

Modeling and Simulations of Tubular Nanowires

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ABSTRACT

Here, we present theoretical investigations on tubular nanowires. In order to have a better understanding of the physical properties of the nanowires in different sizes and to have a better comparison with the other nanowire forms a systematic study is performed. Atomic models of tubular aluminum nanowires in different radii and thickness are created. To obtain typical atomic structures of the tubes, molecular dynamics (MD) simulation method is used and annealing - quenching simulations are performed. For tubes in large diameters, periodic boundary conditions are modified and angular boundary conditions are used. An important question related with the tubular nanowires is their structural stability. Energetics and stability of these nanowires and their dependence on the radius and thickness are studied.

Keywords: Nanowires, Coating, Molecular Dynamics

1 INTRODUCTION

Metallic nanowires have attracted great interest due to their interesting low-dimensional physics and due to possible future technological applications. Nanowires and contacts having radius in the range of the Fermi wavelength λ_F have been fabricated and have shown novel electronic and mechanical properties [1-3]. Ultrathin nanowires suspended between two metal electrodes have been produced [4-9]. Previous theoretical investigations include studies on quantum point contacts [10-13] as well as the structural, vibrational and electronic properties of metallic nanowires [14-17]. Most of these investigations were related with atomic scale nanowires. Recently, metallic tubular nanowires (nanotubes or tubes) in different radii and lengths were created using physical vapor deposition techniques. Polymeric nanofibers were coated with aluminum and then the polymer cores were removed that leaved tubular nanowires of coating material [18]. The smallest inner radii were around 10 nm and the approximate thickness of the tubes was controlled by the sputtering process. The tubes did not collapsed after the removal of the polymer core. Beside these tubular nanowires, epitaxial core-shell nanowire heterostructures [19] and single-walled nanotube (SWNT) coatings with tin oxide [20] or different

metallic nanoparticles such as Au, Ti, Ni Pd, Al were reported [21-23].

Here, we present theoretical investigations on the structural properties of the tubular aluminum nanowires. In order to have a better understanding of the properties of the nanowires in different sizes and to have a better comparison with the other nanowire forms a systematic study is performed. Atomic models of tubular aluminum nanowires in different diameters and thickness are created. To obtain typical structures, molecular dynamics (MD) simulation method is used and annealing - quenching simulations are performed. For tubular nanowires in large diameters, periodic boundary conditions are modified. An important question related with the tubular nanowires is their structural stability. Energetics and stability of these nanowires and their dependence on the diameter and thickness are studied. In section two, the details of the models are given. Section three is for the presentation of the results on the structure and stability of the tubes and it is followed by our conclusions in section four.

2 MODEL

Atomistic simulations, which provide the methodologies for detailed microscopic modeling, are powerful and widely used tools in physics, chemistry and materials science. Directly from the atomic nature of the system, they offer prediction of mechanical and electronic properties of materials. In order to study the structural properties of tubular aluminum nanowires, an atomic model of a slice or angular region of the tube is created. A well-tested state-of-the art embedded-atom-type interaction potential [24] is used for the Al-Al atom interactions. As the radii of the tubes can be quite large, angular portions of tubes in larger diameters are simulated using modified periodic boundary conditions. For atomic displacements perpendicular to the axis of the tubes, angular boundary conditions are used. On the other side, regular periodic boundary conditions are employed for the atomic displacements along the axis of the tubes. Thus, the tubes were modeled as if they are perfectly cylindrical and infinitely long. Then, molecular dynamics simulations were performed and structures are relaxed at different constant temperature ranging from 100 K to 300 K using velocity scaling algorithm. The time steps are taken as 2.0 fs. In addition, to obtain typical atomic structures, annealing and quenching simulations are performed.

