Interaction and Multiscale Mechanics, Vol. 5, No. 2 (2012) 115-129
DOI: http://dx.doi.org/10.12989/imm.2012.5.2.115

Numerical investigation of mechanical properties of nanowires: a review

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(Received July 31, 2011, Revised November 14, 2011, Accepted April 5, 2012)

Abstract. Nanowires (NWs) have attracted intensive researches owing to the broad applications that arise from their remarkable properties. Over the last decade, immense numerical studies have been conducted for the numerical investigation of mechanical properties of NWs. Among these numerical simulations, the molecular dynamics (MD) plays a key role. Herein we present a brief review on the current state of the MD investigation of nanowires. Emphasis will be placed on the FCC metal NWs, especially the Cu NWs. MD investigations of perfect NWs' mechanical properties under different deformation conditions including tension, compression, torsion and bending are firstly revisited. Following in succession, the studies for defected NWs including the defects of twin boundaries (TBs) and pre-existing defects are discussed. The different deformation mechanism incurred by the presentation of defects is explored and discussed. This review reveals that the numerical simulation is an important tool to investigate the properties of NWs. However, the substantial gaps between the experimental measurements and MD results suggest the urgent need of multi-scale simulation technique.

Keywords: mechanical properties; nanowires; molecular dynamic simulation; defects; surface effects.

1. Introduction

Metals and semiconductor nanowires (NWs), as one type of the most exciting nanomaterials, have attracted intensive research owing to their remarkable mechanical, optical, electrical and other properties (Xia *et al.* 2003). Wide applications have been expected from such distinct characteristics, such as the building blocks of nanoelectromechanical systems (NEMS) (Ekinci and Roukes 2005) and the critical part of the solar energy conversion devices (Bierman and Jin 2009). To explore the mechanical properties of NWs, abundant experimental studies have been conducted. For example, Wu *et al*. (Wu *et al.* 2005) employed the atomic force microscope (AFM)-based experiments to measure the Young's modulus and yield strength of Au NWs under bending. Marszalek *et al*. (Marszalek *et al.* 2000) demonstrated that experiments could provide direct evidence for the mechanism underlying the plastic deformation of a NW. Recently, Richter *et al*. (Richter *et al.* 2009) reported the fabrication of high aspect ratio FCC single crystalline NWs using a high temperature molecular beam epitaxy method and found the Cu NWs' strengths are close to

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the theoretical upper limit under tensile tests.

Due to the extreme small scale of NW, the controlling of experimental conditions is supposed with inherent complexities and unknowns (McDowell *et al.* 2008). Therefore, numerical investigations of NWs' properties are frequently employed by researchers, including theoretical calculations (Lim *et al.* 2009), multi-scale simulations (Chen and Lee 2010) and molecular dynamics (MD) simulation. In view of the immense numerical studies that been conducted are mainly by MD simulation, herein we present a brief review on the current state of the MD investigation of NWs. Emphasis will be placed on FCC metal NWs, especially the Cu NWs. In particular, MD studies of perfect NWs' mechanical properties under different deformation conditions, including tension, compression, torsion and bending are revisited at first, and then the effects of defects for Cu NWs are discussed in details. These defects include twin boundaries (TBs) and pre-existing defects. Certain overall conclusions and recommendations are provided at the end of this paper. To note that, despite the tremendous MD investigations being carried out, a substantial gap is still existed between experimental measurements and MD results. Upon such circumstance, multi-scale simulation technique, which could not only provide experimental comparable results, but also capture nanoscale deformation mechanisms, is urgently required.

2. Mechanical properties of perfect nanowire

Although considerable MD simulations of NWs have been carried out, very few work has pursued the NWs' properties under combined loading conditions, therefore, this review focuses on single loading condition.

2.1 Tensile properties

Due to the ease of tensile stress analysis in the atomistic framework, numerical investigations of NWs subjected to axial tension have been frequently conducted. Many researches can be found regarding to the tensile properties of different NWs, such as the FCC (Cu, Au, Al and Ni) and BCC (Fe, Cr and W) NWs (Komanduri *et al.* 2001). Fig. 1 shows a Cu NW simulation model during tensile deformation. The NW is constructed as a regular FCC lattice with the lateral directions as [100] and [010], and the axial direction of [001]. Hereafter, we refer NWs with such orientations as <100> NW. As different boundary conditions (BCs) would obviously change the simulation results. Hence, it is necessary to mention the different BCs that being applied during MD simulation by different researchers. Accordingly, two kinds of BCs have been considered for the simulation of NWs. One referred as S-S-P with shrink-wrapped BCs (free BCs) at two lateral directions and periodic BC in the axial direction. The other referred as S-S-S with free BCs in all three directions.

