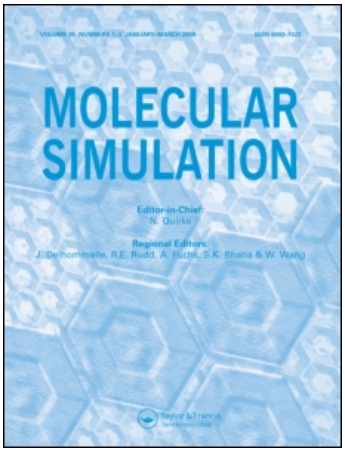

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G. Bilalbegovic[a]
[a] Department of Physics, University of Rijeka, Rijeka, Croatia

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MULTISHELLED GOLD NANOWIRES

G. BILALBEGOVIC*

Department of Physics, University of Rijeka,
Omladinska 14, 51 000 Rijeka, Croatia

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The current miniaturization of electronic devices raises many questions about the properties of various materials at nanometre-scales. Recent molecular dynamics computer simulations have shown that small finite nanowires of gold exist as multishelled structures of lasting stability. These classical simulations are based on a well-tested embedded atom potential. Molecular dynamics simulation studies of metallic nanowires should help in developing methods for their fabrication, such as electron-beam litography and scanning tunneling microscopy.

Keywords: Molecular dynamics simulation; nanowires; gold; embedded-atom potential; metals

INTRODUCTION

One-dimensional and quasi one-dimensional metallic structures are often used in various electronic devices. Wires of nanometre diameters and micrometre lengths are produced and studied for some time. Recent advances in experimental techniques, such as Scanning Tunneling Microscopy (STM) [1, 2] and electron-beam litography [3], are giving rise to fabrication of wires with nanometre lengths. Many important results were recently obtained for nanowires of different materials. For example, multishelled nanostructures were found in experiments for carbon [4], WS_2 [5], MoS_2 [6] and $NiCl_2$ [7]. In the jellium model calculation multishelled structures were obtained for sodium nanowires [8].

The results of Molecular Dynamics (MD) simulation [9] have shown that a gold wire with length 4 nm and radius of 0.9 nm, at $T = 300$ K,

*e-mail: goranka@phy.hr

consists of the three coaxial cylindrical shells and the thin core. Here we present an analysis of two additional multiwalled gold nanowires. We also propose that unusual strands of gold atoms recently formed in STM and observed by a transmission electron microscope (TEM) [1] are the image of cylindrical walls of multishelled gold nanowires. An explanation of the thinning process for the STM supported multishelled gold nanowires is given.

METHOD

To simulate metals by the classical MD method one should use many-body potentials. Several implementations of these potentials are available, as for example ones developed within the embedded-atom and effective medium theories [10]. Gold nanowires were simulated using the glue realization of the embedded atom potentials [11]. This potential is well-tested and produces a good agreement with diversity of experimental results for bulk, surfaces, and clusters. In contrast to most other potentials, it reproduces different reconstructions on all low-index gold surfaces [11]. Therefore, it is expected that simulated gold nanowires of more than ~ 50 atoms realistically model natural structures. A time step of 7.14×10^{-15} s was employed in simulation. The temperature was controlled by rescaling particle velocities.

We started from ideal face centered cubic nanowires with the (111) oriented cross-section at $T = 0$ K, and included in the cylindrical MD boxes all particles whose distance from the nanowire axis was smaller than 1.2 nm for the first nanowire, and 0.9 nm for the second one. The initial lengths of nanowires were 6 and 12 layers, whereas the number of atoms were 689 and 784. The samples were first relaxed, then annealed and quenched. To prevent melting and collapse into a drop, instead of usual heating to 1000 K used in MD simulation of gold nanostructures, our finite nanowires were heated only to 600 K. Such a procedure gives the atoms a possibility to find local minima and models a constrained dynamical evolution present in fabricated nanowires. The structures were analyzed after a long MD run at $T = 300$ K.

RESULTS AND DISCUSSION

Figure 1 shows the shape of the MD box for a nanowire of 784 atoms after 7.1 ns of simulation at $T = 300$ K.

Top views of the particle trajectories in the whole MD boxes for two nanowires are shown in Figures 2 and 3. While the presence of a

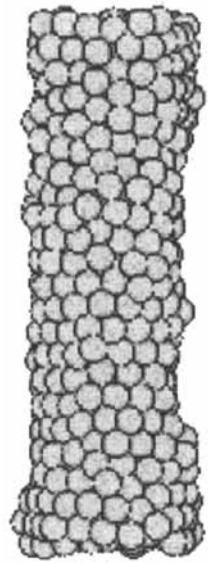

FIGURE 1 Atomic positions for a nanowire with length 5.4 nm, and a radius of 0.9 nm.

FIGURE 2 Top view of the MD box for a nanowire shown in Figure 1. Here and in Figure 3 the whole thickness of the wire along its axis is shown after 7.1 ns of simulation.

