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Deformation mechanisms and slip-twin interactions in nanotwinned body-centered cubic iron by molecular dynamics simulations

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ABSTRACT

Deformation mechanisms in nanotwinned face-centered cubic (fcc) materials have been extensively studied due to the successful fabrication of nanotwinned fcc materials and the advance in experimental techniques and atomistic simulations. However, less attention has been paid to nanotwinned body-centered cubic (bcc) materials despite that deformation twinning has been widely observed in bcc materials both in experiments and computer simulations. Here we investigate the mechanical behaviour of nanotwinned Fe with various twin spacing under tensile deformation as a function of the inclination angle between the twin boundaries (TBs) and the loading direction using large scale molecular dynamics simulations. Our simulations reveal that the twin orientation determines the deformation mechanisms of nanotwinned Fe. When the TBs are parallel or inclined by an angle smaller than 20° to the loading direction, the samples fracture in an almost brittle manner. When the TBs are inclined by a medium angle between 20° and 70°, TB migration takes over the role of the main deformation mechanism and two possible pathways accounting for the disappearance of TBs, namely twinning or detwinning are distinguished. When the TBs are inclined by an angle larger than 70° or nearly perpendicular to the loading axis, plastic deformation is dominated by abundant slip-twin interactions. The dynamic transition in deformation mechanisms is discussed based on Schmid factor analysis and generalised planar fault energy. Moreover, we systematically summarise the plausible slip-twin interactions in bcc materials and determine the energy barriers according the Frank rule. The dislocation reactions at the TBs are compared with experimental observations.

1. Introduction

Nanocrystalline materials exhibit exceptional strength and hardness but at the expense of ductility [1,2]. To overcome the strength-ductility trade-off [3], coherent twin boundaries (TBs) with twin spacing of less than 100 nm have been successfully engineered into metals or alloys to achieve ultrahigh strength and high ductility simultaneously [4–7]. Such efforts have been focused on nanotwinned face-centered cubic (fcc) materials, which have been successfully fabricated in the form of one-dimensional nanowires [8], columnar structured thin films [9] and full three-dimensional bulk samples [10–12]. The strength of polycrystalline nanotwinned Cu first increases with decreasing twin spacing and then decreases if the twin spacing is refined below a critical value [11]. The ultrahigh strength is attributed to the interactions between dislocations and TBs, while the softening phenomena result from TB migration, which involves the nucleation and propagation of twinning dislocations along the twin plane [13,14]. Recent studies on ⟨1 1 1⟩ textured nanotwinned Cu and nanowires reveal that twin orientation also plays an important role in the deformation of nanotwinned fcc materials [15]. Deformation mechanisms transit dynamically from slip transfer to TB migration to slip-twin interactions as the TB orientation changes [16]. It can be seen that the deformation mechanisms in nanotwinned fcc materials have been well established thanks to advances in experimental techniques as well as atomistic simulations [13,17–19]. But relatively fewer studies has been carried out on nanotwinned body-centered cubic (bcc) metals.

Deformation twinning is an important deformation mode in addition to dislocation slip in bcc materials [20–24] and a number of models have been proposed to rationalize the formation of deformation twins [20,25–28]. Dislocation was reported to initiate twinning under high stress in Fe [29]. Recent in situ experiments and computer simulations revealed that deformation twinning dominates the plastic deformation of nanocrystalline W [30] and reversible detwinning occurs during the unloading process

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[30,31]. Deformation twinning is promoted by high strain rates and low temperature. Twinning tendency also largely depend on the stacking fault energy. The high stacking fault energy of bcc materials restrict the synthesis of nanotwinned bcc materials through conventional growth methods [5,32], therefore less attention was paid to nanotwinned bcc materials. Molecular dynamics (MD) simulations have also revealed massive deformation twinning in nanocrystalline bcc materials, including Fe [33], Mo [34–36], Ta [37–39] and Nb [40,41]. Ojha et al. [42,43] determined the TB migration stress in bcc metals and alloys and investigated the twin-twin reactions. Song et al. [44] reported that severe irradiation enhances TB migration in Fe. Very limited MD simulations have been performed to study the mechanical response of nanotwinned bcc materials with twin planes perpendicular to the loading direction. Sainath et al. [45] studied the mechanical behaviour of Fe nanopillars containing nanoscale twins under tensile and compressive deformation and analysed the twin-twin and slip-twin interactions. Xu et al. [32] revealed the size-dependent plastic deformation of twinned W nanopillars. The effect of twin spacing and twin orientation on mechanical response of bcc materials is far from being understood compared to fcc materials. The mechanical behaviour of nanotwinned fcc materials is determined by the slip-twin interactions and it is of great importance to investigate the slip-twin reactions in bcc materials.

Given that experimental studies of the mechanical behaviour of nanotwinned bcc materials at the atomic level are still difficult, we systematically investigate the effects of twin orientation and twin spacing on the mechanical behaviour of nanotwinned bcc materials using MD simulations. Fe is the most widely used structural materials and the dislocation motion in Fe has been extensively studied [29,46,47], therefore we choose Fe as a typical bcc material. Here we successfully construct nanotwinned Fe with various twin orientation and twin thickness. The simulation cells contain a high density of nanoscale twins with specific orientation. Therefore, it is not difficult to identify the origins of the mechanical properties without the influence of grain boundaries, randomly oriented TBs and other defects [8]. We elucidate the deformation mechanisms in nanotwinned Fe with different orientations and analyse the atomistic mechanisms involved in slip-twin interactions.