It should be noted here that different interatomic potentials would lead to different behaviours of NWs in MD simulation. Early researches already claimed that pair potential was inaccurate in calculation involving surfaces, or defects (Daw and Baskes 1984). Under nanoindentation simulation, Ziegenhain *et al*. (Ziegenhain *et al.* 2009) found that pair potentials (L-J and Morse potentials) predict a severe overestimation of work hardening. It is evident that, a many-body potential is more realistic for FCC metals. In fact, the EAM potential (Daw and Baskes 1984) is the most popular potential employed during MD simulations. Thus, in this work, the EAM potential is applied to ensure comparable results with previous researchers. It should be noted here different

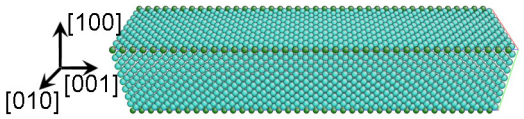

Fig 1. A Cu NW modelled by embedded atom method (EAM) potential for tensile deformation

potentials are suitable for different materials, for example, silicon usually uses Tersoff potential (Zhao and Aluru 2008).

As is well known, NWs have a significant surface-to-volume ratio and the surface atoms possessing different electron densities and a lower coordination number than bulk atoms. MD studies have unveiled a plethora of novel mechanical behaviours of NWs due to the surface effect. Such novel behaviours include phase transformations (Diao *et al.* 2003, Park 2006), pseudoelastic behaviour (Liang *et al.* 2005) and shape memory effect (Park *et al.* 2005, Park and Ji 2006). Since these surface-driven phenomena have already been systematically reviewed (Park *et al.* 2009), we intend to exclude them from the scope of this article.

It is reported by many researchers that the stress of the stress-strain curve is not from zero, indicating the existence of the initial stress or initial strain. For example, Liang and Zhou (Liang and Zhou 2004) advised a initial stress value around 0.4~1.6 GPa for Cu NWs. Our recent research (Zhan and Gu 2011c) suggests that, this initial stress is originated from the surface stress. We find that for a NW with the BC of S-S-S, the NW would be stress free after energy minimization (getting an equilibrium configuration). However, for a NW with S-S-P BC, the axial stress will show an inverse proportional relation with the cross-sectional size after energy minimization. This observation is reasonable, as the NW will not be stress free due to the periodic BC in the axial direction. In particular, Diao *et al*. (Diao *et al.* 2004) proposed that, for a <100> NW with square cross-section, the initial axial stress can be estimated as: $\sigma_{in} = 4fd/A = 4f/d$, where f is the surface stress, d is the cross-sectional size and supposing the cross-sectional area $A = d^2$. This estimation is employed in our simulation, we get a surface stress $f = 0.786$ J·m^{-2}, which is very close to the value provided by Streitz *et al*. (Streitz *et al.* 1994) as 0.896 J·m^{-2}. Typically, it is found that the surface stress is tensile for FCC metals (Wan *et al.* 1999), but compressive for semiconductor NWs (Shim *et al.* 2005).

Yield strength (stress at which plastic deformation initials) and Young's modulus are two mostly discussed mechanical properties. Researchers (Gall *et al.* 2004) found that the yield strength of NWs is considerably higher than bulk materials. To investigate the dependence of yield strength and Young's modulus with different factors, such as temperature, size (cross-sectional size when the BC is S-S-P, both cross-sectional size and length when the BC is S-S-S), strain rate or loading rate and geometry of the NW (crystalline orientation or cross-sectional shape), vast MD investigations have been carried out. Several consistent conclusions have been drawn for NWs with both BCs of S-S-P and S-S-S, i.e.,: (1) both Young's modulus and yield strength decrease with increasing temperature; (2) Young's modulus is almost independent of strain rate and yield strength increases with increasing strain rate; (3) yield strength decreases with increasing cross-sectional size; (4) the mechanical behaviour of NWs is strongly dependent on the cross-sectional geometry and surface orientation, e.g. non-square NWs exhibit lower yield strength and strains, and appear a propensity to deform via twinning. (Gu and Zhan 2010, Zhan *et al.* 2010, Setoodeh *et al.* 2008, Yuan *et al.* 2007, Liang and Zhou 2003, Wang *et al.* 2008, Ji and Park 2006a, Leach *et al.* 2007). Apart from the above consistent conclusions, certain discrepancies should also be mentioned. First, for the BC of S-

