twin lamella causes local thinning at the active slip planes that eventually leads to lamella fracture. Since the crack is periodically deflected by twin boundaries, a zigzag crack path develops in MD simulations, which is consistent with the previous experimental observation through in situ TEM [17], as shown in Fig. 1(a).

To understand the fracture mechanism of zigzag cracking, we note that in the 2D projected view of the film (Fig. 2), the $\{1\,1\,1\}$ pre-crack has its edge along the $\langle 1\,1\,2\rangle_M$ direction. We choose to create such $\{1\,1\,1\}$ pre-crack in order to facilitate cleavage fracture on the close-packed $\{1\,1\,1\}$ planes. However, it is unexpected to observe in Fig. 3 that the edges of the growing crack in MD simulations are primarily aligned with the $\langle 1\,1\,0\rangle$ directions in all lamellas. This footprint of $\langle 1\,1\,0\rangle$ crack edges indicates that fracture does not occur by cleavage of $\{1\,1\,1\}$ planes, which otherwise would produce crack edges along the $\langle 1\,1\,2\rangle$ directions.

A detailed analysis of MD results reveals that fracture occurs through a process of dislocation-mediated local thinning instead of cleavage. This is a unique mode of mechanical failure of thin films in the absence of out-of-plane constraints. More specifically, Fig. 4(a) shows a 3D view of the atomic configuration of a partially cracked film. Fig. 4(b1) and (b2) respectively expose the (1 1 1) cross sections of the film that are cut at two different locations along the crack path, such that the onset and growth of the local thinning can be clearly seen. As schematically shown in Fig. 4(c), the local thinning is mediated by dislocation glide. That is, an extended dislocation, which splits into the leading and trailing partials in FCC Cu, can glide on the conjugate $\{1\,1\,1\}_M$ and $\{1\,1\,1\}_T$ slip planes in the adjoining matrix and twin crystals. Such type of dislocations have the Burgers vector $\mathbf{b} = \langle 1\,1\,0\rangle/2$ with the non-zero component in the thickness direction of the film. As a result, gliding of those dislocations on $\{1\,1\,1\}_M$ and $\{1\,1\,1\}_T$ slip planes causes the decrease of film thickness, responsible for the local thinning and final rupture of the film. Because of symmetry, the in-plane tensile loading along the [1 1 2] direction can activate dislocations on all the equivalent inclined $\{1\,1\,1\}_M$ and $\{1\,1\,1\}_T$ slip planes symmetric about the (1 1 0) plane of the film, which eventually produce