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Orientation- and microstructure-dependent deformation in metal nanowires under bending

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Abstract

Device miniaturization requires the bending of nanowires (NWs) on the nanoscale. To explore the mechanical behavior the mechanisms of plastic deformation of nickel nanowires of different orientations, sizes and twin structures under bending were investigated by means of molecular dynamics simulation. We show that plastic deformation can be either homogeneous or heterogeneous, depending on the NW orientation. Bending $\langle 1\,2\,1\rangle$ oriented NW leads to homogeneous plastic flow, attributed to the large capacity for storage of axial extended dislocations (AEDs). AEDs are formed by constriction and cross-slip of inclined extended dislocations to the neutral $(1\,1\,1)$ planes. The stacking of AEDs forms new defect structures, such as micro-twins and small hcp embryos. More localized deformation appears in NWs with $\langle 1\,1\,1\rangle$ and $\langle 0\,1\,0\rangle$ orientations at large bending angles, which is mainly caused by the pile-up and escape of inclined dislocations. The mechanical behavior of NWs is altered by introducing preset nano-twins,. The strength increases monotonically as the twin boundary spacing decreases. Among the three orientations the $\langle 1\,2\,1\rangle$ oriented NWs with twin structure have been demonstrated to possess both high strength and ductility. A theoretical model based on geometrically necessary dislocations is proposed to quantify the contribution of various defects to the plastic deformation under bending, which links the continuum theory and atomistic simulations.

Keywords: Nanowire; Dislocation; Plasticity; Molecular dynamics simulation; Geometrically necessary dislocations

1. Introduction

Metallic nanostructures, such as thin metal films [1], grooves [2], and nanowires [3–10], have been widely investigated as guides of surface plasmon polaritons in nano-photonic devices due to the efficiency of high field localization on the nanoscale. Among the various types of nanostructures metallic nanowires (NWs) are promising candidates due to their high crystallinity and smooth surfaces. Bending NWs into highly curved shapes is desirable for accommodating these wires into nanoscale circuits. The bending strength and plasticity of NWs on the nanometer scale are also of great interest as they relate to the reliability and manufacturability of flexible electronics [11–14] and piezoelectric nanogenerators [15–17]. Tremendous effort has been put into understanding the underlying atomistic mechanisms in tensile and compressive deformation. Surprisingly, little is known about NW behavior under bending. Preliminary works indicated a size effect on the elastic limit and incipient plasticity of metallic NWs under bending [18–23]. It has been found that surface stress and surface energy contribute to the size-dependent elastic properties of gold NWs upon bending deformation [21]. Fivefold deformation twins were detected at the onset of bending plasticity on the tensile surface of square cross-section copper NWs with hollow cores [22]. To date the deformation mechanisms in NWs under bending have not been investigated, either by simulation or experiment.

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In this work we use a computational approach to determine the atomistic mechanisms and mechanical behavior of bending plasticity of both single crystalline and nano-twinned nickel NWs of different sizes and orientations. Among all the factors, NW orientation has the most significant effect on the mechanical behavior. For ⟨1 2 1⟩ oriented NWs homogeneous plastic flow has been observed in both single crystal and nano-twinned structures, as a consequence of the large capacity for dislocation storage. The primary deformation modes are dislocation constriction and cross-slip, in contrast to their tensile behavior. More localized deformation develops in NWs with ⟨1 1 1⟩ and ⟨0 1 0⟩ orientations at large bending angles, which is mainly caused by the pile-up and the escape of inclined dislocations. A theoretical model based on geometrically necessary dislocations (GNDs), is proposed to correlate the dislocation density with the non-recoverable curvature. The consistency between the model and simulations validates the application of continuum theory down to the atomic scale.

2. Method

A parallel molecular dynamics (MD) scheme, an improvement on the LAMMPS package [24] (http://lammps.sandia.gov), is used for the simulation and visualized using Visual Molecular Dynamics code [25]. The embedded atom method (EAM) potential, developed by Daw and Baskes [26,27], is used to model the interactions between nickel atoms [28,29]. The EAM potential correctly predicts the basic properties (Table 1), including lattice constants, elastic modulus and the stacking fault energy, which are important factors in determining both the mechanical response and the defect structures. The ambient temperature remained 300 K during the whole simulation employing the Nose–Hoover thermostat [30–32]. All atoms were equilibrated for 200 ps before loading. The MD time step was fixed at 1 fs.

