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Brittle versus ductile behaviour of nanotwinned copper: A molecular dynamics study

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Abstract—Nanotwinned copper (Cu) exhibits an unusual combination of ultra-high yield strength and high ductility. A brittle-to-ductile transition was previously experimentally observed in nanotwinned Cu despite Cu being an intrinsically ductile metal. However, the atomic mechanisms responsible for brittle fracture and ductile fracture in nanotwinned Cu are still not clear. In this study, molecular dynamics (MD) simulations at different temperatures have been performed to investigate the fracture behaviour of a nanotwinned Cu specimen with a single-edge-notched crack whose surface coincides with a twin boundary. Three temperature ranges are identified, indicative of distinct fracture regimes, under tensile straining perpendicular to the twin boundary. Below 1.1 K, the crack propagates in a brittle fashion. Between 2 K and 30 K a dynamic brittle-to-ductile transition is observed. Above 40 K the crack propagates in a ductile mode. A detailed analysis has been carried out to understand the atomic fracture mechanism in each fracture regime.
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1. Introduction

The fracture of a material is usually categorised into brittle fracture and ductile fracture. A brittle fracture propagates along a crystallographic plane by cleavage due to high stress concentration at the crack tip. A ductile fracture is accompanied by plastic deformation characterised by dislocation nucleation and dislocation mobility [1]. Transition from brittle to ductile fracture has been observed in a range of materials over different temperature ranges. The accepted mechanism governing the brittle-to-ductile transition is the competition between loss of inter-atomic bonds and dislocation processes at or near the crack tip [2–6]. The study of the atomic-scale fracture process around the crack tip is a central issue in understanding fracture ductility, fracture embrittlement and the associated transition regime in materials having different microstructures.

Rice and Thomson [3], followed by Anderson and Rice [7] and Li [8], compared the brittle and ductile fracture response on the basis of the energy competition between propagation of a Griffith cleavage and a dislocation nucleated at a crack tip. When the energy release rate associated with the emission of a single dislocation was less than the Griffith cleavage energy, it was assumed that a dislocation would be spontaneously emitted before cleavage, and vice versa. Rice [5] used the ratio of surface energy to the unstable stacking fault energy to predict the brittle and ductile response of Face Centred Cubic (fcc) and Body Centred Cubic (bcc) metals. Zhou and Thomson [9] proposed that ledges on cracks could be efficient sources for dislocation emission at loads well below the critical load. The dislocations could be more easily emitted compared to homogenous dislocations because of the existing finite lengths of dislocations at the ledge. Freund and Hutchinson [10] found that the brittle-to-ductile transition could be determined by the crack's ability to overrun the active plastic zones. As pointed out by Argon [11], it is possible to nucleate dislocations from the tip of a propagating cleavage crack at finite temperatures in many intrinsically brittle solids. While the cleavage process at the crack tip is primarily independent of temperature, the initiation of dislocation loops from the crack tip can be significantly assisted by thermal activation. At a given temperature, and at a crack velocity below a critical value, more dislocation emissions from the crack tip lower the crack tip stress below the level necessary for continued cleavage, resulting in a brittle-to-ductile transition.

Atomistic simulations have been widely used to examine fracture propagation in solids. Knap and Sieradzki [12] conducted Molecular dynamics (MD) simulations for fcc solids subjected to Mode I and Mode II loadings. Their observations of dislocation nucleation from Mode II fracture simulations were in reasonably good agreement with Rice's prediction [5]. In Mode I, Rice's continuum formulation

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underestimated the stress intensity for dislocation emission by almost a factor of 2 compared to the MD results. Cleri et al. [13] reported that the Burgers vectors of the straight edge dislocations nucleated from the crack tip and the slip plane inclination with respect to the crack plane observed in atomistic simulations were consistent with the predictions of the continuum elasticity theory. However, they suggested that the unstable-stacking energy in Rice's formulation, which was based on the concept of a homogeneous displacement field, should be replaced by a suitably defined energy barrier for dislocation nucleation that fully incorporates the displacement inhomogeneity in the vicinity of the nucleating dislocation. Abraham and Gao [14] found from MD simulations that the fcc crystal failed by brittle cleavage for cracking on a {1 1 0} plane growing in the [1 1 0] direction and by ductile plasticity for cracking on a {1 1 1} plane growing in the [1 1 0] direction. Comparison of equilibrium surface energies on the crack plane and Schmid factors on the primary slip systems indicated that the classical theories of fracture gave predictions in contradiction with the simulation results. A hyper-elasticity model was proposed by Abraham and Gao [14] to explain this discrepancy. It has also been found that if the speed of the (1 1 0) brittle crack reached approximately one-third of the Rayleigh sound speed, a dynamic brittle-to-ductile transition occurred [15]. Zhang et al. [16] reported that the geometry of the crack and crystal orientations had a strong effect on the processes at the crack tip. Kimizuka et al. [17] studied the dynamic behaviour of dislocations near a crack tip in fcc metals. Results obtained for copper and aluminium showed multiple emissions of dislocation loops from the crack tip and incipient evolution of plastic deformation during crack extension. Cui and Beom [18] investigated single Cu and Al crystals with edge cracks under Mode I loading conditions using MD simulations. In their simulation model a crack with its front along the [0 1 1] direction was inserted on the (1 0 0) plane. Five different crack lengths were employed to examine the effect of crack length on the fracture behaviour of each material. The results indicated that Cu and Al exhibited different fracture mechanisms. The above literature review shows that most investigations on brittle versus ductile behaviour using MD simulations were carried out on single crystals.