S-S, some researchers (Liang and Zhou 2003) found that Young's modulus is insensitive or independent to NWs' cross-sectional size. However, with the increase of cross-sectional size, Yang *et al*. (Yang *et al.* 2009) reported that, Young's modulus decreases for <110> Cu and <110> Ni NWs, but increases for <111> Cu and <111> Ni NWs. Second, for the BC of S-S-P, Wu (Wu 2006a) reported that Young's modulus increases with increasing cross-sectional size for <100> Cu NW. However, according to Agrawal *et al*. (Agrawal *et al.* 2008), Young's modulus is found deceasing with increasing diameter of [0001] oriented ZnO NW. Our own simulation revelas that, for <100> Cu NW with the BC of S-S-P, Young's modulus appears insensitive to the cross-sectional size. While, for <100> Au and Ag NWs with the BC of S-S-S, Young's modulus decreases and yield strength increases with increasing length, respectively. Finally, for different crystalline orientations or geometry of the NW, Ji and Park (Ji and Park 2007) reported that non-square Cu NWs generally exhibit lower yield strength and toughness.

Massive MD simulations have been carried out to investigate the NWs' tensile deformation mechanisms (Park and Zimmerman 2005). Park *et al*. (Park *et al.* 2006a) reported that the tensile deformation mechanisms of NWs are a function of the intrinsic material properties, applied stress state, axial crystallographic orientation and exposed transverse surfaces. It is found that, with extreme high strain rate, NWs will change to an amorphous phase. This phenomenon has been found in many different NWs, such as the Pt and Au NWs (Koh and Lee 2006), Ni and NiCu NWs (Ikeda *et al.* 1999). For low strain rate, the tensile deformation is dominated by the nucleation and propagation of partial dislocations (slip dominate deformation process). Lin and Pen (Lin and Pen 2007) found that, the tension of <100> Cu NW induces the formation of twin and consequently cause geometrical softening, while for <110> NW, the generation of twin bands causes geometrical hardening. Researchers found that Cu NWs with non-square cross-section have a propensity to deform via twinning under tension (Ji and Park 2006b, Ji and Park 2007).

In most publications relating to the NWs' tensile deformation, a saw-toothed (Wu 2006b, Liang and Zhou 2003) or a zigzag (Yuan *et al.* 2007, Wen *et al.* 2005) stress curve during the plastic deformation is reported. Our recent work (Zhan *et al.* 2011b) reveals that, during the plastic deformation of both perfect and defected NWs, decrease regions of the stress curve are accompanied with stacking faults (SFs) generation and migration activities, but during stress increase, the structure of the NW appears almost unchanged.

2.2 Compressive properties

Besides of the tensile deformation, the MD investigation of NWs' mechanical behaviours under compression is also being frequently employed. For example, researchers observed the single step phase transformation from B2 to body-centred-tetragonal (BCT) of CuZr NW under compression (Sutrakar and Mahapatra 2010), and Ni NWs with helical multi-shell structure show greater yield strength than that of macroscopic solid (Wang *et al.* 2005). Usually, for the NWs compression simulation, the applied BC is S-S-S with free BCs at two lateral directions, and clamped ends at the axial direction. Researchers have discussed the dependence of critical stress and Young's modulus with different factors (temperature, strain rate and size) and the deformation mechanism is also being extensively explained.

It is reported that, the tensile yield strength is much larger than the compressive yield strength for small <100> Au NWs, while for small <111> Au NWs, tensile and compressive yield strengths have similar magnitude (Diao *et al.* 2006). For Ni NWs, Setoodeh *et al*. (Setoodeh *et al.* 2008)

found the compressive critical stress (yield strength) and Young's modulus are lower than those obtained from tensile deformation. Similar findings are also reported in other work (Tschopp and McDowell 2007), for orientations of [110] and [111], higher yield stress is required for compression, but for the orientation of [100], a higher yield stress is required for tension.

