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LETTER TO THE EDITOR

NANOMETER-SCALE CAPACITORS

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Dedicated to Professor Boran Leontić on the occasion of his 70th birthday

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Molecular-dynamics computer simulations which employ the embedded-atom potential show that nanowires of gold exist as multishelled structures. We simulate double-walled gold nanowires and calculate the capacitance of a finite nanometer-size cylindrical capacitor. For the sizes for which multishelled nanowires appear in simulations we find the capacitances below one attofarad.

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Finite-size systems of atomic-scale dimensions are attracting a great attention. Interest is focused on fundamental aspects as well as on applications. The remarkable physical properties of nanostructures allow one to design nano-scale electrical and mechanical devices. The continuing miniaturization of engineering devices leads to a technological revolution. Research on the properties of cylindrical nanostructures of various materials, e.g., nanowires, has been an especially active field.

Multishelled nanostructures have been produced of carbon clusters and wires [1, 2], as well as wires of WS_2, MoS_2, and $NiCl_2$ [3]. Gold nanowires are made by Scanning Tunneling Microscopy (STM) [4, 5] and electron-beam litography [6]. In recent molecular-dynamics (MD) computer simulation, multishelled cylindrical nanostructures of gold were analysed [7]. Wires with radii around a nanometer and of a length/diameter ratio between 1 and 3 were studied. It was found that multiwalled structures exist for longer of these nanowires, i.e., for a length/diameter ratio of 2 and 3. The formation of shells has also been found in a jellium-model calculation for finite sodium nanowires [8]. This was confirmed by the conductance measurements [9]. We simulate here cylindrical double-walled gold nanowires and study the capacitance for this geometry.

It is well known that an application of a many-body potential is necessary for an accurate description of metallic bonding by the MD simulation method [10]. We used (as in Ref. [7]) an embedded-atom potential for gold which produces a good agreement with the available experimental results for bulk, surfaces and nanoparticles [11]. A time step of 7.14×10^{-15} s was employed in the simulation. The temperature was controlled by rescaling the particle velocities. We started from an ideal fcc (111) structure at $T = 0$ K, and included in the cylindrical MD box all particles whose distance from the nanowire axis was smaller than 1.2 nm. The length of the sample of 689 atoms was 6 layers. We also studied a nanowire of 9 layers and 1032 particles. 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, as in Ref. [7], 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. Figure 1 shows the shape of the MD box for a nanowire of 689 atoms after 3.55 ns of simulation. The top view of the whole cylindrical MD box for this

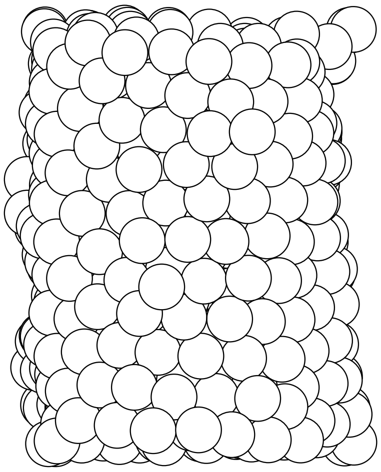

Fig. 1. Atomic positions (side view) for a nanowire with length 2.6 nm *and an external radius of* 1.2 nm.

nanowire is shown in Fig. 2. While the presence of a double-walled and internally filled structure is obvious, the walls are still not completely homogeneous. Several atoms remain close to the walls. Simulation shows that an almost identical structure exists in up to 10^6 time steps, i.e., 7.1 ns [12]. We also found a double-walled structure for nanowire of 1032 atoms. These structures suggest an application of gold nanowires as cylindrical capacitors. Therefore, we calculated the capacitance of a nanometer-scale capacitor for the geometry shown in the inset of Fig. 3.

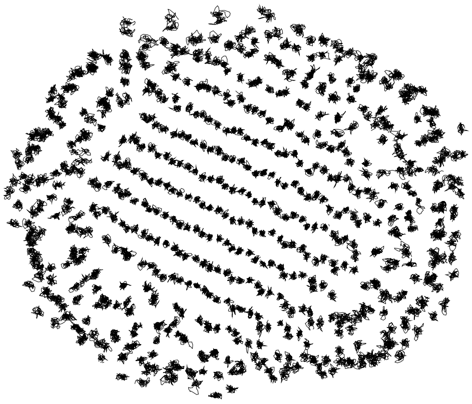

Fig. 2. MD trajectory plot of a top view for a gold nanowire shown in Fig. 1. The whole thickness of the wire along its axis is shown after 3.55 ns *of simulation. This nanowire consists of the two coaxial near walls and a large filled core.*

