Twinning to slip transition in ultrathin BCC Fe nanowires

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Abstract

We report twinning to slip transition with decreasing size and increasing temperature in ultrathin <100> BCC Fe nanowires. Molecular dynamics simulations have been performed on different nanowire size in the range 0.404-3.634 nm at temperatures ranging from 10 to 900 K. The results indicate that slip mode dominates at low sizes and high temperatures, while deformation twinning is promoted at high sizes and low temperatures. The temperature, at which the nanowires show twinning to slip transition, increases with increasing size. The different modes of deformation are also reflected appropriately in the respective stress-strain behaviour of the nanowires.

Keywords: Molecular dynamics, BCC Fe nanowire, Size effects, Twinning, Dislocation slip

1 Introduction

Dislocation slip and deformation twinning are two important deformation mechanisms in crystalline materials. In general, plastic deformation occurs by the slip of dislocations at room temperature and conventional strain rates, while twinning is observed in conditions that lead to high stresses such as high strain rates and/or low temperatures. However, it is now well established that the deformation behaviour of single crystals with dimensions reduced to nanoscale is qualitatively different from their bulk counterparts [1]. At nanoscale, the size in addition to temperature and strain rate also plays an important role on the deformation behaviour [2]. In this regard, understanding the size dependence of deformation behaviour in metallic nanowires becomes important and hence attracted huge interest among the materials community.

Experimental and molecular dynamics (MD) simulation studies have shown that the size influences the elastic modulus [3], yield and flow stresses [4], dislocation nucleation and character [5,6], deformation mechanisms [5–9] and failure behaviour [10]. With decreasing size, a transition in deformation mechanisms from dislocation slip to twinning has been reported in many FCC nanowires [5–9]. For example, a transition from full dislocation slip to twinning/partial dislocations has been demonstrated in Cu nanowires for sizes ranging from 70 to 1000 nm [5]. In Cu nanowires of size higher than 150 nm, deformation remains dominated by the slip of full dislocations, while partial dislocations/twinning has been observed below 150 nm [5]. In Ag nanowires of size 11 nm and above, dominance of slip of full dislocations has been observed, while stacking faults and twins governs plastic deformation in 5-8 nm nanowires [6]. Interestingly, with further decrease in size to less than 3 nm, plastic deformation accommodated by relative slip between two adjacent {111} planes without any dislocations has been reported [6]. A similar transition has also been observed in Au thin films, nanowires and nanopillers [7–9]. These results suggest that there exist a clear transition in deformation mechanisms in FCC nanowires. Contrary to this, Yu et al. [11] demonstrated a reverse transition from twinning at higher sizes to dislocation slip at smaller sizes in HCP Ti. Using in-situ experiments, deformation twinning has been observed in HCP Ti single crystal of size 1 μm and above [11]. Below this size, twinning is entirely replaced by the slip of dislocations [11]. These observations strongly suggest that there is a size limit below which twinning does not occur in HCP Ti. In this context, it is important to understand how the size influences the deformation behaviour in BCC nanowires.

In the past, many MD simulations have been carried out to understand the deformation mechanisms in BCC Fe and Mo nanowires [12–17]. All these studies have concluded that the deformation in <100> BCC Fe and Mo nanowires occurs by deformation twinning. The twinning in BCC nanowires is confirmed by the recent experimental observation in <100> W nanowires of size 15 nm [18]. The Schmid factor calculations also predict twinning in <100> BCC crystals [18]. However, here we show that, when the nanowire size is reduced below 3.23 nm, the twinning in <100>/\{110\} BCC Fe nanowires is completely replaced by dislocation slip at high temperatures. MD simulations have been carried out on nanowires with cross section width (d) ranging from 0.404 to 3.634 nm for temperatures in the range 10-900 K. The combined influence of size and tem-

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perature twinning to slip transition for ultra-thin size along with stress-strain behaviour of $<100>$ BCC Fe nanowires has been presented.

2 Simulation Details

Molecular dynamics (MD) simulations have been performed using LAMMPS package [19] employing an embedded atom method (EAM) potential for BCC Fe given by Mendelev and co-workers [20]. Earlier several studies have shown that this potential appropriately describes the deformation behaviour of BCC Fe nanowires [13–15,17].

BCC Fe nanowires oriented in $<100>$ axial direction with $\{110\}$ as side surfaces have been considered in this study. MD Simulations have been performed on nanowires with cross section width ($d$) ranging from 0.404 to 3.634 nm. In all the nanowires, the length ($l$) was twice the cross section width ($d$). Periodic boundary conditions have been chosen along the nanowire length direction, while the other directions were kept free in order to mimic an infinitely long nanowire. After the initial construction of nanowire, energy minimization was performed by conjugate gradient method to obtain a stable structure. To put the sample at the required temperature, all the atoms have been assigned initial velocities according to the Gaussian distribution. Following this, the nanowire system was thermally equilibrated to a required temperature for 125 ps in canonical ensemble using Nose-Hoover thermostat. The Velocity Verlet algorithm was used to integrate the equations of motion with a time step of 5 fs.

