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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 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.

Keywords: Fracture; Twin; Phase transformation; Ledge

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 the ledge formation [1] and phase transformation [2, 5]. Previous experiments showed that the bulk or coarse-grained Face Centred Cubic (FCC) materials tended to be 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 the opposite phenomenon that the fracture transition occurs as twin boundary spacing decreases and increases. The 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 both 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 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 the temperature at expected temperatures 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 dynamic BDT. In Group 3 (≥200 K), the crack propagates in a ductile manner.

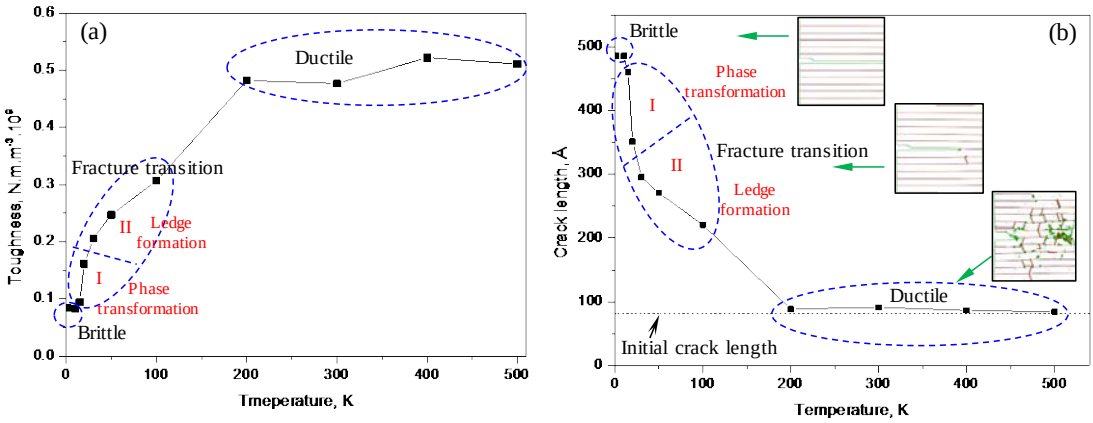

Fig. 1. Crack characteristics of nanotwinned Ni subjected to tensile deformation: (a) toughness-temperature curve; (b) crack length-temperature curve, where FCC crystal atoms are filtered in insets.

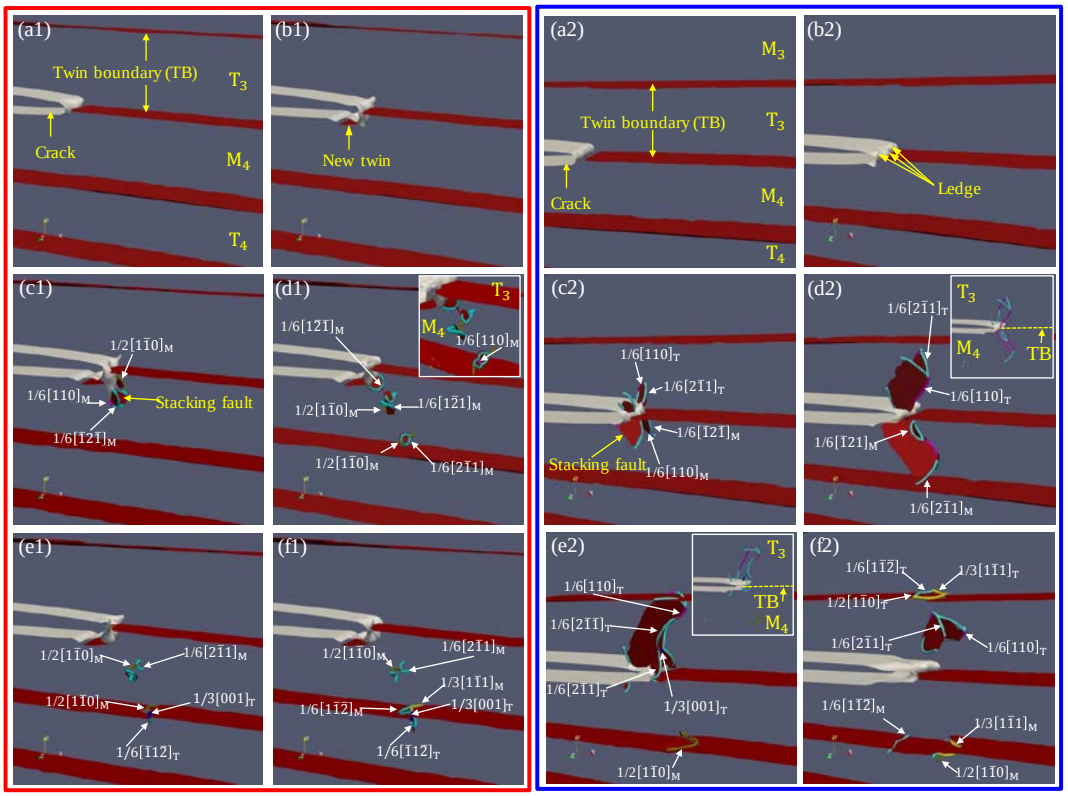

Fig. 2. Snapshots of dislocation activities around the crack tip for (a1-f1) 20 K and (a2-f2) 50 K. The crack surface and stacking faults including twin, intrinsic and extrinsic stacking faults are shown by envelope surfaces in grey and red respectively. The solid lines with different colours represent different types of dislocations.

