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The fracture stabilities of ultrathin gold nanowires

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ABSTRACT

The fracture and corresponding failure of ultrathin gold nanowires have attracted much attention due to its applicable reliability of nanoelectromechanical devices, so understanding the fracture stability is critical especially when the width reduces to ultrathin scale. Here, we studied the fracture stabilities of ultrathin gold nanowires subjected to uniaxial tension. The statistical mechanical properties show that the stabilities result from size effects, in which, the width of 4.5*a* ("*a*" means lattice constant, 0.408 nm for gold) is shown as a critical and transitional size. Less than 4.5*a*, the strong mechanical strength is obviously unstable, attributing to surface dislocation nucleation; Larger than 4.5*a*, the mechanical stabilities have been enhanced. However, the fracture stabilities are demonstrated to be extrinsic at large sizes because of the dominated action of small aspect ratios. With macro-broken position distributions at the effects of sizes and atomic vacancies, the intrinsic and extrinsic fracture stabilities are further found to be related with the damaged degrees of crystalline lattices and propagated styles of the tensile waves. Lastly, the atomic vacancy sensitivities show the extrinsic fracture stabilities of large sizes are from a competition of bulk atoms and the strong shock induced by small aspect ratio.

1. Introduction

Ultrathin metallic nanowires are of great interest for nano-engineering as well as for nanotechnology owing to their special mechanical, thermal and electrical properties [1–3]. In applications ranging from electronics, nanoconnectors and active components of nanoelectromechanical system [4], a stringent control of deformation and fracture is critical to insure the reliability of ultrathin metallic nanowires. It is, therefore, significant that how to manipulate the mechanical stabilities and to control the failure of ultrathin metallic nanowires. However, comprehensive realization of ultrathin metallic nanowires in nanoelectromechanical devices requires a reliable study of their deformation fracture behaviors and corresponding fracture stabilities. As proposed by Hemker [5], the functionality and reliability of emerging nanoscale devices were closely tied to constructed nanocrystalline materials, whose reliability should be based on good understanding of the operative deformation. Detecting the deformation fracture of ultrathin metallic nanowires usually applies experimental means of atomic force microscopy (AFM), high resolution transmission electron microscopy (HRTEM) and mechanically controllable break junctions (MCBJ) [1,6,7]. However, the tendencies of shrinking critical sizes to develop high performance of devices have brought some difficulties that seriously hinder their observing at such small scales [5]. Especially, the existences of some defects such as

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grain boundary, amorphous and atomic vacancies could induce the moving uncertainties of crystalline enhancing the difficulty of observing the fracture failure [8].

In contrast, molecular dynamics (MD) simulation, which solves Newton's equation of motion by collecting interacted atoms over a number of time steps [9,10], is a reliable and effective method to study the crystalline stabilities and corresponding properties of metallic nanowires. Under effects of sizes and defects, the fracture and mechanical stabilities of metallic nanowires have been studied with MD simulations. For the influence of sizes on ultrathin gold nanowires, wrinkling of atomic planes in ultrathin Au nanowires showed the bulk suffered strain in order to balance the surface stress owing to surface effects [11]. The unexpected brittle-like fracture of ultrathin gold nanowire was tied to shear-induced twin structures, confirming the experimentally observed difference of surface dislocation nucleation [1]. Ductile-to-brittle crystalline could be provoked at a critical size (2.8 nm) of ultrahigh density twins of gold nanowires, inducing brittle-like materials with near-ideal strength [12]. Subjected to unixial tension, the nanowire width 2.0 nm was also found to be a transitional and critical size for mechanical stabilities of ultrathin gold nanowires [13]. At such small nanoscale, structural imperfection could increase atomic potential energy and facilitate crystalline slip under critical stress [14]. Due to the instability of crystalline, the irreversible plastic response also rapidly appeared in decreasing sizes of ultrathin gold nanowire, taking along the enhanced mechanical strength [15]. With instabilities of nanoscale materials, the sensitivities of atomic vacancies on the fracture of gold nanowires were proved to be based on a competition between vacancy ratios and deformed crystalline states at different strain rates, sizes and temperatures [16–18]. For ultrathin gold nanowires as activate components of nanoscale devices, one appearing problem is which factors dominate the mechanical fracture stabilities of such small-sized nanowires, and how to maintain the material reliability. To make devices applicable and avoid the material failure, the stabilities of ultrathin metallic nanowires should be considered in advance.