Two kinds of deformation behaviours for NWs during compression have been proposed. The first behaviour is plastic deformation for short or medium NWs, during which NWs no longer retain their original structure. According to Park *et al*. (Park *et al.* 2006a), for <100>/{100} NW, the compression deformation is dominated by twinning, with partial dislocation for <100>/{110} NW and full and partial dislocations for <110> NW. Similarly, for Au NWs under compression, researchers found the yielding via Shockley partial dislocation that nucleated from the surface (Rabkin *et al.* 2007, Wen *et al.* 2010). The second is elastic deformation, namely buckling phenomenon, during which NWs retain their original atomic structures. It is observed that (Jiang and Batra 2009), after complete unloading of a buckled NW, the average axial stresses and the total potential energy will fully recover to their original state (reference configurations). The critical stresses that extracted from MD simulations with the predictions from conventional Euler theory (Timoshenko and Gere 1961) are compared. Researchers found both values are very close to each other when NWs' lengths are longer than a certain value. However, for NWs with shorter lengths, the critical stress obtained from MD is much smaller than that given by the conventional Euler theory, and the critical strength shows less dependence on the wire length (Wang *et al.* 2008, Olsson and Park 2011).

Recently, based on the conventional Euler theory, Wang and Feng (Wang and Feng 2009) proposed a modified Euler model (M-Euler) to predict NWs' critical stress. The M-Euler theory takes account of the influence from the surface elasticity and the residual surface tension. Our recent work (Zhan and Gu 2011b) employed the M-Euler model to fit with the critical stresses for <100> Cu NWs obtained from MD simulation. It is found that, for NWs with the slenderness ratio (L/a) larger than 10, M-Euler function fits well with the values obtained from MD. However, large differences between the values given by MD and M-Euler function are found for the slenderness ratio smaller than 10. This conclusion is reasonable, as M-Euler theory only predicts the critical buckling stress, and it will lead to significant error in the prediction when the failure mode of NW under compression changes from buckling to yielding mode when the slenderness decreases. In the contrast, a direct comparison between the MD results and the M-Euler for Au NWs conducted by Olsson and Park (Olsson and Park 2011) suggests that the M-Euler model may not be accurate for the buckling force prediction.

Generally, the critical stress decreases with increasing temperature and length, but increases with strain rate and cross-sectional size. In the meanwhile, Young's modulus is found decreasing with the increase of temperature and insensitive to strain rate. Although, Young's modulus is observed dependent on the NWs' length, the dependence is expected reduced when the length of NWs is much larger than the cross-sectional size (Jing *et al.* 2009, Wang *et al.* 2008). One should note that according to the recent buckling study of Au NWs, the critical stress is found increasing with the increase of cross-sectional size for both the <100>/{100} and <100>/{110} NWs, whereas, it decreases for <110>/{110}{100} NWs (Olsson and Park 2011).

2.3 Torsional properties

NWs mechanical properties under torsion have also been investigated by researchers. Different

cross-sectional shapes have been considered, including square, circular and hollow square cross-section. The usually applied BC is S-S-S, with a pair of torsional load applied to the two ends.

The critical torsional angle (the angle value when dislocations begin to emit) is the most discussed properties. Our recent work (Zhan *et al.* 2011a) reveals that during elastic deformation stage, the relation between the strain energy and torsional angle is well described by a parabolic curve as $\Delta E = k\varphi^2/2$. Here, ΔE is the strain energy and is defined as $\Delta E = E_t - E_o$, with E_t and E_o as the energy of the strained and initial system, respectively. φ is the torsional angle, and $k = GI_p/l$ with l as the NW's length and GI_p as the torsional rigidity. It is supposed that, based on the strain energy versus torsional angle curve from MD simulation, we could estimate the torsional rigidity for a given NW. Our simulations for perfect <100> Cu NWs reveal that, the parabolic curve fits well with the strain energy versus torsional angle curve.

