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A dual fracture transition mechanism in nanotwinned Ni

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ABSTRACT

Molecular dynamic simulation was used to study the brittle versus ductile fracture behaviour in nanotwinned Ni at various temperatures. The simulation results show that three temperature regimes correspond to three different fracture behaviours: brittle, brittle-to-ductile transition and ductile. A dual fracture transition mechanism in nanotwinned Ni within a small temperature interval was observed: (1) local phase transformation and (2) ledge formation ahead of the crack tip induced a sharp fracture transition from brittle mode to ductile mode. Our simulation results reveal that the very rare double fracture transition mechanisms could be transformed quickly in nanotwinned Ni within a narrow temperature interval, suggesting a new interpretation of fracture and deformation of nanotwinned Face Centred Cubic metals.

1. Introduction

Many researchers have observed brittle fracture and brittle-to-ductile transition (BDT) by experiments and simulations in materials, such as Silicon [1,2], Body Centred Cubic (BCC) [3–5] and glass [6], where the BDT was attributed to ledge formation [1] and phase transformation [2,5]. Previous experiments showed that the bulk or coarse-grained Face Centred Cubic (FCC) materials tended to show a ductile fracture. However, the nanocrystalline materials show a different scenario. In the case of size- [7] and twin boundary spacing-induced [8,9] BDT of FCC materials, it has been reported that the brittle fracture or BDT would occur as these parameters reach critical values. However, very few studies could fundamentally explain why FCC metals can fail in two distinct modes, and what is the underlying atomistic mechanism of BDT? For example, Li [8] and Wang et al. [9] found an opposite phenomenon that fracture transition occurs as twin boundary spacing decreases and increases. Phase transformation and ledge formation appear to be rarely applicable to induce the BDT in FCC metals. In this letter, our work reveals a new finding that two mechanisms based on phase transformation and ledge formation can occur and shift towards each other in a very narrow temperature range in FCC structured Ni metal, which they are all able to trigger the dislocation activity and further induce the BDT.

2. Molecular dynamics simulation model

An initially semi-infinite crack and a set of twins were introduced into single Ni crystal. A relatively large twin boundary spacing of 4.06 nm was chosen to ensure a brittle fracture mode at low temperature. Twinned crystal was labelled T_1–T_6 and the matrix crystal was labelled M_1–M_6. The atomic model size was 491.49 Å × 487.75 Å × 24.89 Å in the *X*, *Y* and *Z* directions respectively. A periodic boundary condition was imposed along the crack front (*Z* axis) and tensile direction (*Y* axis). The EAM interatomic potential [10] was adopted. After the model was constructed, the sample was minimised by the conjugate gradient algorithm, and then the model was relaxed through the Nose-Hoover thermostat and Parrinello-Rahman barostat (NPT) method for 105 time steps prior to tensile deformation. A multiple time algorithm was used with a time step of 3 femtoseconds. Eleven simulation cases at temperatures (1.1 ~ 500 K) were conducted. A constant strain rate of 1×10^8 s^{-1} was applied along the *Y* axis. As the model stretched, the NPT method was used to control temperature at an expected temperature and external pressure at zero in the *Z* direction.

3. Results and discussion

Toughness- and crack length-temperature curves for nanotwinned Ni are depicted in Fig. 1. Both curves consistently show that there are three groups of fracture. In Group 1 (1.1 K and 10 K), the fracture propagates in a perfect brittle mode without dislocation activity. In Group 2 (15 ~ 100 K), the fracture exhibits a

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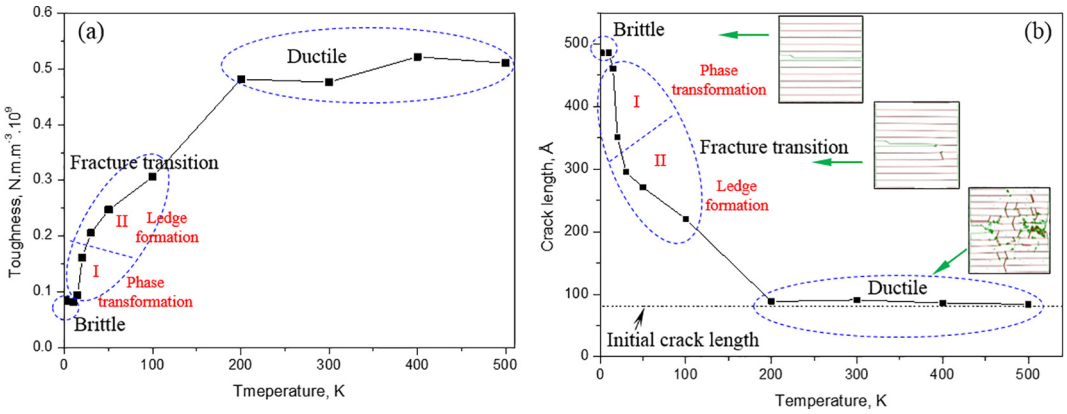

Fig. 1. Crack characteristics of nanotwinned Ni subjected to tensile deformation: (a) toughness-temperature curve; (b) crack length-temperature curve, where FCC crystal atoms are filtered in insets.

