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Molecular dynamics study of the mechanical behavior of nickel nanowire: Strain rate effects

Yu-Hua Wen [a,b], Zi-Zhong Zhu [a,*], Ru-Zeng Zhu [b]

[a] Department of Physics, and Institute of Theoretical Physics and Astrophysics, Xiamen University, Xiamen 361005, China
[b] LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

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Abstract

We present the analysis of uniaxial deformation of nickel nanowires using molecular dynamics simulations, and address the strain rate effects on mechanical responses and deformation behavior. The applied strain rate is ranging from 1×10^{8} s^{-1} to 1.4×10^{11} s^{-1}. The results show that two critical strain rates, i.e., 5×10^{9} s^{-1} and 8×10^{10} s^{-1}, are observed to play a pivotal role in switching between plastic deformation modes. At strain rate below 5×10^{9} s^{-1}, Ni nanowire maintains its crystalline structure with neck occurring at the end of loading, and the plastic deformation is characterized by {1 1 1} slippages associated with Shockley partial dislocations and rearrangements of atoms close to necking region. At strain rate above 8×10^{10} s^{-1}, Ni nanowire transforms from a fcc crystal into a completely amorphous state once beyond the yield point, and hereafter it deforms uniformly without obvious necking until the end of simulation. For strain rate between 5×10^{9} s^{-1} and 8×10^{10} s^{-1}, only part of the nanowire exhibits amorphous state after yielding while the other part remains crystalline state. Both the {1 1 1} slippages in ordered region and homogenous deformation in amorphous region contribute to the plastic deformation.

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1. Introduction

In the past decade, nanometer-sized structures have attracted a great deal of interests due to its unique mechanical, electronic, optical, and magnetic properties, opening up a broad view of applications [1,2]. As one of the most important one-dimensional (1-D) nanostructures, metallic nanowires have been expected to play an important role in future electronic, optical and nanoelectromechanical devices. Metallic nanowires have been also employed as catalysis, superconductor, nanopipette probes, and reinforcing fibers in high-strength/light-weight composite materials, etc. [3–8].

Characterization of mechanical properties of nanowires is an increasingly important area of materials science, not only from scientific interests, but also from implications for constructing materials with specific mechanical properties. However, this work is a challenge to existing testing and measuring techniques because of the tiny dimension of a nanowire making the manipulation rather difficult [9,10]. In recent years, the mechanical deformation of nanowires have been studied by molecular dynamics simulations using either embodied-atom-method (EAM) [11–15] or effective-medium theory (EMT) [16] as well as first-principles method based on density functional theory (DFT) [17–20]. These studies focus on investigations of the structural transformation under uniaxial strain, stress–strain relationship, the conductance, and the correlation of the force (associated with the changes in the bonding of nanowires). Many studies have been dedicated to

* Corresponding author. Tel.: +86 592 2182248; fax: +86 592 2189426.
E-mail addresses: yhwen@xmu.edu.cn (Y.-H. Wen), zzhu@xmu.edu.cn (Z.-Z. Zhu).

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ascertaining the properties of gold nanowires, and show that the Au nanowires, before breaking under tensile stress, can get as thin as one-atom chains, and as long as five suspended atoms [17,20,21]. Nickel nanowires show superplastic behavior at lower strain rates, while at sufficiently high strain rates, it can transform continuously to an amorphous metal at constant temperature [12–14,22]. Recently, shape memory effect (SME) and pseudoelastic behavior are observed in Cu and Ag nanowires in molecular dynamics simulations [23–25]. Some works also investigate temperature, size and strain-rate effects on the axial elongation and transverse shear behavior of copper nanowires [26–29].

Because of the unique properties of metallic nanowires, they are important in next-generation structural materials, biosensors and future nanoscale devices. It is necessary to develop a quantitative understanding of the mechanical and structural properties of such metallic nanowires. Although much research had been done to quantify the mechanical behavior of metallic nanowires, few have been dedicated to the study of strain rate effects on the mechanical properties of metallic nanowires. In this paper, we will address these effects by using molecular dynamics calculations to simulate the uniaxial tensile mechanical deformation of metallic nanowire, and investigating the structural evolution of the mechanical deformation process. Details of the MD simulation are presented in the following section. We present a brief discussion of the MD results and comparison with other results in Section 3. The main conclusions are summarized in Section 4.