Several works have been dedicated to explore the plastic deformation of metal NWs under torsion. (Weinberger and Cai 2010a, Weinberger and Cai 2010b) reported that the plastic deformation of NWs under torsion can be either homogeneous or heterogeneous, regardless of size, depending on the wire orientation. Particularly, homogeneous deformation is found for NWs oriented along <110>. In contrast, NWs oriented along <111> and <100> are found deformed through the formation of twist boundaries and tend not to recover when high angle twist boundaries are formed. One recent work reported by Jiang *et al*. (Jiang *et al.* 2010) suggested that elastic pre-loading conditions can induce a distinct weakening on the resistance against plastic deformation under later applied loads. They observed the formation of fivefold twins in Cu NWs subjected to tensile deformation with pre-torsion.

Generally, researchers drew the following conclusions: First, the critical torsional angle increases with the increase of loading rate and length, but decreases with temperature and cross-sectional size. Second, most of the atoms in the necking region are found experiencing a phase transformation from regular lattice structure (For example, FCC for Cu NWs) to amorphous, and then rearranged to regular lattice structure again. Such deformation processes are more obvious at higher loading rates. Third, the torsional buckling behaviour is observed, and the buckling modes are highly affected by the wire length and temperature (Wang *et al.* 2008, Gao *et al.* 2010, Jiang *et al.* 2009). In the end, it is worth to mention that, according to the potential energy versus torsional angle curves given by previous researchers and the aforementioned parabolic curve, the torsional rigidity is expected to be insensitive to different loading rates. Further investigation of the dependence of the torsional rigidity with the factors of temperature, size and cross-sectional shape will be reported in our future work, as well as the theoretical calculation of the torsional rigidity.

2.4 Bending properties

Bending experimental test at nanoscale is widely used in mechanical characterizations of NWs because of its manipulation convenience (Wu *et al.* 2005, Ni *et al.* 2006). However, comparing with the tremendous numerical investigation of NWs' mechanical properties under uniaxial loading, the MD simulation of NWs bending deformation is still very few, and requiring a more complete development.

Usually, for the simulation of bending, the NWs' BC is S-S-S with no periodic BC applied in any direction. To date, several kinds of bending simulation have been reported, such as four-point bending and three-point bending. Generally, the nominal Young's modulus that obtained from bending and tension is found different (Wu 2004). An early work conducted by Miller and Shenoy

(Miller and Shenoy 2000) suggested that, the significance of size effect in bending is larger than that in uniaxial tension. Consistent conclusions have also been reported by Wang *et al*. (Wang *et al.* 2010), i.e., the surface-induced size-dependent nominal Young's modulus is more significant under bending than that under tension or compression.

As a matter of fact, researchers got different results when they investigated the cross-sectional size effect to the nominal Young's modulus. For example, Chan *et al*. (Chan *et al.* 2008) found that the nominal Young's modulus is lower as the cross-sectional size became smaller for SiC NWs. However, McDowell *et al*. (McDowell *et al.* 2008) reported that, for Ag NWs with a <110> axial orientation, Young's modulus increases with increasing cross-sectional size, while for <100> axial orientation, it decreases with cross-sectional size. Another interesting finding about bending is the formation of two conjoint fivefold deformation twins (DTs) in the hollow square cross-section Cu NWs (Zheng *et al.* 2008), which implies that fivefold DTs could be formed without introducing initial imperfections.

3. Mechanical properties of defected nanowire

Several studies have also been conducted to investigate the defects effect to NWs. In this section, MD studies of effect from two kinds of defects are reviewed. One is twin boundaries (TBs), the other is pre-existing surface and internal defects that being investigated by our recent work.

3.1 Twin boundaries effect

TBs is supposed to be ubiquitous for both synthesis and properties in nano-enhanced FCC metals (Sansoz *et al.* 2008). Particularly, TBs are observed exerting great influence to the properties of NWs (Wu *et al.* 2006). It is of great importance to investigate their roles in NWs. Currently, a serial of studies have been carried out to study the TBs influence. Cao and his group members studied the twinned Cu NWs under tensile deformation (Cao and Wei 2006, Cao *et al.* 2007). They found that, the fivefold twinned NW has higher yield strength than the perfect <110> NW, but appear brittle failure and low elongation ductility. For twinned Cu NWs with <111> growth orientation and nearly square cross-section, they observed the smaller the TBs, the higher the twinned NW yield strength. Further, TBs are found acting as barrier for dislocation movements and lead to hardening effects but turn out to be dislocation sources with further deformation.