FIGURE 3 Top view of the whole MD box for a nanowire of 689 atoms, with length 2.6 nm, and a radius of 1.2 nm.

multishelled structure is obvious, after 10^6 time steps of simulation the walls are still not completely homogeneous. Several atoms remain about the walls. Three cylindrical shells exist for the nanowire shown in Figure 2.

The nanowire presented in Figure 3 consists of the two coaxial near walls and a large filled core. The filled core is well ordered and its parallel vertical planes are at the spacing of 0.18 nm. This double-walled structure suggests an application of similar gold nanowires as cylindrical capacitors. Therefore, we calculated the capacitance of finite nanometre-scale cylindrical capacitors and found the values of the order of 0.5 aF for the sizes for which multishelled nanowires appear in simulations [12].

As always in computer simulations of real materials, it is important to compare results with experiments. Gold nanostructures were the subject of recent STM studies [1, 2]. Unusual strands of gold atoms (down to one row) were simultaneously observed by an electron microscope [1]. The structure of the strands and understanding of the thinning process for these tip-supported nanostructures were left for future studies. The MD

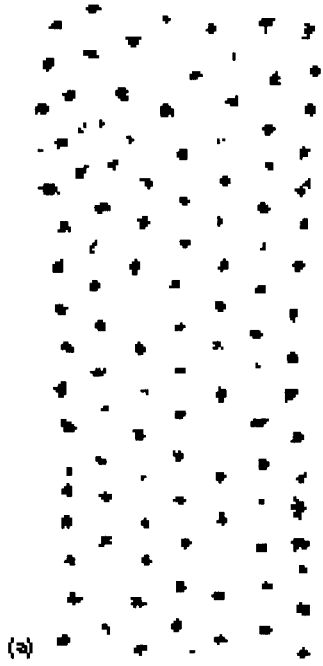

FIGURE 4 Vertical slice through a multishelled gold nanowire: (a) for a nanowire from [9] (588 atoms, length 4 nm, radius 0.9 nm), (b) for a nanowire shown here in Figures 1 and 2. Vertical rows of gold atoms are the image of coaxial cylindrical shells. Similar structures were recently formed in STM and observed by an electron microscope [1].

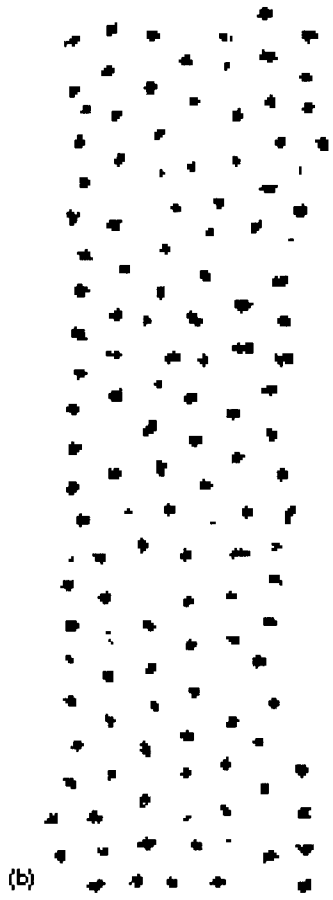

FIGURE 4 (Continued).

trajectory plots of atoms in the vertical slice of the box shown in Figure 4 resemble strands of gold atoms in Figure 2 of [1]. Therefore, we propose that strands formed in STM are the image of the cylindrical walls of multishelled gold nanowires [13]. Figure 4 shows that defects exist on some rows. Gold rows with a defect were sometimes observed by electron microscope (see Fig. 2(a) in [1]).

The thinning process for a multishelled nanowire should start from its central part, either the filled thin core (Fig. 1 from [9]), the central part of a large filled core (Fig. 3 here), or an empty interior cylinder which first shrinks into a thin filled core (Fig. 2 here). When this central part is removed by diffusion of atoms to the tip, the next interior cylindrical wall

shrinks into a new core, and then the process repeats. Therefore, the number of rows decreases by one as observed in the experiment [1]. At a final stage of the shrinkage processes an empty cylinder shrinks to one row of atoms. For multishelled nanowires the shrinkage of an internal cylinder is followed by the decrease of the radii of external cylinders and the whole nanostructure thins down with time. A mechanism of plastic deformation cycles of filled nanowires was suggested to explain the shape of necks formed in STM [14]. In this model plastic deformation starts from the central cylindrical slab of a filled nanowire which acts as a weakest spot. For multishelled nanowires a such central cylindrical weak spot most often naturally forms. In STM/TEM experiments [1] it was noted that the gap between the dark lines of their Figure 2(d) is greatly enlarged. This should be related to the special situation where the multishelled structure is lost and only two rows, *i.e.*, an empty cylinder is present. After that, at a final stage of the shrinkage processes, one atomic chain remains.

CONCLUSIONS

MD computer simulation based on the well-established embedded-atom potential shows that finite gold wires of nanometre dimensions are often multishelled. Recently, similar gold nanostructures were formed in STM and observed by TEM [1]. The model of multishelled gold nanowires should be considered in explanation of the conductance measured in STM [1, 2]. Results of computer simulations enable fabrication of similar metallic nanowires which will be used in nanoelectronic and nanomechanical devices.

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