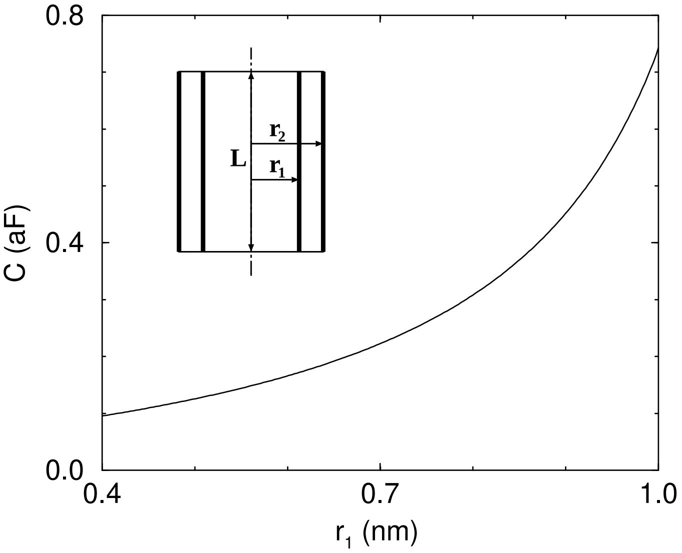

Fig. 3. Capacitance of a capacitor as a function of an internal radius r_1, for $L = 2.6$ nm, *and an external radius $r_2 = 1.2$* nm. *Inset: the geometry of a nanometer-scale cylindrical capacitor.*

The calculation starts from the electrical potential $\phi(r, z)$ in the space between two coaxial cylinders of radii r_1 and r_2 ($r_1 < r_2$), of a finite length L in the z

direction [13]

$$\phi(r,z) = V\frac{4}{\pi}\sum_{k=1,3,5,\dots}\frac{\sin\nu_k z}{k}\frac{I_0(\nu_k r)K_0(\nu_k r_1) - I_0(\nu_k r_1)K_0(\nu_k r)}{I_0(\nu_k r_2)K_0(\nu_k r_1) - I_0(\nu_k r_1)K_0(\nu_k r_2)}, \tag{1}$$

where $\nu_k = k\pi/L$ and $0 \le z \le L$. The parameter V is the potential difference applied between the two cylinders, whereas $I_i(x)$ and $K_i(x)$ (here and below) are the modified Bessel functions of the order i [14]. The capacitance $C = (r_1, r_2, L)$ of the structure is obtained from

$$C = \frac{2\pi r_1\epsilon_0}{V}\int_0^L \left(\frac{\partial\phi}{\partial r}\right)_{r=r_1} \mathrm{d}z, \tag{2}$$

where $\epsilon_0 = 8,854\times10^{-12}$ Fm^{-1} is the electric permittivity of vacuum. The result is

$$C = 16 r_1\epsilon_0 \sum_{k=1,3,5,\dots}\frac{1}{k}\frac{I_0(\nu_k r_1)K_1(\nu_k r_1) + I_1(\nu_k r_1)K_0(\nu_k r_1)}{I_0(\nu_k r_1)K_0(\nu_k r_2) - I_0(\nu_k r_2)K_0(\nu_k r_1)}\,. \tag{3}$$

Using Eq. (3), we calculated the capacitance for several sizes typical for structures obtained in MD simulations. The results are presented in Fig. 3 and in Table 1.

Table 1. Capacitance C of a nanometer-scale capacitor with an external radius $r_2 = 1.2$ nm, an internal radius $r_1 = 0.9$ nm, for several lengths L.

L (nm)	2.0	2.2	2.4	2.6	2.8	3.0
C (aF)	0.336	0.374	0.413	0.452	0.490	0.529

In summary, molecular-dynamics computer simulation based on the well-established embedded-atom potential [7] shows that gold wires of nanometer dimensions form double-walled structures. Motivated by this result, we calculated the capacitance of a finite nanometer-scale cylindrical capacitor. Our calculations of the capacitance is based on the classical electrodynamics. However, on very small scales the quantum corrections appear. This is the point we are pursuing now [15]. It is known that typical inhomogeneous electric fields used in the polarizability measurements for metallic clusters are of the order of 10^5 Vcm^{-1} and field gradients are $\approx 10^5$ Vcm^{-2} [16]. These fields induce a dipole moment and slightly deform the clusters. Therefore, in order to strictly preserve the shape of a nanometer-scale capacitor weaker and homogeneous fields should be applied in an electronic device. An STM could be used to manipulate gold atoms and assemble small nanowires [4, 5]. The STM experiments show that gold nanostructures can sustain large fields of up to 1 V [5]. Wires produced by electron-beam litography will approach the smallest nanometer-scales discussed here. It is possible to fill the space between two cylindrical electrodes with various insulators and obtain nanometer-scale capacitors with different capacitances. Similar filling of carbon nanotubes with metals was recently realized [17, 18]. Moreover, fabrication of metallic nanowires using carbon multishelled nanotubes as templates could be used to produce nanometer-scale cylindrical capacitors not only of gold, but also of other metals.

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NANOMETARSKI KAPACITORI

Računalne simulacije molekulskom dinamikom, koje primjenjuju višečestični potencijal, pokazuju da postoje višeslojne nanožice od zlata. Simulirali smo dvoslojne zlatne nanožice i izračunali kapacitet takvog konačnog cilindričnog kapacitora. Za veličine kapacitora koje se nalaze u simulacijama višeslojnih nanožica dobivamo kapacitete ispod jednog atofarada.