The TBs effect has also been extensively studied by Sansoz and his group members for Au and other metal NWs (Deng and Sansoz 2009c, Deng and Sansoz 2009a, Deng and Sansoz 2009b). They found the coherent TBs in NWs could cause strengthening effects, weakening effects and even no effects, as a function of both twin spacing and sample diameter. They also observed the enabled significant strain hardening and ultrahigh flow stresses in twinned Au NWs when NW diameter increase of, conversely, the TB spacing decrease at the nanoscale. Recently, Zhang and Huang (Zhang and Huang 2009) reported that whether TBs strengthen NWs depends on the surface morphologies. TBs would soften NWs if they have circular cross-section or strength NWs when they have square cross-section. Accordingly, many works have been carried out to explore the TBs effect to NWs' properties. However, we notice that most of the current MD studies of TBs are under the deformation of tension or compression (Afanasyev and Sansoz 2007). To get a more systematic understanding of TBs effect, the studies of twinned NWs under other loading conditions are expected.

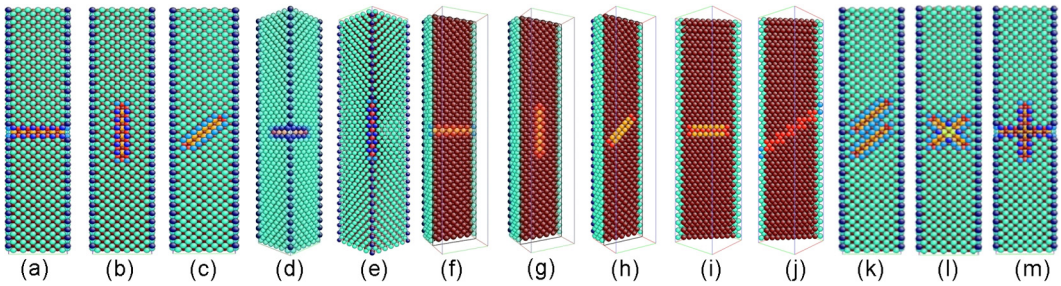

Fig. 2 Cu NWs with different pre-existing defects. (a) Defect I: surface horizon defect; (b) Defect II: surface vertical defect; (c) Defect III: surface 45° defect; (d) Defect IV: surface corner defect; (e) Defect V: surface edge defect; (f) Defect VI: horizon defect in internal (100) plane; (g) Defect VII: vertical defect in internal (100) plane; (h) Defect VIII: 45° defect in internal (100) plane; (i) Defect IX: horizon defect in internal (110) plane; (j) Defect X: diagonal defect in internal (110) plane; (k) Defect XI: surface parallel 45° defects; (l) Defect XII: surface crossed 45° defects; (m) Defect XIII: surface horizon and vertical defect. Figs. (f) to (j) are sectional views

3.2 Surface and internal defects effect

It is well known that, imperfections would be introduced to the NW during the fabrication or manufacturing processes. Using large scale MD simulations, Chen *et al*. (Chen *et al.* 2010) reported that, during the machining and stretching of single crystal Cu, SFs will be generated inside the specimen, which will greatly affect the specimen's properties under tension. Therefore, it is crucial to investigate the defects effect for a better understanding of NWs' properties. Recently, we carried out a serial study of the pre-existing defects effect to Cu NWs. Some of the main conclusions under different deformation conditions have been summarised in this section. Different surface defects on Cu NWs have been considered. To investigate further of the defects effect, several different internal defects have also been considered as an academia analysis. On the whole, thirteen different defects have been studied, which are denoted as defect 'I', 'II' … 'XIII' for discussion convenience, as illustrated in Fig. 2. Different defects are introduced to NWs by removing certain number of atoms according to different orientations. Note that, the surface defects that we considered is more like a surface notch that been investigated by Doyama (Doyama 1995), and also similar to the defect of vacancies studied by Chang (Chang 2003).

3.2.1 Defects' effect under tension

The defects' effect under tension has been systematically investigated in our recent works (Zhan *et al.* 2011c, Zhan and Gu 2011a, Zhan and Gu 2011c). We considered the above thirteen different defects, different fractions of defects, as well as different orientated NWs with surface defects. Major conclusions are given as follows.

