Numerical Exploration of the Defect's Effect on Mechanical Properties of Nanowires under Torsion

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Abstract. Molecular dynamics (MD) simulations have been carried out to investigate the defect's effect on the mechanical properties of single-crystal copper nanowire with different surface defects, under torsion deformation. The torsional rigidity is found insensitive to the surface defects and the critical angle appears an obvious decrease due to the surface defects, the largest decrease is found for the nanowire with surface horizon defect. The deformation mechanism appears different degrees of influence due to surface defects. The surface defects play a role of dislocation sources. Comparing with single intrinsic stacking faults formation for the perfect nanowire, much affluent deformation processes have been activated because of surface defects, for instance, we find the twins formation for the nanowire with a surface 45^o defect.

Introduction

Due to their excellent mechanical, electrical, optical and other properties, nanowires are attracting increasing attentions [1]. They have been applied as active components of nanoelectromechanical systems (NEMS) including high frequency resonator, force and pressure sensing, and other devices [2]. To explore the revolutionary characteristics of nanowires, massive numerical studies have been carried out. For instance, the size, strain rate, temperature effects to tensile deformation of nanowires have been carried out [3]. McDowell et al. [4] studied the bending deformation of metallic nanowires, and the buckling phenomena of nanowires have also been investigated [5]. Since the nanowires possess significant surface-to-volume ratio, which exert great influence on the structure and properties of nanowires [6]. Researchers reported the surface-stress-induced phase transformation [7], pseudoelastic behaviour [8] and a novel memory effect [9] in nanowires.

It is believed that materials used in engineering always contain imperfections, like grain boundaries, surface defects, nano-cavities and others, which may be induced during the fabrication or manufacturing processes. Owing to the nanometre size scale, the defects appear as one of the most influential factors in determining the nanomaterials' properties. For example, significant stress concentrations can occur at the tip of notches in the surfaces, which would eventually result the propagation of cracks through the system and degradation of mechanical behaviour [10]. Therefore, studying the defect's effect is crucial to enhance the utility of nanowires. Several numerical studies of defects on nanowires have been reported, for example, the studies of the deformation mechanism and mechanical tensile behaviour of the twinned metal nanowires [11], which illustrated the effect of grain boundaries. Although, in our previous work [12], we extensively studied the defect's effect on the nanowire's properties under tensile deformation. It appears that systematic investigations of the defect's effect on the nanowire's properties still calls for significant development, such as under other loading conditions, like bending, compression deformation or vibration.

Therefore, in this work, we will employ the molecular dynamics (MD) simulation to explore the deformation mechanism of surface defected single-crystal copper nanowires under torsion deformation. As some of previous works [13, 14] have already perused the size, temperature and loading rate effects on the mechanical behaviour of perfect nanowires under torsion, thus, we will concentre on the defect's effect on the deformation mechanism.

Numerical Implementation

MD simulations are carried out on single-crystal copper nanowires under the torsion deformation. The square cross-section nanowire with the initial atomic configuration positioned at the FCC lattice site has been considered, and the x, y, z coordinate axes represent the lattice direction of $[100],[010],[001]$, respectively. Four different cases have been considered with the same size of $2.169\times2.169\times18.075nm^3$, as shown in Fig. 1. Non-periodic boundary condition is applied. The nanowire is first relaxed to a minimum energy state using conjugate gradient energy minimization and then the Nose-Hoover thermostat is employed to equilibrate the nanowires at 0.01K. In all the simulations, a constant torsional loading rate is applied, as $9.053\times10^7 rads^{-1}nm^{-1}$.

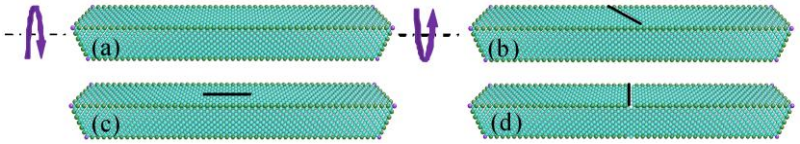

Fig. 1. Simulation models. (a) Case *a*: perfect nanowire; (b) Case *b*: surface 45^o defect; (c) Case *c*: surface vertical defect; (d) Case *d*: surface horizon defect. The defects' schematics are highlighted by straight solid lines.