Following thermal equilibration, the tensile deformation was performed at a constant strain rate of $1 \times 10^8 \text{ s}^{-1}$ along the axis of the nanowire. For each cross section width ($d$) of nanowires, MD simulations have been performed at different temperatures ranging from 10 K to 900 K. Further, at each size and temperature conditions, five independent MD simulations with different random number seeds have been performed to make statistically meaningful conclusions. The stress was calculated from the Virial definition of stress [21,22]. The visualization of atomic configurations was performed using AtomEye [23] and OVITO [24].

3 Results and Discussion

Figure 1 shows stress-strain behaviour of $<100>/\{110\}$ BCC Fe nanowires with $d = 1.615$ nm at different temperatures ranging from 10 to 500 K. It can be seen that at all temperatures, the nanowires undergo an initial elastic deformation up to a peak stress followed by an abrupt drop in flow stress due to yielding. Following yielding, the stress-strain behaviour of the nanowires depends strongly on the temperature. At low temperatures of 10 and 100 K, the stress-strain behaviour during plastic deformation exhibits uniform flow stress oscillations about a constant mean value up to a strain of 0.4 (Figure 1a). Following this, the nanowires display second elastic peak followed by stress drop and continuous decrease in stress till failure. On the other hand, at high temperatures i.e. at 200 K and above, the nanowires don’t show any second elastic peak (Figure 1b). During plastic deformation, a continuous decrease in stress with large fluctuations (jerky flow) till failure can be seen (Figure 1b). The observed significant difference in the stress-strain behaviour clearly suggests that different deformation mechanisms are operative at low (i.e., 10 and 100 K) and high (i.e., at 200 K and above) temperatures during tensile deformation in $<100>$ BCC Fe nanowires.

In order to understand the difference in stress-strain behaviour, the atomic configurations have been analysed as a function of strain at various temperatures. Figure 2 shows the deformation behaviour in nanowire with $d = 1.615$ nm at the lowest temperature of 10 K. It can be seen that initially perfect nanowire (Figure 2a) yields by the nucleation of a twin embryo, associated with an abrupt drop in flow stress. Following yielding, the stress-strain behaviour of the nanowires depends strongly on the temperature. At low temperatures of 10 and 100 K, the stress-strain behaviour during plastic deformation exhibits uniform flow stress oscillations about a constant mean value up to a strain of 0.4 (Figure 1a). Following this, the nanowires display second elastic peak followed by stress drop and continuous decrease in stress till failure. On the other hand, at high temperatures i.e. at 200 K and above, the nanowires don’t show any second elastic peak (Figure 1b). During plastic deformation, a continuous decrease in stress with large fluctuations (jerky flow) till failure can be seen (Figure 1b). The observed significant difference in the stress-strain behaviour clearly suggests that different deformation mechanisms are operative at low (i.e., 10 and 100 K) and high (i.e., at 200 K and above) temperatures during tensile deformation in $<100>$ BCC Fe nanowires.

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The typical deformation behaviour by twinning mechanism under the tensile loading of \(<100>/\{110}\) BCC Fe nanowire with \(d = 1.615\) nm at the lowest temperature of 10 K. The snapshots in top row are coloured according to the atom’s coordination number and indicates the changes in surface orientation due to twinning. In bottom row, the colour is according to the common neighbour analysis and it clearly shows the presence of twin boundaries.

Once the twin completely sweeps the \(<100>/\{110}\) nanowires, orientation of the nanowire changes to \(<110>\) tensile axis having \(\{100\}\) and \(\{110\}\) as side surfaces (Figure 2d). It can be clearly seen that the new \(<110>\) reoriented nanowire is completely defect free (Figure 2d) and with increasing deformation, it undergoes an elastic deformation once again as reflected in the occurrence of second elastic peak in the stress-strain curve (Figure 1a). Following the second elastic deformation, the reoriented nanowire deforms by full dislocation slip leading to neck formation and final failure (Figure 2e) at relatively higher values of strain. Similar stress-strain behaviour and deformation dominated by twinning mechanism have been observed up to 150 K.

Contrary to deformation by twinning at low temperatures, deformation dominated by dislocation slip at relatively higher temperatures (200 K and above) is shown for 300 K in Figure 3 as an example. The initially perfect nanowire (Figure 3a) yields by the nucleation of 1/2\(<111>\) full dislocations and with increasing strain, dislocations glide on their respective slip planes and finally annihilate at the opposite surface. As a result of deformation by full dislocation slip, the slip steps have been observed on the surface of the nanowire (Figure 3b-c). The absence of surface reorientation clearly indicates that no twinning occurred at 200 K and above. The discrete events of nucleation, glide and annihilation of dislocations is responsible for the observed jerky flow in the stress-strain curve (Figure 1b). Following plastic deformation, the nanowire fails by shear along the dominant slip plane at relatively lower values of strain to failure (Figure 3d). These results clearly suggest that the BCC Fe nanowire undergoes twinning to slip transition with increasing temperature. The different modes of deformation are also reflected in the respective stress-strain behaviour of the nanowires (Figure 1). In case of twinning mode of deformation, a plateau in the flow stress is generally observed, and the occurrence of second elastic peak necessarily suggests twinning followed by reorientation [12, 17]. On the other hand, deformation dominated by full dislocation slip results in continuous decrease in flow stress along with jerky flow [12].