First of all, for NWs with the ten single defects, Young's modulus is found insensitive to different defects. A similar result has been found by Zhao *et al*. (Zhao *et al.* 2009), who reported the Young's modulus is independent of the nano-void in a periodic unit cell subjected to the uniaxial tension. However, contradiction is found for an earlier work done by Chang (Chang 2003), who revealed that the Young's modulus decreases with increasing vacancy fraction. Such discrepancy is expected resulting from the Lennard-Jones (L-J) potential that he employed, as the L-J potential is supposed

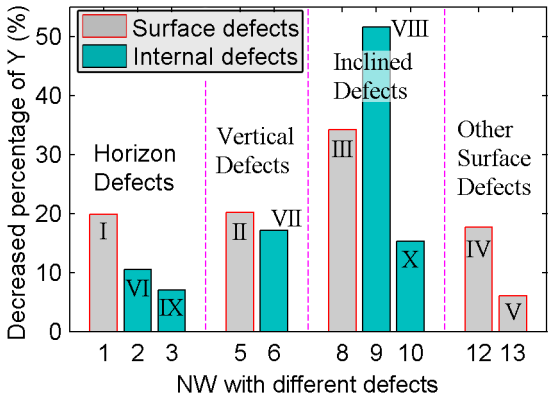

Fig. 3 Comparison of the decreased percentage of the yield strength (Y) for Cu NWs with different defects

to have significant problems when the local environment is substantially different from the uniform bulk, such as surfaces, grain boundaries, internal voids and fracture process (Foiles *et al.* 1986).

According to Fig. 3, yield strength appears obvious decrease due to different single defects. Particularly, the biggest yield strength decrease is found in NW with defect VIII, with about 51.46% reduction. In the meanwhile, we find NWs with defect V and IX have the least decrease. Furthermore, it is observed that, usually the same features defects located on the surface exert bigger decrease to the yield strength than those located in the internal. It is concluded that the defect that lies on the slip planes tend to introduce larger decrease to the wire yield strength than other defects.

For the deformation mechanism, we find the formation of twins, hexagonal close packed (HCP) structure and even phase transformation (from FCC to HCP and then change back to FCC) for NWs with different defects and the defects have played a role of dislocation sources. Different deformation mechanisms that triggered by different single defects have been summarised in Table 1. For convenience, we refer intrinsic SFs and extrinsic SFs as iSFs and eSFs, respectively. Twin refers to twinning process, and HCP refers to the formation of a small fraction of HCP structure with the phase transformation shorted as PT. Obviously, due to the existence of defects, more affluent deformation mechanisms have been activated. Another interesting point to mention is that, for NWs with Defect V (surface edge defect), the generation of two conjoint fivefold deformation twins (FDT) is observed.

Second, for NWs with three surface bi-defects (defects XI, XII and XIII), we find Young's modulus is still insensitive to such defects, and yield strength appears an obvious decrease. Regarding to the abundant deformation processes in NWs with single defects, we find the generation of iSFs, eSFs, twins and HCP structure happened for NWs with surface bi-defects.

Third, we considered NWs with three different cross-sectional sizes, with the same length but have different fractions of defect III. Again, it is found that Young's modulus is insensitive to different fractions of defects, with yield strength showing an apparent decrease. Furthermore, larger decrease of the yield strength is induced with larger fraction of defects.

Fourth, surface defected NWs with three different crystalline orientations have been investigated. It is found that Young's modulus is insensitive to the defect, even when the NWs' crystalline orientations are different, and an obvious decrease for yield strength is observed. The defects are

Table 1 Deformation mechanisms that observed in NWs with different defects under tension

Perfect	Defect I	Defect II	Defect III	Defect IV	Defect V
iSFs, eSFs	iSFs, eSFs Twin, HCP	iSFs, eSFs HCP	iSFs, eSFs Twin	iSFs, eSFs HCP, Twin, GB	iSFs, eSFs HCP, Twin, GB, PT
	Defect VI	Defect VII	Defect VIII	Defect IX	Defect X
	iSFs, eSFs HCP, Twin, PT	iSFs, eSFs HCP, Twin, PT	iSFs, eSFs Twin	iSFs, eSFs HCP, Twin, GB	iSFs, eSFs HCP, Twin

observed as a role of dislocation sources, and exert different influences to the deformation mechanisms when the NWs' crystalline orientations are different.