The embedded-atom-method (EAM) potential developed for copper by Mishin [15] is used to describe the atomic interactions during these simulations and the equations of motion are integrated with time using a Velocity Verlet algorithm. In order to analyse the partial dislocation and stacking faults (SFs) during the torsion deformation, the centro-symmetry parameter (*csp*) is used [16], which increases from 0 for perfect FCC lattice to positive values for defects and for atoms close to free surfaces. During this work, $0.5<csp\le3$, $3<csp\le12$, and $csp>12$ will be assigned to identify the partial dislocations, SFs and surface atoms, respectively. According to the *csp* value, the intrinsic SFs will have two adjacent SFs layers and for the extrinsic SFs or twins, only two translated SFs layers will be observed with atoms between the top and bottom layers still in the FCC environment.

Deformation Mechanisms Analysis

Perfect Nanowire. Fig. 2(a) shows the strain energy versus torsional angle curve of the perfect nanowire under torsion deformation. The strain energy ΔE is defined as $\Delta E=E_t-E_o$, where E_t and E_o are the energy of the strained and initial system, respectively. Following the continuum mechanics [17], during the elastic stage, the torque is a linear function of the torsional angle, means $M=k\varphi$, here, M is the torque, φ is the torsional angle, and k is the constant value for a given nanowire. As the temperature of the system is controlled by NVT ensemble in our simulation, thus, consider the principle of conservation of energy, we can expect that the work W done by M equals the strain energy, therefore, we have, $\Delta E=W=M\varphi/2$, means, $\Delta E=k\varphi^2/2$. That is, a parabolic relationship should be found between the strain energy and torsional angle during the elastic stage, which is consistent with our result in Fig. 2(a) and also results from previous researchers [18]. The value of k can be obtained by fitting the elastic region of the curve in Fig.2(a). In fact, for a traditional torsion of rectangular cross-section bar, the torsional angle is given by equation $\varphi=(Ml)/(GI_p)$, where l is the length of the bar, and GI_p is the torsional rigidity, thus, we get, $k=GI_p/l$. Comparing with the single analysis of the critical angle during torsion deformation in previous work [13, 19], eq. of $k=GI_p/l$ provides us another way to analysis the differences of elastic deformation between different cases, basing on the strain energy and torsional angle curve.

Surface Defected Nanowires. Fig. 2(b) shows the strain energy versus torsional angle curves of three surface defected nanowires. We find that during the elastic region, the strain energy versus torsional angle curves of the defected nanowires are highly consistent with that of the perfect nanowire. As the lengths of the four cases are the same, which means, according to $k = GI_p / l$, we will get an approximately same value of k for all cases, indicating a same value of torsional rigidity GI_p. Therefore, it can be concluded that the torsional rigidity is insensitive to the surface defects, which is similar as our previous studies of tensile deformation [12], as the Young's modulus is found insensitive to both the surface and centro-plane defects. On the contrary, the critical angle shows an obvious decrease due to the surface defects. Specifically, the critical angle for the perfect nanowire is about 1.365*rad*, with the critical angle values about 1.209*rad*, 1.224*rad*, 1.175*rad* for Case *b*, *c* and *d*, respectively. The largest decrease in Case *d* suggests the surface horizon defect appears as the most influential surface defect.