Considering the intrinsic instability of nanoscale materials, different initial equilibrium states induced by different relaxing loops are designed to investigate statistically the fracture stabilities of ultrathin gold nanowires. A parallel series of sizes are compared to reveal the critical dimensions of dominating the fracture reliability of gold nanowires. In this study, the fracture stability further shows that, 1) the size dependence is not only from different heights or widths [13,18], but also from the ratio of structural dimensions and a strong competition between sizes and mechanical tension; 2) Correspondingly, the intrinsic and extrinsic characters of fracture stabilities have been shown under size effects, which are different from the previous study that the large-sized characters are always stable [18]; 3) With macro-broken position distributions of ultrathin gold nanowires, we further found that such intrinsic and extrinsic fracture stabilities are related with the damaged degrees of crystalline lattices and different propagated styles of the tensile waves.

2. Methodology

MD simulations were performed to investigate the tensile deformation behaviors and mechanical stabilities of ultrathin gold nanowires at different sizes and atomic vacancy ratios. As shown in Fig. 1a, the geometric model of the gold nanowire was generated along the [100] crystallographic orientations. In this study, the structural dimension of the gold nanowire was set as $Wa \times Wa \times 15a$ ($Wa \times Wa$ is the cross section, Wa stands for the width of the nanowire, and a stands for lattice constant, 0.408 nm for gold.), and the width of the nanowire varied from $3a$ (1.224 nm) to $12a$ (4.896 nm). According to the theoretical and experimental testing that 2 nm diameter of the gold nanowire is critical to its mechanical behavior and suitability as interconnects [18,19], the size regions from $3.5a$ (1.4 nm) to $4.5a$ (1.8 nm) and $5.0a$ (2.0 nm) were especially considered in this study. In addition, to compare the influence of structural dimensions on mechanical stabilities of gold nanowires, Model A ($Wa \times Wa \times 15a$) was parallel compared with Model B ($Wa \times Wa \times 3Wa$) [13]. For Model A in Fig. 1a, both ends with three lattices were set as fixed layers, and the middle region was the thermal controlled layers of the gold nanowire. Under zero traction (xy-plane) and zero stress (z-direction), the gold nanowires were firstly relaxed to quasi-equilibrium states, according with the stable recorded average potential energy per atom of the nanowire. From radial distribution function (RDF) of Fig. 1a, different sizes obviously showed different crystalline degrees before stretching of gold nanowires. Upon stretching, the uniaxial tension along z-direction was performed via moving two fixed layers, and the tensile strain rate was 1.00% ps^{-1} [16]. Considering nanoscale unstable deformation characters of ultrathin gold nanowires, enough and different initial equilibrium states were chose to statistically analyze the deformation, fracture and mechanical properties. Here, the most probable broken position (MPBP) or most probable broken positions (MPBPs) were got from broken position distributions of ultrathin gold nanowires. According to the MPBP and MPBPs at different sizes, atomic vacancies were both set in the middle part of the gold nanowire. For example, the MPBPs of the size ($4a \times 4a \times 15a$) showed a transitional and unstable distribution, and the size ($10a \times 10a \times 15a$) showed a middle fracture distribution with a stable style. To study the vacancy sensitivities on broken styles, atomic vacancies were both set around the middle single-layer crystalline plane (0.5, the normalized length) at two selected typical sizes, and two fixed layers were considered as around 0.0 and 1.0 of the normalized length. The vacancy ratio was the one between atomic vacancies and all atoms in a single-layer crystalline plane. As shown in Fig. 1b and c, atomic vacancies were in a scattered, but uniformed distribution. The ratios were from 3% to 25% at the size ($4a \times 4a \times 15a$), and it was from 0.5% to 25% at the size ($10a \times 10a \times 15a$). The ratios of 3% and 0.5% corresponded to one atomic vacancy at two different sizes, respectively. Table 1 showed the detailed conditions of ultrathin gold nanowires (Model A).

With the software NanoMD [20], ultrathin gold nanowires subjected to uniaxial tension were calculated by moving two fixed crystalline layers uniformly in z-direction. Under the free boundary condition, the motion equation integrations of velocity and trajectories of atoms were performed with the Verlet leapfrog algorithm. Nośe-Hoover thermostat [21–23] as a

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