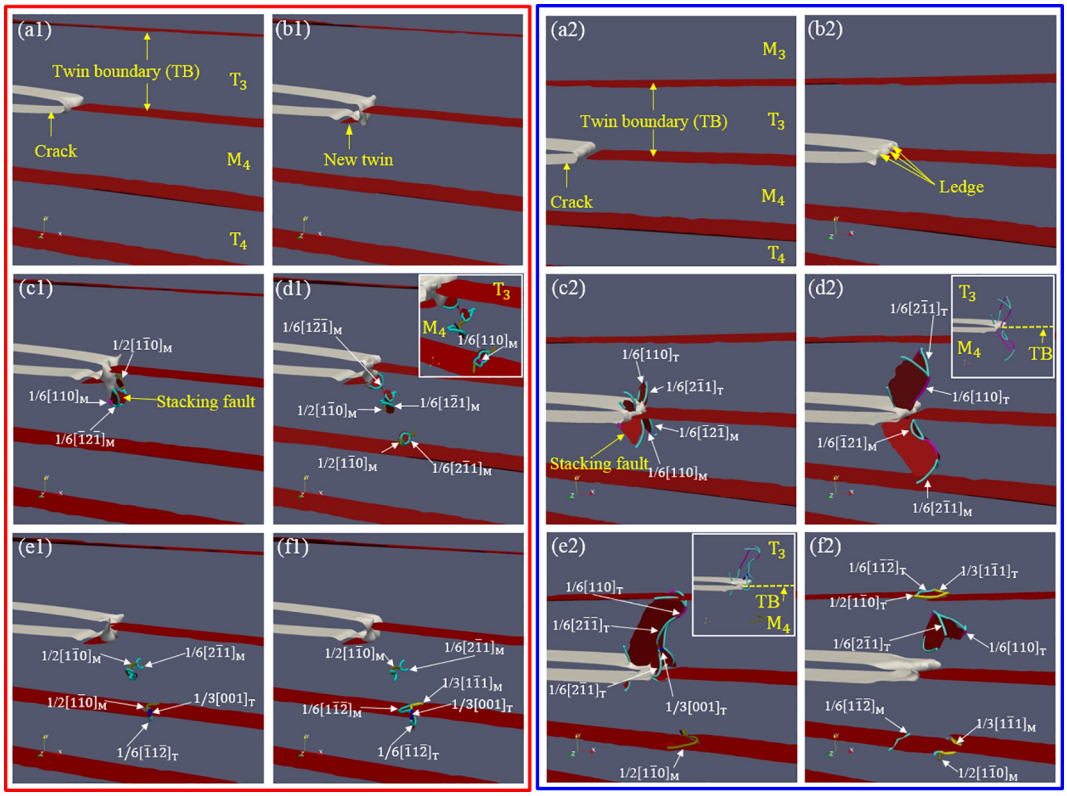

Fig. 2. Snapshots of dislocation activities around the crack tip for (a1–f1) 20 K and (a2–f2) 50 K. The crack surface and stacking faults including twin, intrinsic and extrinsic stacking faults are shown by envelope surfaces in grey and red respectively. The solid lines with different colours represent different types of dislocations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

dynamic BDT. In Group 3 (≥200 K), the crack propagates in a ductile manner.

Fig. 2 shows the dislocations emit from the crack tip for representative cases of 20 K and 50 K. In Fig. 2(a1–f1), the crack propagates in a brittle mode first without dislocations, but as the strain increases, a new twin parallel to the envelope surface of crack is formed. Then a $1/2[1\bar{1}0]_M$ perfect dislocation ahead of the twin is nucleated from the crack tip. The dislocation grows into a complicated structure, moving collectively towards TB and interacting with it. In comparison, in Fig. 2(a2–f2), the crack propagates in a brittle mode and its front gradually becomes rough with ledges on it. Two defective structures consisting of dislocations are emitted from the ledges into the matrix and twin crystal.

The occurrence of dislocations emitted from the crack tip contributes to a final BDT. The atomic mechanism at the crack tip responsible for dislocation nucleation is necessarily understood. Atom C_3 is formerly located at the second (110) plane in Fig. 3 (a1) and moves towards the first (110) plane along the negative Z direction in Fig. 3(a2). This results in that five atoms C_2, B_3, C_4, D_3 and C_3 are roughly located at the same (110) plane. A careful examination reveals that a base-centred orthorhombic structure with lattice constants $a \approx 2.40$ Å, $b \approx 4.14$ Å and $c \approx 2.49$ Å has been locally formed in the entire Z direction. More local structural transforms occur in the wake of local deformation around the crack tip while the Atoms like C_4, C_5, C_6 shuffle along the Z direction, and are unstable as strain increases. The consequence of these activities