3 RESULTS AND DISCUSSION

In order to simulate tubular aluminum nanowires that have similar geometrical features with the experiments [18], tubes that have 10-25 nm radii and 1-5nm thicknesses are selected. In figure 1, atomic structure of a tube in 17 nm radius and in 5 nm thickness is shown. The simulation cell includes a 30° portion of the tube that contains 6112 atoms. The initial structure is created from an fcc Al crystal structure with (111) surface facing radially outwards. The positions of the atoms that are in a certain radial distance interval to the tube's axis (in 0.5 nm shell) are fixed. As it can be seen in the figure, the tube's structure can be considered as a poly-crystalline nanostructure. After relaxing the tube's atomic structure at constant $T=100\text{K}$ and 300K temperatures, we found that the tube preserved its shape and only the atoms in or close to the boundary regions had significant displacements. Further increasing temperature of the structure to 500K did not alter this result.

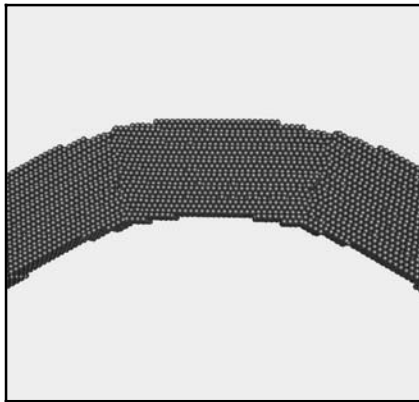


Figure 1: Top view of a region of an aluminum tube with radius 17 nm and thickness 5 nm after equilibration at $T=100\text{K}$.

In order to investigate the structural stability of these tubular nanowires a systematic simulation study is performed. Atomic structures of the tubes in different radii and thickness are equilibrated at $T=100\text{K}$. When the inner shells of the tubes are kept rigid, the structures of the tubes preserved their selves and only relatively small atomic displacements were observed. This simulation case corresponds to the existence of support for the thinner tubes such as nanofibers at the core region or it corresponds to the relaxation of only outer surfaces or shells of thicker tubular structures. On the other side, when all the atoms of the tubes were relaxed, significant structural changes occurred especially in the case of thinner tubes with thickness less than 2.5 nm (for 17 nm radius).

Calculation and analysis of potential energy of nanostructures provide important information related with the nanostructures' stability. In figure 2, variation of

potential energy of the tubes as functions of tube thickness and radius are shown. In these calculations, the atoms in the inner 0.5 nm shell of the tubes were fixed and the rest of the atoms were allowed to move. After equilibration of the atomic structures, further MD simulation runs were performed and average atomic potential energy values were obtained. As it can be seen in figure 2(a), for a fixed tube radius (17 nm), average potential energy of the atoms decreases with the increase of the tube thickness. This is directly related with the surface to volume ratio of these tubular nanostructures. Relaxing both inner and outer surfaces of the tubes resulted with relatively lower potential energy values due to significant deformations in the case of thinner tubes. In figure 2(b), average potential energy values of the atoms as a function of tube's radius is shown for constant tube thickness of 3.0 nm. As the tube's radius increases, the average potential per atom is found to be decreasing, however, to have a better understanding of the overall variation of potential energy of the tubes with radius, a more systematic study is required and the two limiting cases (solid cylinder and completely flat slab) must be taken into account.