2. Potential model and simulation methods

In this work, MD simulations have been performed with the quantum corrected Sutten–Chen (Q-SC) type many-body force field modified by Kimura et al. [30] in which the parameters were optimized to describe the lattice parameter, cohesive energy, bulk modulus, elastic constants, phonon dispersion, vacancy formation energy, and surface energy, leading to an accurate description of many properties of metals and their alloys [31,32]. For the SC type force field, the total potential energy for a system of atoms can be written as

$$U = \sum_{i}^{N} U_i = \sum_{i}^{N} \lambda \left[\frac{1}{2} \sum_{j \neq i}^{N} V(R_{ij}) - c\sqrt{\rho_i} \right]. \quad (1)$$

Here $V(R_{ij})$ is a pair interaction function defined by the following equation:

$$V(R_{ij}) = \left(\frac{a}{R_{ij}} \right)^n, \quad (2)$$

accounting for the repulsion between the i and j atomic cores; ρ_i is a local electron density accounting for cohesion associated with atom i defined by

$$\rho_i = \sum_{j \neq i}^{N} \phi(R_{ij}) = \sum_{j \neq i}^{N} \left(\frac{a}{R_{ij}} \right)^m. \quad (3)$$

In Eqs. (1)–(3), R_{ij} is the distance between atoms i and j, a is a length parameter scaling all spacings (leading to dimensionless V and ρ); c is a dimensionless parameter scaling the attractive terms; λ sets the overall energy scale; n and m are integer parameters such that $n > m$. Given the exponents (n, m), c is determined by the equilibrium lattice parameter, and λ is determined by the total cohesive energy. The Q-SC potentials have already been used to study structural transitions between various phases of Ni, Cu and other face-centered-cubic (fcc) metals [13,26,33]. For the Q-SC type potential of Ni, the parameters are given as follows: $n = 10$, $m = 5$, $\lambda = 7.3767$ meV, $c = 84.745$, and $a = 3.5157$ Å.

The initial geometry of Ni nanowire is constructed from a large cubic fcc single crystal of nickel using certain cylindrical cutoff radii centered at a cubic interstitial site, in which the crystallographic orientations in the X-, Y- and Z-axis are taken to be in the directions of [1 0 0], [0 1 0], and [0 0 1], respectively. In the X and Y directions, the Ni nanowire spans a finite number of unit cells, while in the Z-direction an infinite wire was obtained by applying the periodic boundary condition. In the present paper, the diameter of the nanowire is 2.53 nm (~7.2 fcc unit cells), and the length of the nanowire as constructed is initially 24.61 nm (~70 fcc unit cells in z-direction), forming a 11 270-atom nickel nanowire. The wire was first thermally relaxed by running 50 000 steps with a time step of 1 fs in order to eliminate unfavorable configurations. During the relaxation process, the temperature is kept constant at 300 K based on Nose–Hoover thermostat [34], and the diameter and length of the nanowire are allowed to shrink (or expand) at zero press based on the Berendsen approach [35]. After relaxation, the diameter expands to ~2.592 nm, and the length contracts to ~24.035 nm. The contraction in axial direction and expansion in radial directions are attributed to surface relaxation phenomenon, in which lost symmetry of surface atoms results in surface tension under initial state. The nanowire contraction due to surface tension effect is determined by allowing the initial nanowire to relax to a zero stress state [29].

We have simulated the uniaxial deformation process of Ni nanowire, and emphasized the strain rate effects. The uniaxial tensile deformation of the nanowire is simulated at room temperature (300 K) and constant strain rate in which the length (in the Z-direction) of the nanowire is increased gradually. Different strain rates, from 1.0×10^8 s^{-1} to 1.4×10^{11} s^{-1}, are applied on the nanowire to study their effects on the deformation mechanism. It should be emphasized that the loading process of the tensile strain is different from those described in Refs. [12,13], where the tensile strain was applied with increment of 0.5% (or 0.4%) in its total length after some time steps. In the present work, the tensile strain in each time step along Z-direction is increased by $\Delta\varepsilon_z = \dot{\varepsilon}\Delta t$, where Δt is the time step, and $\dot{\varepsilon}$ the strain rate. During the deformation process, the temperature is kept constant based on Nose–Hoover chain dynamics [34], and the diameter of the nanowire is