2. Methods

Fig. 1 shows the processes of introducing nanoscale twins into bcc Fe. Parts of a perfect bcc model were continuously displaced on adjacent {1 1 2} planes with the magnitude of $1/6 < \bar{1}\,\bar{1}\,1 >$to produce a symmetric twin while keeping the matrix unchanged [20,48]. Different from the fully coherent twin interface in fcc materials, the coincident twin interface in bcc materials that consists of three layers of atoms was not stable and translated to isosceles interfaces [20,41,45,49] after energy minimization with the reflection symmetry being destroyed (Fig. 1h). The samples were produced with four twin thicknesses: 1.98 nm (T2), 3.96 nm (T4), 5.94 nm (T6) and 7.92 nm (T8). In all samples, the twin and matrix were spaced uniformly. Then the nanotwinned model was rotated clockwise about $[1\,\bar{1}\,0]$ direction through various inclination angles (0°, 15.8°, 30°, 45°, 60°, 74.2° and 90°) to obtain different twin orientations. Fig. 2 shows the fabricated samples T4A0, T4A30, T4A60 and T4A90. The prepared samples are around 30 nm long in X direction and the thickness was fixed at 12.11 nm in Z direction to save computing time, with the width varying in Y direction to satisfy periodic boundary conditions.

MD simulations were performed using the parallel MD package LAMMPS [50] at a constant temperature of 300 K. A uniaxial tensile strain was applied by continuously scaling the atomic coordinates and box size at a constant engineering strain rate of 5×10^8 s^{-1} along the X direction. Along the other two directions, a Nose-Hoover thermostat and barostat (NPT ensemble) was used to keep the stress around zero so that the system can shrink or expand freely. Periodic boundary conditions were imposed in all three directions to simulate the behaviour of bulk materials.

The simulation results strongly depend on the accuracy of the interatomic potentials and several potentials for Fe have been developed. We compared the performance of four recent semi-empirical potentials, developed by Ackland et al. [51] (denoted as A97), Mendelev et al. [52] (denoted as M03), Mishin et al. [53] (denoted as M06) and Marinica et al. [54] (denoted as MCM11). The simulation results are given in the Supplementary Information (Supplementary Figs. S1–S16). The response of A97 and M03 are similar in many ways. Previous studies also revealed that the Mendelev-type potential is the best choice for large scale simulations and this potential was widely adopted in previous simulations [46,55,56] Therefore, we chose the embedded atom method (EAM) potential by Mendelev et al. [52] to describe the atomic interactions between Fe atoms. This potential accurately reproduces many material properties, including lattice parameters, elastic constants, point defect energies and bcc–fcc transformation energy.

The simulated configurations were visualized using the scientific software package Open Visualization Tool (OVITO) [57]. Common neighbour analysis (CNA) was used to colour the atoms according to the local crystalline order. This technique combined with coordination number defines four different types of atoms: grey represents perfect bcc atoms, dark grey indicates fcc atoms, red stands for atoms of non-bcc structure and with a coordination number of 14 (corresponding to TBs and dislocation cores in bcc materials), and green indicates other defected atoms (corresponding to grain boundaries and other defects). The atomic-level strain tensors were calculated based on the deformed and the initial configuration of the system in OVITO [57]. Then the von Mises local shear invariant part of the strain tensor was calculated and was used to trace the evolution of microstructure. For the sake of clarity, perfect bcc atoms that are not involved in the plastic deformation were eliminated in the analysis of the dislocation structures. The dislocations were identified by the dislocation extraction algorithm (DXA) implemented in OVITO [58], which extracts the dislocation lines and their Burgers vector. The modified Thompson tetrahedron was used to determine the slip planes, which enable us to carry out a detailed analysis of the dislocation reactions.

The slip system in nanotwinned bcc materials can be described with the aid of the modified double Thompson tetrahedron [20] as shown in Fig. 3a, because the reciprocal lattice of bcc lattice is fcc lattice [59]. The planes of the tetrahedron correspond to ⟨1 1 1⟩ slip directions and the directions in the tetrahedron correspond to {1 1 0} and {1 1 2} slip planes in bcc lattice. For a $(1\,1\,2)[\bar{1}\,\bar{1}\,1]$ twin, TB is the (1 1 2) or (Dγ) slip plane, shared by the twin above and the matrix below. The lower Thompson tetrahedron ABCD below the twin plane represents matrix slip systems, while the symmetric upper tetrahedron A′B′C′D′ shows slip systems in the twin, where A′ = B, B′ = A, C′ and D′ is the reflection of C and D. Slip systems in nanotwinned bcc materials are listed in Table 1. In this study, the dislocation reactions are represented by Burgers vector equations expressed in terms of the modified double Thompson tetrahedron, and the same equation in vector form is also given [20]. Indices relative to the twin lattice are given the superscript T. For simplicity, the energy of a dislocation is considered to be proportional to the square of the Burgers vector. The energy barrier is determined by the difference between the energy of the reacting dislocations and the resulting dislocations according to the Frank rule [59,60]. Due to the non-planar core configuration of the screw