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 the base-centred orthorhombic structure with lattice constants a ≈ 2.40 Å, b ≈ 4.14 Å and c ≈ 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 is that a new twin forms. The newly formed twin structure is approved to shield atoms at the crack tip and impede stress concentrating at this region, leading to an incremental crack tip blunting and almost no atomic bonds breaking around the crack tip. This newly twinned region has a mismatched boundary with M_4. This mismatched boundary is a weak link where sliding can easily occur under stretching, and therefore as the imposed strain continues, the relative movement at the mismatched boundary can trigger the nucleation of a perfect dislocation on $(001)_M$ plane.

Unlike at 20 K where a local phase transformation accompanied by a formation of new twin contributes to the dislocation process, the dislocation activity at 50 K arises from ledges that form on the crack tip. The crack tip is located at Atom A_2' in Fig. 4(a), while the crack tip is at Atom A_3' in Fig. 4(b). This indicates that the crack front is non-synchronous in X or Z direction, i.e., the crack front is rough, and ledges form on it. Many studies have proved that the ledge is an effective source for dislocation core nucleation [1, 11]. As a result, the formed ledges trigger dislocations nucleating on them. The reason for ledge formation distinguishing from phase transformation in a small temperature range may attribute to three factors: (i) The larger thermal fluctuation at

higher temperature activates atomic bonds to break into different crystallographic $(1\bar{1}1)_T$ planes along the *Y* direction, or break at different positions along the *X* and *Z* directions on the same $(1\bar{1}1)_T$ plane. (ii) The crack front wave causes the variations in toughness along the crack front due to the wave speeding up and slowing down to distort the crack front [12]. (iii) The dynamical instability increases the roughness of crack surface as the crack speed increases [13, 14]. The case with a higher temperature of 30 K or 50 K has a faster crack propagation speed and larger thermal fluctuation than the one with a lower temperature of 15 K or 20 K. This means that the ledge can form easier or earlier than the onset of phase transformation within a narrow temperature interval, leading to two distinct fracture transition mechanisms from phase transformation-induced to ledge-induced transition.