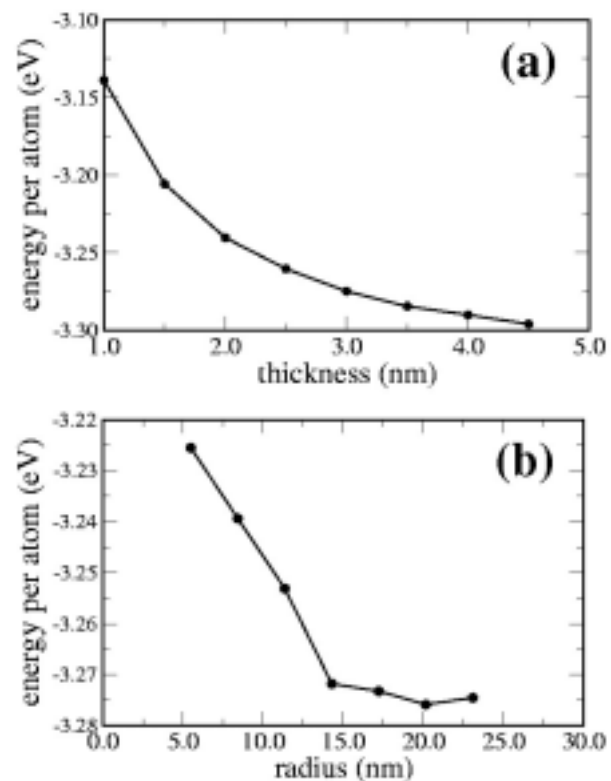


Figure 2: (a) Average potential energy per atom as a function of tube's thickness for a fixed radius of 17 nm. (b) Average potential energy per atom vs. tube's radius for a fixed tube thickness of 3.0 nm.

Transmission electron microscope (TEM) images of tubular nanowires observed in the experiments showed that the surfaces of the tubes may not be smooth and may

contain islands or asperities depending on growth conditions [18]. To study the energetics of the tubes with asperities, two atomic models of tubes with the same inner radii (17nm) and the number of atoms (7364 atoms in 30° region) are created. One of the models contains a pyramidal asperity that has 364 asperity atoms and 2.6 nm height. In the other model, the asperity atoms are distributed on the

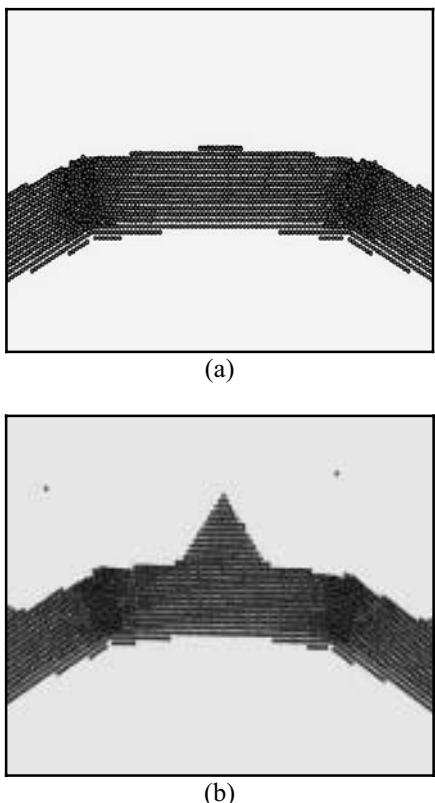


Figure 3: Top views of tubular nanowires (a) without asperities and (b) with asperities. Both structures contain same number of atoms and relaxed at constant T=300 K temperature.

outer surface of the tube. Both structures are equilibrated at constant T=300 K temperature. In figure 3, the top views of the tubes' atomic structures are shown. It is found that the potential energy difference between two structures is 59 eV and the energy of the structure with no asperity is lower. Thus, smooth tube surfaces are energetically more favorable. On the other side, asperities or islands that are grown may exist depending on their sizes, as their atoms may not diffuse on the tubes' surfaces at relatively low temperatures.

4 CONCLUSIONS

Theoretical investigations on tubular nanowires are presented. In order to have a better understanding of the physical properties of the nanowires in different sizes and to have a better comparison with the other nanowire forms a systematic study is performed. To obtain typical structures, molecular dynamics (MD) simulation method is used and annealing - quenching simulations are performed. For tubular nanowires in large diameters, periodic boundary conditions are modified. Energetics and stability of these tubes and their dependence on the radius and thickness are studied. It is found that, as increase in tubes' radius or thickness results with decrease in the potential energy. Although they were observed in TEM images, islands or asperities on the surface of the tubes are not energetically favorable.

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