Fig. 1 shows the loading scheme. The bending deformation is realized by rotating two pairs of rigid body regions ((a, b) and (c, d) in Fig. 1) at both ends with the same angular velocity of $0.01°\ ps^{-1}$ around their centers A and B, respectively. The distance between two neighboring rigid body regions is allowed to freely adjust. In this way only the bending moments are transferred to the NW, in contrast to bending deformation by axial buckling or by three point bending [23,33]. We considered square cross-sectional NWs with three different axial orientations, including ⟨1 2 1⟩, ⟨1 1 1⟩ and ⟨0 1 0⟩, as synthesized in Tian et al. [34], Wang et al. [35], and Florian et al. [36]. The lateral (D) and longitudinal (L) dimensions were taken to be 5×50 nm and 10×100 nm, termed D5L50 and D10L100, respectively. As a comparison, nano-twins were introduced into NWs by inserting multiple {1 1 1} twin boundaries (TBs). The TBs were parallel to the axial direction of ⟨1 2 1⟩ oriented NWs and perpendicular to that of ⟨1 1 1⟩ oriented NWs. The nominal surface strain rates were $\sim 1.7 \times 10^7\ s^{-1}$ for both D5L50 and D10L100 NWs, which is much lower than most reported MD simulations (generally 10^7–$10^9\ s^{-1}$). Such a strain rate has been confirmed to be useful in MD simulations for understanding plasticity in metallic nano-structures [37]. Severe plastic deformation was introduced by bending NWs to large angles. The long simulation duration (8 ns) ensures the exhibition of all mechanisms.

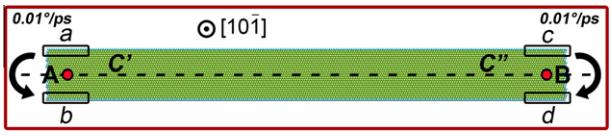

Fig. 1. Loading scheme for bending of nickel NWs. Two pairs of rigid body regions ((a, b) and (c, d)) at both ends rotate with an equal angular velocity of 0.01° per ps around their centers A and B. The rigid translation is removed by keeping the line AB horizontal.

Table 1
A comparison of the calculated properties using EAM potentials with the experimental or DFT data.

	Experiment or DFT	EAM potential used in this work
Lattice constant a (Å)	3.52 [46]	3.52
Elastic constants (10^{11} Pa)		
c_{11}	2.47 [47]	2.47
c_{12}	1.47 [47]	1.48
c_{44}	1.25 [47]	1.25
Stacking fault energy ($mJ\ m^{-2}$)		
γ_{SF}	125 [48]	125
γ_{us}	350 [49]	366

Defects are identified by coloring atoms according to the local crystalline order method [38,39], which examines both the atom type and the coordination number by topological analysis. Atoms having fcc stacking are colored green. Atoms having a local hcp stacking order are identified as a stacking fault and colored blue. Both fcc and hcp atoms have a coordination number of 12. Pink atoms, located at dislocation cores, have the same coordination number 12, but different atomic arrangements from hcp and fcc. Blue atoms have a coordination number other than 12 and are generally identified in the vicinity of vacancies or free boundaries.

3. Results and discussion

3.1. Mechanical response under bending

Fig. 2 plots the loading curves of D5L50 NWs with orientations of ⟨1 2 1⟩, ⟨1 1 1⟩ and ⟨0 1 0⟩ under bending. Incipient plasticity occurs at different yield strains, indicating a close relation of plastic deformation to orientation. In the plastic deformation region homogeneous flow is only observed in ⟨1 2 1⟩ oriented NWs. Mechanical instability, as indicated by violent oscillations in the curves, indicates the discrete nature of plasticity on the nano scale. Detailed mechanisms are analyzed in the following sections.