



Defect engineering, a path to make ultra-high strength low-dimensional nanostructures

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ABSTRACT

A current understanding is that materials with perfect structures have better mechanical properties. Thus, lowering the defect concentration, particularly by reducing the size of synthesized materials such as nanowires (NWs), is one of the key goals in the fabrication of new materials. In contrast, here we demonstrate the possibility of enhancing the mechanical properties of the low-dimensional nanostructures by engineering defects using the classical molecular dynamics technique. Our results show that NWs with high-density of I_1 stacking faults (I_1 -SFs) have higher Young's Module (up to 14% in compression) and critical stress (about 37% under compression) in comparison to the perfect structure over a wide range of temperatures. This enhancement is in agreement with the in-situ experimental measurements of highly defective NWs and is explained by the interplay between surface stresses and the stress field of immobile SFs. The overlap of SF-induced stresses in regions confined by SFs partially relaxes with increasing temperature, while it remains the main reason for this non-trivial strengthening. Furthermore, a unique stress relaxation mechanism, twin boundary formation, is revealed for highly defective NWs. The twin boundary formation postpones the phase transition and increases the resilience of the nanostructure over a wide range of temperatures, which results in a stress plateau in a highly defective NW and an increase in ductility. Defect engineering is demonstrated as a new route for synthesizing advanced materials with superior mechanical properties, and increasing their stiffness, strength, and ductility for applications under extreme environments.

1. Introduction

One-dimensional nanomaterials, nanotubes (NT), nanowires (NWs), nanorods (NRs), and nanobelts (NBs), are promising candidates for sensors [1], lasers [2], optoelectronics [3], and photocatalysts [4]. The response of these one-dimensional (1D) materials highly depends on the size, defect concentration, and structure. Therefore, to achieve the desired characteristics (e.g., electrical, mechanical, and optical), the growth condition should be controlled. There is a long-standing notion among researchers that the perfect structure is the ideal form of material in terms of mechanical properties, and intrinsic defects (e.g., point and planar defects) degrade the mechanical properties. So, defects have been treated as unwanted constituents that should be removed from the material or have their concentration reduced, e.g., by precise controlling of the growth process [5,6]. Here, our main goal is to understand the correlation between defect structure and properties in low-dimensional materials and seek a way to enhance mechanical performance of this class of materials by engineering inherent structural

defects. This will open up a new avenue for design materials with tunable properties and subsequently expand the design space.

The tuning of material properties by modifying defect concentration has recently attracted a great deal of attention in the research community. This topic is of great importance when one deals with nanostructured materials, because their response highly depends on the defect size, type, and concentration, e.g., doping the nanostructures with specific elements can change their electrical properties [7]. Furthermore, experimental [8] and numerical studies [9] show that the radiation tolerance of nanocrystalline SiC (nc-SiC) with a high density of SFs can be enhanced by an order of magnitude. A few experimental studies show that systematically introducing nano-twin boundaries in Cu [10] or stacking faults (SFs) [11,12] in GaAs NWs enhances the mechanical properties that can be achieved by precise control over the synthesizing process [13]. Also, introducing twins in Ag [14] and Ni [15] NW alters the deformation mechanism -i.e. plasticity and dislocation nucleation. Additionally, MD simulations confirmed this strengthening mechanism in SiC [16] and ZnO NWs [17] at $T = 0$ K and

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relatively low density of the SFs. These studies predicted the strengthening mechanism, although the stress relaxation mechanism is still unchanged; the stress drops due to the phase transition or fracture. This careful engineering of internal defects creates barriers for dislocation motion or phase transition and subsequently alters the physical properties of nanostructures. Despite the fact that manipulating internal defects, e.g., adding precipitates or grain refinement to enhance the yield strength, is a common method at the macroscale level, it has not been well-studied at the nanoscale level. It is worth mentioning that the strengthening methods in macroscale have their own setbacks, like a reduction in ductility [18] that can be overcome in nanoscale. However, on the other side of the spectrum, there is a long-standing notion that these defects are the root cause of structural weakening [19–24]; consequently, there is not a consensus on the exact effects of the defects on mechanical properties. Therefore, understanding the underlying physics opens a new avenue through which to predict, design, and fabricate a new class of one-dimensional materials with superior properties. Here, we showed that this enhancement in mechanical properties can be achieved over a wide temperature range, $T = 100\text{--}500\text{ K}$. Also, a new stress relaxation mechanism for ZnO NWs, twin formation, was predicted for high density of SFs, which is unprecedented.

2. Computational model

In order to study the potential strengthening mechanism in defect-engineered low-dimensional materials, ZnO NWs are chosen as the model material due to their technological importance [25–28]. The stable structure for ZnO NWs is Wurtzite (WZ) that consists of stacking ABABABAB; each letter corresponds to a layer including zinc and oxygen atom. The I_1 -SF is the most common planar defect in ZnO NWs [29], which changes the stacking sequence to ABAB|CBCB so that the fault is placed between layer B and C. This planar defect was frequently observed in synthesized NWs due to their low formation energy [30]. The I_1 -SF burger vector $R = (1/3)[01\bar{1}0] + (1/2)[0001]$ [29] can be generated by removing a layer from the perfect crystal and moving the other portion of NW by R . The schematic for faulted NW is shown in Fig. 1a.