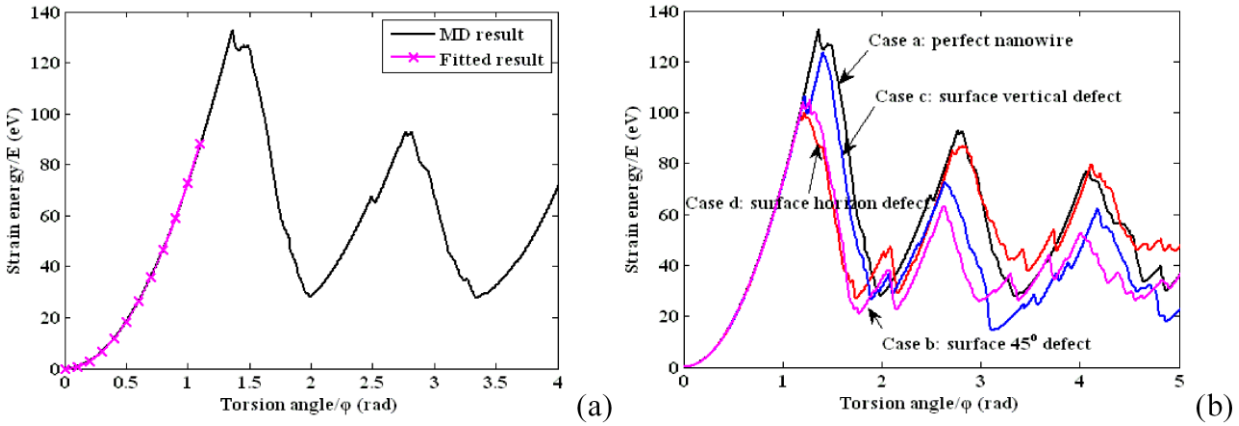

Fig. 2. Strain energy versus torsional angle: (a) Perfect nanowire; (b) Surface defected nanowires.

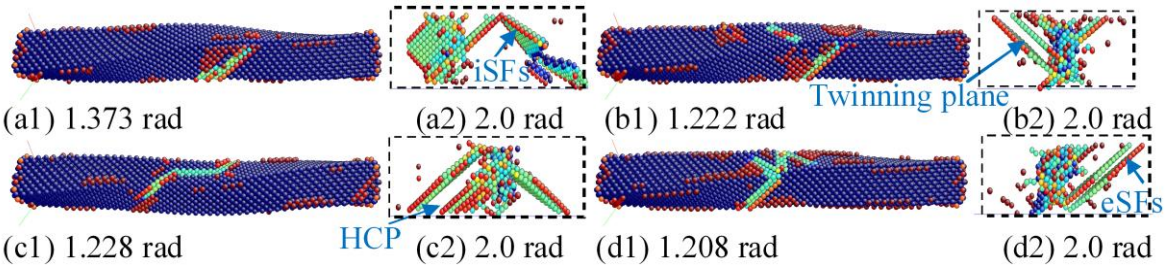

Fig. 3. Atomic configurations. (a1)~(a2): perfect nanowire; (b1)~b(2): surface 45° defect; (c1)~(c3): surface vertical defect; (d1)~d(2): surface horizon defect. Atoms with the *csp* value between 0~12 and 0.5~12 are visualised in the first and third columns and for the rest, respectively.

Fig. 3 presents several snapshots of the nanowires during torsion deformation for both perfect and defected nanowires, different torsion angles are chosen to best clarify the deformation mechanism. As the dislocation generation and propagation processes are concentred around the middle of the nanowire, therefore, only the part with dislocations are kept in the second and fourth column in Fig. 3. Basically, we find the deformation of perfect nanowire is dominated by intrinsic stacking faults (iSFs), which is first generated from one corner of the nanowire as illustrated in Fig. 3(a1). However, for the surface defected nanowires, distinct deformation processes have been observed. Firstly, the SFs are found generated around the surface defect (Fig. 3(b1), (c1) and (d1)), which implies that the surface defects play a role of dislocation sources. Secondly, due to the existence of surface defects, much affluent deformation processes have been triggered, such as the formation of extrinsic stacking faults (eSFs), twins and HCP structure. In detail, for Case *b*, the twins are formed as seen in Fig. 3(b2). For Case *c*, we find the formation of HCP structure as shown in Fig. 3(c2), which disappeared after further deformation. Actually, the whole deformation process of Case *c* is very similar to the perfect nanowire, which is also indicated by the similar strain energy versus torsional angle curves in Fig. 2(b). For Case *d*, we find the existence of eSFs,

as illustrated in Fig. 3(d2). In all, obvious influences to the deformation mechanism are resulted from surface defects.

Conclusions

MD simulations have been carried out to investigate the defect's effect on the mechanical properties of single-crystal copper nanowires with different surface defects, under torsion deformation. The deformation process has been investigated, major findings are summarised as follows:

(1). The torsional rigidity is found insensitive to the surface defects;

(2). The critical angle appears an obvious decrease due to the surface defects, the largest decrease is found for the nanowire with surface horizon defect;

(3). The deformation mechanism appears different degrees of influence due to the surface defects. In particular, the surface defects play a role of dislocation sources. Much affluent deformation processes have been activated, for instance, we find the twins formation for the nanowire with a surface 45^{o} defect.

Conclusively, this study provides a fundamental understanding of the mechanical behaviour of nanowires under torsion deformation when surface defects are presented. The defects' effect to the elastic and plastic deformation has been discussed, which will enrich the current numerical study of nanowires.

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