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Resistance of copper nanowires and comparison with carbon nanotube bundles for interconnect applications using first principles calculations

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Abstract

We have studied the electronic properties and the band structure of copper nanowires for various diameters using first principles density functional methods and a supercell approach. The resistances of copper nanowires were computed on the basis of the Landauer formalism and compared with those obtained from an empirical approach. The fundamental resistances of small copper nanowires (~ 60 nm diameter) are found to be larger than those predicted by Ohm's law. In parallel, we have computed the fundamental resistances for bundles of single walled carbon nanotubes and compared them with that of a single copper wire of similar dimensions. We find that the resistance of carbon nanotube bundles is smaller than that of the copper wires for dimensions below 60 nm. Our results are discussed in light of recent experiments.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The ever shrinking size in commercially integrated circuits has now reached the nanoscale limit and its continuous scaling beyond the 90 nm node has proved to be a great challenge [1]. It is well recognized that, there are difficulties in producing reliable materials with controlled properties at this scale, as quantum effects such as tunneling and contact resistance may severely affect the performance of these smaller nanoelectronics devices. There are also other issues that future electronic devices must overcome in an integrated circuit, such as those related to the material and also their processing for interconnect purposes. The role of the interconnect in an integrated circuit is to enable effective passing of clock and other signals in addition to providing power to various parts of the circuit on a chip. Copper, which is

presently used as the interconnect material, faces two critical problems: one related to its inability to carry high current density and the other being its increased electrical resistivity due to surface scattering of electrons, and problems due to grain boundaries [1]. It should be pointed out that the electronic transport through copper wires at the nanoscale requires a full quantum mechanical description and the present understanding of the increase in the resistance of copper wires with decreasing dimension is based on an empirical approach [2]. However, experiments are beginning to provide microscopic understanding of electron transport in nanoscale copper wires. In this context, a full quantum mechanical description of electronic transport in copper wires is not only important for fundamental understanding but also will have impact on practical applications.

In a related context, carbon nanotubes (CNTs), due to their large current carrying capacity and electron mean free path, have potential to be used as interconnects [3–10]. However,

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due to the low density of states in CNTs near the Fermi energy, the resistivity becomes comparable to that of copper, whose mean free path of electron in bulk is considerably smaller (~ 40 nm) compared to CNTs (~ 1 μm). Hence it has been suggested that the CNT bundles may be able to overcome this difficulty by providing parallel channels for conduction despite the coupling between individual nanotubes of the bundle [11, 12].

Electronic transport in metallic nanowires and clusters where the size is comparable to the electron mean free path are of great interest both from a fundamental point of view and also for its potential in nano device applications [13]. Copper nanowires are particularly of interest as they are used as interconnects in electronic devices. In nanometer dimensions, electronic transport is mostly considered ballistic [14], and according to the Landauer formalism [15], conductance of a nanowire is understood as electronic transport through channels and is calculated as a function of transmission probability for each channel of the nanowire. Recently, there have been some experiments to measure the resistance of the copper nanowires [2, 14, 16–19] which aids in a better understanding of the transport mechanism. However, few first principle studies have studied copper nanowires, which may have great impact for its use as interconnects. The macroscopic Ohm's law, which is typically used to calculate the resistance of a bulk conductor, breaks down due to the various effects brought on by the finite size effect. Here one needs to study the transport behavior of nanowires using a quantum mechanical description. Such an effort will not only enrich our fundamental understanding of the electron transport at the nanoscale, but also provide various parameters for its use in circuit design. In this paper, we present a comprehensive study of electronic and transport properties of copper nanowires with different diameters using first principles density functional methods and the Landauer formalism. The resistance of the copper nanowire was then compared to single walled carbon nanotube (5, 5) bundles, and we find that the resistance of the CNT bundles was much smaller than that of the copper nanowire, making it a better choice for interconnects.

2. Computational methods

Our calculations were based on first principle density functional methods. In particular, we have used the generalized gradient corrected approximation of Perdew and Wang (PW91) [20]. As the exchange and correlation functional. The calculations were based on a super cell approach and the wavefunctions were expanded using plane waves. The ionic cores were replaced by ultrasoft pseudopotentials [21] and the accuracy of pseudopotentials scheme was tested for carbon and copper systems by comparing the results with that obtained using the PAW method [22]. We have used an energy cutoff of 330 eV and the Monkhorst–Pack scheme for k -point sampling. The total energy is converged to within 0.01 meV. The calculations were carried out using VASP code [21]. The structures of the copper nanowires were created from their bulk structures. We have considered wires along (100) direction with ABAB stacking as they were most commonly used in