Initially, the NW was relaxed for 500 ps at various simulation temperatures, $T = 100\text{--}500\text{ K}$, under NVE ensemble to equilibrate the energy. The relaxation time was chosen via an iterative process, ensuring that the stress fields of SFs are relaxed. A maximum temperature of 500 K is chosen that is smaller than $T_m/3 \approx 750\text{ K}$ to avoid the emergence of time-dependent behaviors such as creep. Then, the NPT ensemble with a Nose–Hoover thermostat was used for another 500 ps

to find the relaxed configuration. In the next stage, a constant strain rate of $\pm 0.1\text{ 1/ps}$, to avoid strain-rate dependent responses, was applied along the c -axis, $[0001]$, (Fig. 1a) to model the mechanical response of NW under tension/compression. The time step for all simulation cases was 1 fs. All of the simulated NWs have a diameter of 10 nm and are 40 nm in length. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [31] was employed for MD simulations. Various defect density was introduced in NW; the number of stacking faults varies between 2 and 26 that are separated with equal distances. In the bulk structure, SF is constrained between two partial dislocations and can glide over these partial dislocations [32], but due to the high surface-to-volume ratio of NWs, these planar defects are pinned at the external surfaces and are immobile. The radial distribution function test was performed on the WZ NW to find the lattice parameters; see Fig. 1b. The calculated c/a ratio is 1.55, which is close to the previous DFT calculations ($c/a = 1.6$) [33], MD simulations ($c/a = 1.57$) [33], and experimental measurements ($c/a = 1.606$) [34]. The difference between the obtained ratios is due to the size effect.

To ensure the validity of our simulations, the formation energy of I_1 -SF and the bulk Young's of WZ structure was calculated. At room temperature, Young's Modulus is 146 GPa, which is in agreement with experimental studies, $\approx 140\text{ GPa}$ [35]. Also, the formation energy is 14.1 meV/unit-cell area, which is close to the density functional theory calculations 15 meV/ (unit-cell area) [30]; the detailed calculation can be found in Refs. [17,36].

3. Results and discussion

The stress-strain curve for the perfect 1D-nanostructures follows a sawtooth pattern. The stress increases with increasing strain, and elastic energy gradually accumulates in the material until it reaches a critical value, i.e. critical stress [36–39]. At this point, the structure releases the elastic energy via a stress relaxation mechanism, e.g., dislocation nucleation/phase transition, which can be designated as a critical strain. The simulated stress-strain curves for a perfect and defective NWs with 2, 13, and 26 SFs are plotted in Figs. 2–5 for $T = 300\text{ K}$. Fig. 2 shows the response of a perfect NW under tensile/compression loading and the associated phase transition as a common stress relaxation mechanism in perfect ZnO NWs [33,36,39,40]. In compression, nucleation of hexagonal (HX) polymorph leads to a drop in stress (point P^{C2}), and nucleation of a body center tetragonal polymorph (BCT) (point P^{T2}) releases the stress in tension. The coordination analysis was performed to visualize the nucleation and propagation of new polymorphs (HX and BCT) during loading; see Fig. 2b–c. In a perfect NW, the nucleus of the new phase appears at the free surface due to the atoms at the surface

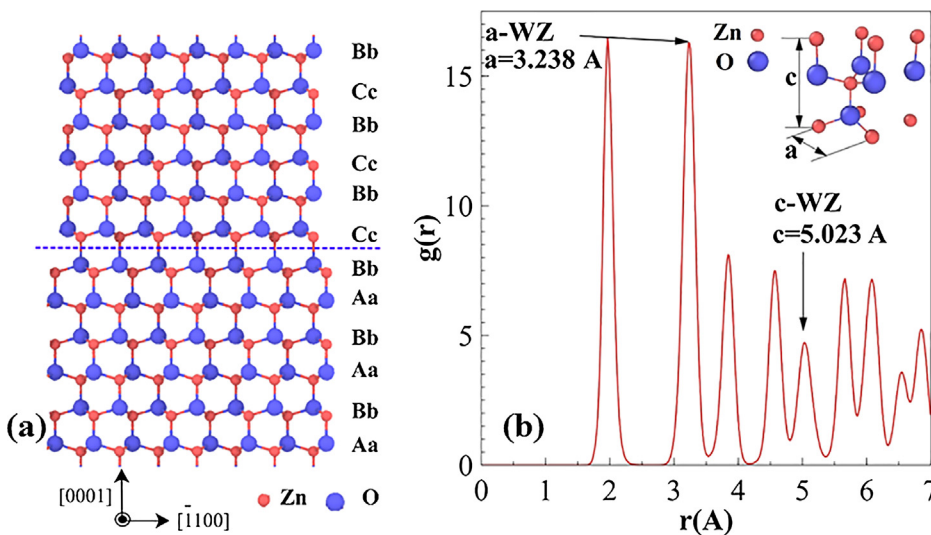


Fig. 1. (a) The I_1 -SF crystal structure. The dashed line shows the SF location along $[0001]$ direction, uppercase letter refers to Zn atoms, and lower case letter stands for O atoms. (b) Radial distribution function for the perfect NW at $T = 300\text{ K}$. The WZ lattice parameters, a and c , were identified on the graph. The WZ unit cell and lattice parameters were shown in the graph inset.

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