In all, we could summarise that: (1) Young's modulus is insensitive to different styles of defects with yield strength appears an obvious decrease; (2) The defects have played a role of dislocation sources, the partial dislocations are first emitted around the locations of the defects; (3) Generally, the surface defect induces bigger decrease to yield strength than the internal defect, and the defect that lies on slip planes leads to larger influence than other defects; (4) The more or larger of the defects, the larger influence appears; (5) Usually, defects intend to enrich the NWs' tensile deformation mechanisms, and different defects exert different influences.

3.2.2 Defects' effect under compression

Recently, we investigated the defects effect to the buckling phenomenon of Cu NW (Zhan and Gu 2011b). Six kinds of pre-existing defects including surface defects of I, II, III and internal defects of VI, VII and VIII have been studied. The NW's BC is S-S-S. Basically, we find that: (1) same as concluded from the NWs' tensile deformation, Young's modulus is insensitive to defects; (2) obvious decreases of the critical stress due to different defects are observed, with the NW with defect II (surface vertical defect) showing the largest decrease and the NW with defect VII (internal vertical defect) leading to the least decrease; (3) the buckling phenomena are observed in all defected NWs and the buckling mode is influenced by different defects. Specifically, NWs are observed deflected in different directions. According to estimated deflection values, we find the NW with defect I (surface horizon defect) has the largest deflection and NW with defect VII (internal 45° defect) has the smallest deflection. In all, the surface defects are found exerting larger influence than internal defects.

3.2.3 Defects' effect under torsion

The investigation of Cu NWs with the surface defects of I, II and III under torsion has also been carried out (Zhan *et al.* 2011a). Defected Cu NWs with the BC of S-S-S are considered. The torsional rigidity, critical torsional angle and the deformation mechanism have been carefully studied. Our study suggests that: First, the torsional rigidity is insensitive to surface defects. Second, the critical angle appears an obvious decrease due to the surface defect and the largest decrease is found for the NW with surface horizon defect. Third, surface defects are found exerting different influence to the deformation mechanisms, which are also observed playing a role of dislocation sources. In particular, much affluent deformation processes are found activated due to the existence of surface defects. For instance, the twinning process is found for the NW with a surface 45° defect.

4. Conclusions

Conclusively, by employing MD simulations, we get a wide fundamental understanding of the deformation mechanisms of NWs. Indubitably, MD simulations have acted as an excellent way not only to the investigation of the elastic and inelastic behaviours and properties of NWs, but also to the prediction of new or unexpected properties.

The discussions for perfect NWs suggest that, majority of the current MD studies are focusing on the NWs deformation under uniaxial loading condition, i.e., tension or compression. Comparing with the commonly utilized experimental approaches, such as bending (Jing *et al.* 2006, Chen *et al.* 2006) and resonance (Feng *et al.* 2007, Tanner *et al.* 2007), a significant development of numerical study of NWs under other loading conditions (like bending and vibration) is required. As aforementioned, materials used in engineering are always not defect-free. Different defects, such as native oxide layers, grain boundaries (GBs) or TBs, impurities, and even pre-existing defect patterns would be introduced during the manufacturing or fabricating processes. The MD investigations of the TBs' and pre-existing defects' effects suggest that the existence of defects would induce large influence to the mechanical properties and deformation mechanisms of NWs. A more systematic and fundamental NWs' defects study calls more research effort.

In the last, as pointed out by Park *et al*. (Park *et al.* 2009), there are obvious inconsistencies between the experimental measurements and MD studies of the NWs' elastic and inelastic properties. We should note that, a large part of the inconsistencies between experimental measurements and MD studies are arisen from the length scale and time scale (Horstemeyer *et al.* 2001). In respect of length scale, inappropriate large simulation system would make it computational impractical. To the time scale, it is well known that the strain rates employed during MD simulations are typically 10-15 orders of magnitude larger than that applied experimentally (Park *et al.* 2009). Certainly, the development of computational science would allow us to deal with larger simulation system. A more realistic way is to develop a multi-scale simulation technique, which would not only accurately catch the properties at nanoscale, but also provide with experimental comparable results. It is glad to see that recently there are already some researches undertaken for multi-scale modelling of NWs (Park *et al.* 2006b, Park and Klein 2007), but the multi-scale modelling is still an open issue.

Acknowledgements

The authors heartily appreciate Professor Harold S. Park at Boston University for his insightful comments and suggestions in preparing this paper. In addition, this work is supported by the ARC Future Fellowship grant (FT100100172).

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