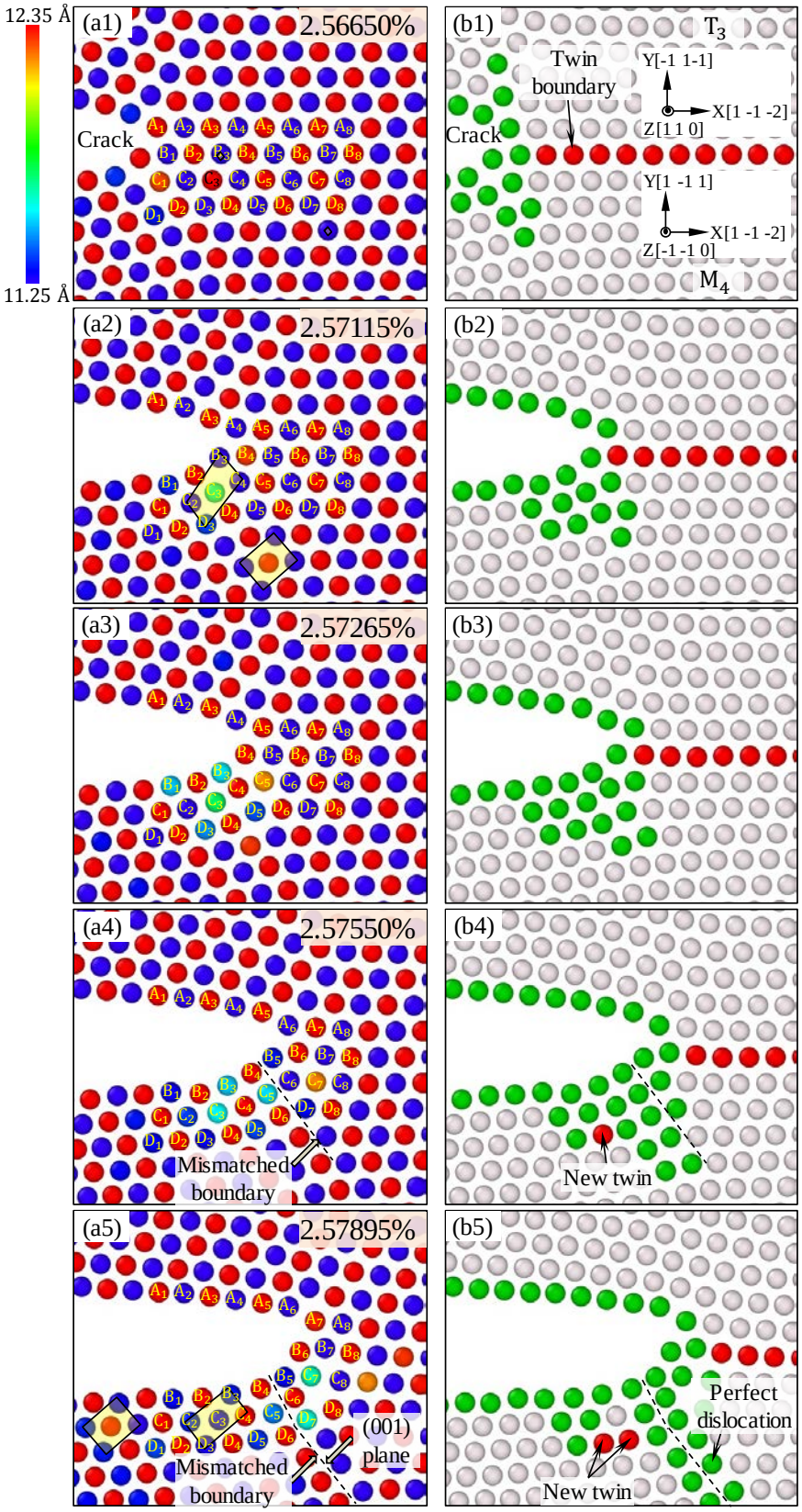

Fig. 3. Atomic configuration (a1-a5) and local crystal structure (b1-b5) around the crack tip for two successive (110) planes in the *Z* direction at 20 K.

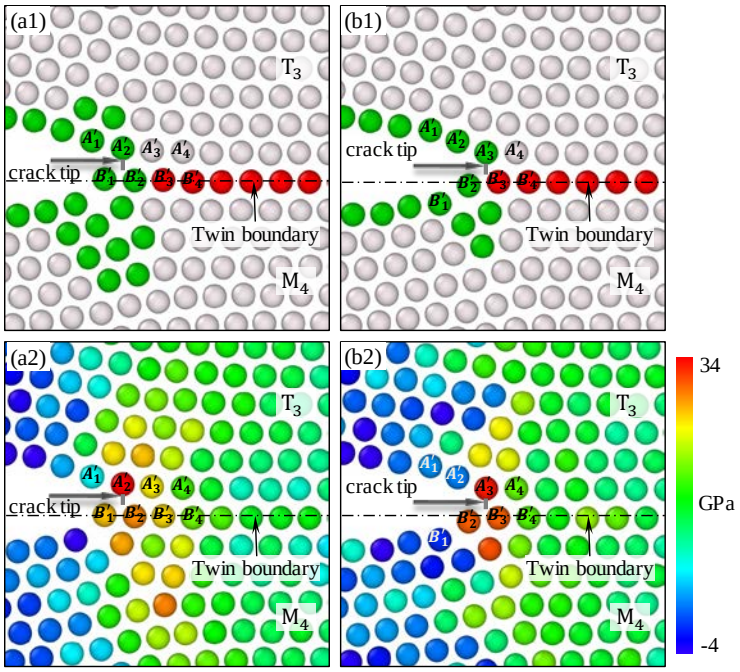

Fig. 4. Atomic configurations for case of 50 K at ε = 2.51055%: (a) 1.45 Å ≤ *Z* ≤ 3.95 Å; (b) 17.15 Å ≤ *Z* ≤ 19.65 Å.

A good link between MD simulation and experiment is still a challenge because of the size-scales and unrealistically high deformation rates. Our atomistic approach offers a new insight that the BDT mechanisms that have been seen in other types of materials can occur in FCC materials and shifted towards each other, which may reveal the possible mechanisms associated with brittle fracture or BDT in experiment for FCC materials [15].

4. Conclusions

MD simulations were used to investigate the fracture behaviour of nanotwinned Ni. Three different temperature-dependent fracture modes were found. The dual fracture transition mechanism within a narrow temperature range is the first time to be observed in nanotwinned FCC metals. (1) Local phase transformation occurs accompanied by a new twin formation and (2) ledge nucleates around the crack tip due to the increasing thermal fluctuation and the increasing dynamic crack speed at higher temperatures, which trigger the dislocations nucleation around these regions, leading to a change from brittle mode to ductile mode.

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