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Molecular dynamics simulation studies on the size dependent tensile deformation and fracture behaviour of body centred cubic iron nanowires

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ABSTRACT

Tensile deformation behaviour of body centred cubic (BCC) iron nanowires with initial orientation of ⟨100⟩/{100} has been investigated using molecular dynamics (MD) simulations. MD simulations were performed at 10 K employing a strain rate of $1 \times 10^8\ s^{-1}$ for the nanowires with cross section width (d) ranging from 1.42 to 24.27 nm. BCC Fe nanowires exhibited two different behaviours as a function of size. Young's modulus, and yield and flow stresses decreased rapidly with increase in nanowire size up to 11.42 nm followed by gradual decrease approaching towards saturation at larger size. The ⟨100⟩/{100} nanowires up to 11.42 nm size deform by twinning at low strains and undergo twinning mediated reorientation to ⟨110⟩/{112} configuration. The reoriented nanowires deform by slip mode at high strains resulting in high ductility and failure by necking. Beyond 11.42 nm size, the reorientation mechanism ceases to operate and the nanowires deform only by twinning exhibiting low ductility and failure by cleavage. The size dependent deformation behaviour has been discussed in terms of the number of active slip systems operating during deformation in Fe nanowires.

1. Introduction

Nanowires, because of their superior electrical, optical and mechanical properties, have large potential for applications in nano/micro electro-mechanical systems (NEMS/MEMS). BCC Fe nanowires exhibit good magnetic properties. This makes it suitable for applications in data-storage media and memory devices, spin electronics, medical sensors and as an enhancement agent for magnetic resonance imaging [1–3]. The high surface area to volume ratio and low defect density provide the nanostructures with mechanical properties different from macroscopic single crystals [4]. Hence, it becomes necessary to understand the deformation behaviour of nanomaterials for applications in multi-functional devices.

Experiments [4–10] have revealed interesting deformation mechanisms characterized by coherent twin propagation [8,10], phase transformation [7,9] and discrete plasticity through dislocations [5,7] operative at nanoscale. It has been observed that the deformation mode and strength in nano-materials are significantly affected by the size due to high surface area to volume ratio [4–6,11]. For example in Ni micro-pillars, the yield strength is found to increase with decreasing size [4]. In-situ transmission electron microscopy experiments on gold revealed that thick films deformed predominantly by perfect dislocations, while the thin films deformed mainly by partial dislocations separated by stacking faults [5]. In HCP metals, it has been shown that the size effects associated with deformation twinning are stronger than the dislocation plasticity [11]. The complexities involved in performing experiments at small length scales prevent the evaluation of mechanical properties using conventional testing methods. Contrary to this, atomistic simulation with suitable inter-atomic potentials can provide appropriate deformation and damage mechanisms operative at nanoscale. In agreement with the experimental observations, atomistic simulations have shown that the different deformation mechanisms in metallic nanowires are slip through perfect and partial dislocations [12,13], twinning [12,14–17] and phase transformation [18,19]. Further, it has been shown that when the deformation occurs by twinning, it gives rise to reorientation [16,20], pseudoelasticity [14], shape memory [14,17] and superelasticity [15]. The difference in deformation mechanisms originates mainly due to crystal structure and its orientation. In addition to crystallographic orientation, the size plays an important role in deformation. For example, in BCC Mo nanowire with ⟨100⟩ orientation, the reorientation ceases to operate when the diameter (d) exceeds 8 nm [21]. Hu et al. [22]

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examined the deformation and fracture behaviour with various boundary conditions and crystal orientations. Olsson et al. [23] have shown a size and orientation dependent Young's modulus in BCC Fe. A decrease in yield strength with increase in temperature has been observed in BCC Fe nanowires [24].

In most of the studies in BCC Fe, the size employed during MD simulations appears to be reasonably low, and a systematic attempt has not been made to examine the influence of size on the tensile behaviour. In addition to above, only a few studies [24–26] are reported on the MD simulation towards the mechanical behaviour of BCC Fe nanowires using suitable inter-atomic potential suggested by Mendelev et al. [27]. In the present investigation, MD simulations using Mendelev EAM potential [27] were carried out on ⟨100⟩/{100} BCC Fe nanowires. Tensile deformation and fracture behaviour as a function of cross section width (d) ranging from 1.42 to 24.27 nm have been examined. The variations in Young's modulus, yield and flow stresses and ductility as a function nanowire size have been presented. The size dependent deformation mechanism and fracture mode have been discussed in terms of the activation of slip/twin system, reorientation and the growth of twins.

2. MD simulation details

In the present work, empirical inter-atomic potential developed by Mendelev et al. [27] was employed. This potential is based on the framework developed by Finnis–Sinclair for many body potential [28]. The potential was fitted to the properties obtained using first-principles calculations in a model liquid configuration and also to other experimentally obtained material properties in BCC Fe. It has been successfully demonstrated that the Mendelev potential can accurately reproduce defect properties such as the self interstitial diffusion [29], the mobility of edge and screw dislocations [30,31] and the six fold symmetry of screw dislocation core [32].