Nanotwinned Cu is a relatively new material with special microstructure. It has been the subject of intensive research due to its unusual combination of ultrahigh yield strength and high ductility [19–21]. The high ductility of nanotwinned Cu has been attributed to the gradual loss of coherency of the Twinning Boundaries (TB) during plastic deformation [22–24]. A brittle-to-ductile transition was experimentally observed in nanotwinned Cu despite Cu being an intrinsically ductile metal. Jang et al. [21] conducted *in situ* Scanning Electron Microscope (SEM) uniaxial tension tests on nanotwinned Cu nanopillars with different twin boundary orientations and twin boundary spacings. The nanopillars with twin boundary spacings up to 2.8 nm exhibited the characteristics of ductile fracture clearly, while those with the larger twin boundary spacing of 4.3 nm failed in a brittle fashion. Jang et al. [21] also performed MD simulations of crack propagation along a twin boundary in nanotwinned Cu to understand the distinct fracture modes observed in their experiments. It was found that when the twin boundaries were spaced sufficiently closely, the high stresses at the crack tip could induce twinning dislocation nucleation and propagation on the twin boundaries in close proximity to the crack tip, leading to a cascade of dislocation activities and eventually ductile failure.

The intriguing findings of the TB-spacing-induced brittle-to-ductile transition in nanotwinned Cu from Jang et al.'s work raises some fundamental questions: (1) can the brittle-to-ductile transition be observed in this material when the temperature varies and (2) what is the atomic mechanism responsible for nucleation and mobility of dislocations emitted from the crack tip? In this paper, we explore these questions for nanotwinned Cu with a pre-existing edge-notched crack using MD simulations at various temperatures.

2. Molecular dynamics simulation model

Molecular dynamics (MD) simulations were performed with the open-source code Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [25]. The MD domain of this study is illustrated in Fig. 1. The domain is 496 Å × 501 Å × 25.16 Å in the X, Y and Z directions respectively. It was filled with Cu atoms arranged in an fcc structure. The original crystal, referred to as the matrix crystal in the following, was aligned along the $[1\,\bar{1}\,\bar{2}]$, $[\bar{1}\,1\,\bar{1}]$ and [1 1 0] crystallographic directions in the X, Y and Z directions respectively. A set of the twinned crystals, labelled $T_1 - T_6$ in Fig. 1, was then introduced by rotating the matrix crystal along its X axis by 180°. This resulted in a set of separated matrix crystals, labelled $M_1 - M_6$. The twinned crystals had crystallographic directions $[1\,\bar{1}\,\bar{2}]$, $[1\,\bar{1}\,1]$ and $[\bar{1}\,\bar{1}\,0]$ in the X, Y and Z directions respectively. All the crystals ($T_1 - T_6$ and $M_1 - M_6$) had the same height of 4.17 nm along the Y direction. In Fig. 1, the dark blue spheres are atoms with perfect fcc structures and light blue spheres are atoms at the Twin Boundary (TB). The coherent TBs between the matrix crystals and the adjacent twinned crystals are marked by light blue colour. A through-thickness crack was created by removing a number of atoms in the middle of the left-hand edge of the simulation cell as shown in Fig. 1. The crack surface was parallel to the TB plane between the T_3 crystal and the M_4 crystal. The crack front was oriented along the Z direction. The initial length of the crack was about 65 Å. Details of the crack tip region are given in the top-right corner of Fig. 1. The atoms surrounding the crack are coloured red. The simulation cell encapsulates over half a million atoms.

The Embedded Atom Method (EAM) interatomic potential developed by Mishin et al. [26] was employed in all simulations. This potential was calibrated using experimental and *ab initio* data for Cu. It has been shown to precisely predict the lattice properties, point and extended defects, various structural energies and transformation paths [26]. The simulations were conducted in a constant NPT ensemble (fixed number of atoms (N), constant pressure (P) and constant temperature (T)). Periodic boundary conditions were applied in the Y and Z directions and free boundary conditions were used in the X direction. In each simulation, random velocities were initially assigned to atoms, followed by a relaxation process for 10^5 time steps. The simulation cell was subsequently stretched at a constant strain rate of 1×10^8 s^{-1} along the Y direction while the normal stress along the Z direction was fixed to zero using the Parinello–Rahman barostat. The equations of the atomic motion were integrated using the velocity Verlet algorithm. The total simulation time was 702 ps with a time step of 0.003 ps, leading to a total strain of 7.02% along the

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