In order to demonstrate the combined influence of size and temperature on twinning to slip transition in \(<100>\) BCC Fe nanowires, the results obtained for different sizes in the range 0.404 to 3.634 nm and for temperatures ranging from 10 to 900 K are shown in Figure 4a. The deformation mechanisms map separating the two different regions of twinning and slip modes of deformation with respect to size and temperature are marked in Figure 4a. It can be clearly seen that the temperature at which the nanowires show twinning to slip transition increases with increase in nanowire size. In other words, at each temperature, there is a critical size below which twinning cannot occur. At low sizes and high temperatures, the slip mode dominates, while at high sizes and low temperatures, deformation twinning is promoted. In the lowest nanowire size of \(d = 0.404\) nm, even though the deformation by slip is observed, but dislocations have not been noticed. Instead of dislocations, the relative slip between the two adjacent slip planes has been seen. In all other sizes, where slip dominates, 1/2\(<111>\) full dislocations have been observed as shown in the bottom row in Figure 3. For nanowire size of 3.23 nm and above, twinning to slip transition has not been observed, and deformation by twinning has been noticed irrespective of temperature. This is also reflected in the flow stress plateaus and occurrence of second elastic peak following re-
The deformation mechanisms map showing the regions dominated by twinning and slip with respect to nanowires size and temperature, and (b) stress-strain behaviour of the nanowire with $d = 3.634$ nm at different temperatures in the range 10-900 K. The analysis of atomic configurations for nanowire size with $d = 3.634$ nm also indicated the dominance of twinning at all temperatures examined. Healy and Ackland [13] have reported dominance of twinning in $<100>$ BCC Fe nanopillar with relatively higher size of 5.8 nm at 300 K. It is important to mention that twinning to slip or slip to twinning transition has not been observed under compressive loading in $<100>$ BCC Fe nanowires, and the deformation remains dominated by dislocation slip for the size and temperature conditions shown in Figure 4a.

Recent large scale MD simulation studies have shown that the deformation by twinning or dislocation slip in BCC crystals depends on many factors such as strain rate, temperature and initial microstructure [25]. It has been shown that in samples free of initial defects, the twinning is inherently favoured at low temperatures and high strain rates [25]. However, the presence of initial dislocations may change the deformation mode from twinning to dislocation slip [25,26]. The occurrence of twinning under tensile loading in $<100>$ BCC Fe nanowires is in agreement with earlier MD simulation studies [13,14,17] and experimental observations on BCC W nanowires of size 15 nm [18]. Generally, the occurrence of twinning at low temperatures can be understood by the fact that, in BCC metals the Peierls stress for perfect dislocations increases more rapidly with decreasing temperature than that for partial dislocations [27]. As a result, the glide of partial dislocations (twinning) is easier at low temperatures. However, the twinning to slip transition with decreasing size in ultrathin $<100>/\{110\}$ BCC Fe nanowires is interesting (Figure 4a) and for the first time such a transition in BCC nanowire is being reported. However, a similar twinning to slip transition with decreasing size has been observed in Ti microcrystals [11]. This size dependence of twinning in Ti has been explained based on the simulated slip model [11]. It has been suggested that a pole of screw dislocation perpendicular to the slip plane acts as a promoter for twin nucleation [11]. Below certain critical size, the dislocations are not high enough to activate twinning and as a result, the twinning is not observed in sample size lower than 1 $\mu$m [11]. The same model cannot be used to explain the observed twinning to slip transition due to the absence of initial dislocations in BCC Fe nanowire. However, the size dependence of twinning in ultrathin pristine nanowires may arise due to highly coordinated nature of twinning mechanism. It is well known that the twin grows by the systematic glide of dislocations having the same Burgers vector on adjacent parallel planes. This coordinated or coherent phenomenon may get disturbed in nanowires of less than a certain size, where the number of surface atoms remains higher than the core atoms. As a result, the twinning is not observed in ultrathin nanowires. Similarly, increasing the temperature have the same effect as that of decreasing the nanowire size, i.e., the high temperature may also disturb the coordinated behaviour of twinning phenomenon in ultra-thin nanowires. The size dependence of twinning has also been observed in nanocrystalline materials [28]. Below certain grain size, it has been reported that the propensity for deformation twinning decreases with decreasing grain size [28].

### 4 Conclusions

We have performed extensive MD simulations on the tensile deformation of ultrathin $<100>/\{110\}$ BCC Fe nanowires for different sizes and temperatures. BCC Fe nanowires with cross-section width less than 3.23 nm deform by twinning mechanisms at low temperatures, while dislocation slip dominates at high temperatures. This indicates that the BCC Fe nanowires undergo twinning to slip transition with decreasing size and increasing temperature. Further, the temperature at which the nanowires show twinning to slip transition, increases with increase in nanowire size, and above 3.23 nm, deformation twinning dominates at all temperatures. The twinning to slip transition has not been observed under the compressive loading of the nanowires.
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