Molecular dynamics simulations have been carried out by using Large scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package developed by Plimpton [33] at Sandia National Laboratories. LAMMPS uses message-passing techniques and a spatial-decomposition of the simulation domain. In MD simulations, cubic simulation box with fixed length to cross section width (d) ratio of 2:1 were used. In order to examine the size dependence of tensile deformation behaviour, MD simulations were performed using different cross-sections width (d) in the range 1.42–24.27 nm. This corresponds to simulating 600–2.4×10^6 atoms. In the present study, fixed aspect ratio of 2:1 (i.e., constant length to cross section width ratio) has been used in all the simulations to avoid the effects associated with aspect or, slenderness ratio on deformation behaviour [34]. Single crystal Fe nanowires oriented in [001] axial direction with {100} as side surfaces were considered for this study. Periodic boundary conditions were chosen along the nanowire length (z) direction, while the other directions (i.e., x and y directions) were kept free in order to mimic an infinitely long nanowire. The initial velocities of the atoms were chosen randomly from a finite temperature Maxwell distribution. After the initial construction of nanowire, energy minimization was performed by conjugate gradient method to obtain a stable structure. Velocity Verlet algorithm was used to integrate the equations of motion with a time step of 5 femto seconds. Finally, the model system was thermally equilibrated to a temperature of 10 K in canonical ensemble (i.e., constant NVT) with a Nose–Hoover thermostat. Following thermal relaxation, there was no change in cross section of the nanowire. It was observed that there were some residual tensile stresses present in the nanowires following equilibration to balance the surface stress arising from the surface tension effects. The magnitudes of these stresses are in the order of GPa, and this effect was more pronounced for small size nanowires having high surface to volume ratio. Following thermal equilibration, the deformation was performed at a strain rate of 1×10^8 s^{-1} with z-axis (⟨001⟩ direction) being the loading direction. Constant strain rate of 1×10^8 s^{-1} was employed in all the MD simulations to avoid the influence of strain rate on plastic deformation behaviour [35]. The strain rate considered during deformation is significantly higher than the typical experimental strain rates. This is due to the inherent timescale limitations from MD simulations. BCC Fe nanowire was allowed to deform naturally at constant strain rate without imposing any stress constraints in the x and y directions. The average stress was calculated from the Virial expression [36]. The visualization of atomic configurations was performed using AtomEye package [37] with coordination number and centro-symmetry parameter (CSP) colouring [38]. Dislocation and defect analysis (slip system determination) was carried out with the help of Dislocation Extraction Algorithm (DXA) developed by Stukowski [39] and Atomviewer [40].

3. Results

3.1. Stress–strain behaviour

Tensile stress–strain curves for ⟨100⟩/{100} BCC Fe nanowires of different cross section widths are shown in Figs. 1 and 2. Since the present study considers only tensile loads, the stress is always positive. The tensile deformation in BCC Fe nanowires shows a characteristic linear elastic regime up to peak stress followed by an abrupt drop in flow stress. Beyond the abrupt drop, large flow stress oscillations about constant mean value occur for small size nanowires in the range 1.42–11.42 nm (Fig. 1). A noticeable decrease in the amplitude of flow stress oscillations with increase in the size of nanowire can be seen in Fig. 1. With further deformation, small size nanowires exhibited occurrence of secondary peaks in the flow stress at intermediate strains (i.e., 68–90% strain) followed by a continuous decrease in the stress values up to failure (Fig. 1). In contrast, secondary peaks were absent and only marginal oscillations in flow stress occur in large size nanowires in the range 12.84–24.27 nm (Fig. 2). Further, the large size nanowires displayed significantly lower tensile ductility (Fig. 2) compared to those for small size nanowires (Fig. 1).

Following thermal equilibrium during simulations at 10 K, presence of residual tensile stresses was noticed in the stress–strain curves (Figs. 1 and 2). The variation in the initial stress with increase in size exhibited a rapid decrease for small size nanowires followed by a gradual decrease to a low saturation value for large

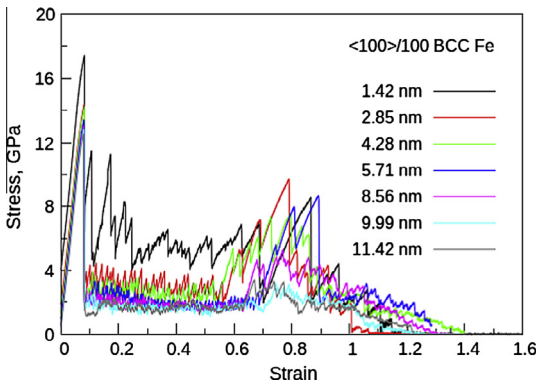

Fig. 1. Stress–strain curves for ⟨100⟩/{100} BCC Fe small size nanowires of different cross section width (d) in the range 1.42–11.42 nm at 10 K.