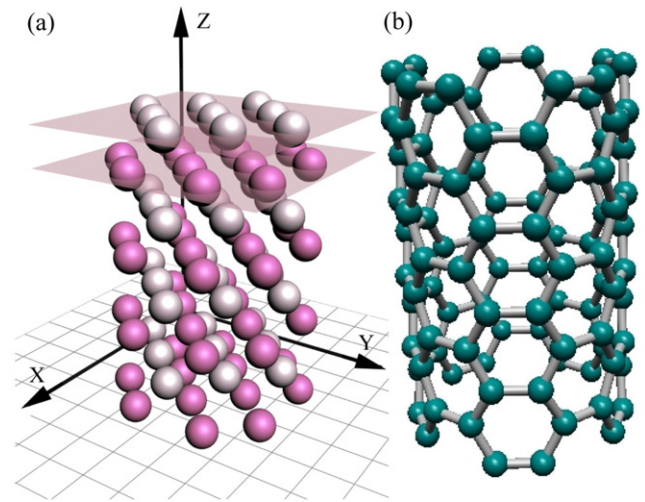


Figure 1. (a) Diagram of the atomic structure of the copper nanowire (9×12). The different colored spheres present the atoms of different planes. (b) Diagram of the atomic configuration of a single walled carbon nanotube (5, 5).

experiments. Electronic properties of these nanowires with different orientation will be of great interest, but is beyond the scope of the present paper.

The distance between the Cu atoms was taken to be 2.56 \AA and the inter-planar distance was 3.62 \AA . The atomic configuration of a typical copper nanowire is shown in figure 1(a). The wires are defined in terms of numbers of atoms in each stacking plane along the z -direction [100] following an earlier convention [16] and for negligible interaction between the wire and its replica, a interwire distance of 5 \AA is established in the xy -direction. We have defined the cross sectional area as the area of the minimum circumscribed circle which can best fit it. The number of atoms in each plane rises from 5 atoms in the A plane to a maximum of 45 and 4 atoms in the B plane to a maximum of 32. The cross sectional area corresponding to 45×32 nanowire is 175\AA^2 .

The electronic structure of the carbon nanotube is computed using a similar approach. In particular, we have considered a (5, 5) carbon nanotube which is metallic in nature. The super cell of this nanotube is shown in figure 1(b). The z -direction represents the axis of the nanotube and is similar to copper nanowires, sufficient vacuum is introduced (at least 5 \AA on each side of the tube along xy -direction) in order to minimize the interaction between the tubes.

Conductance of these wires can be calculated from their electronic structure, which depends on the molecular configuration, dimension, temperature. At room temperature ($T = 300$ K), $k_B T \approx 0.0258$ eV, any two energy levels whose energy difference is smaller than 0.0258 eV will be indistinguishable. For an electron with energy E_i lower than E_f (energy corresponding to the Fermi level), the probability of it appearing at the Fermi level is given by the Fermi distribution function as $p_i = 1/(e^{(E_i - E_f)/k_B T} + 1)$. Thus, the electrons in energy bands close to the Fermi level will be transferred to it and will contribute to conduction. Besides the occupied subbands below E_f , the empty subbands above E_f

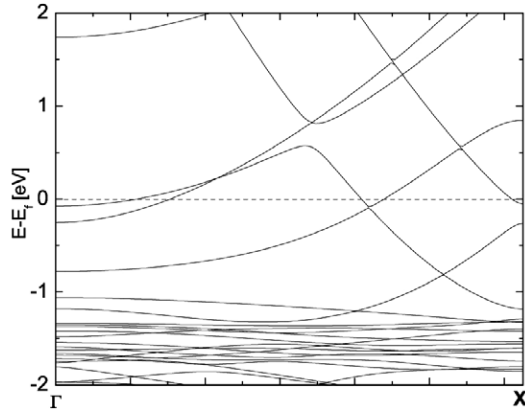


Figure 2. Electronic band structure of the copper nanowire (5×4). Negative energies correspond to valence band states and positive energies correspond to conduction band states.

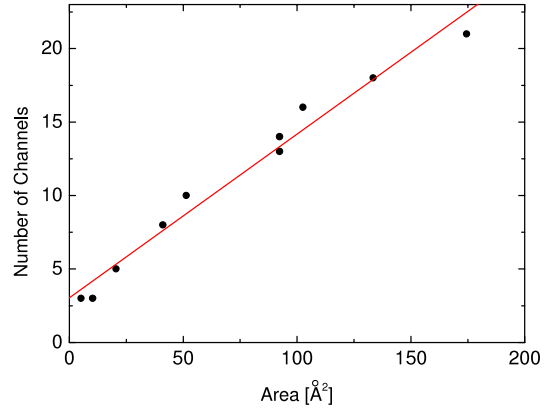


Figure 3. Number of channels for conduction in copper nanowires as a function of the cross sectional area.

also contribute to conduction [23]. Therefore, the sum of the probabilities for all such bands is given by

$$P = \sum_i^{N_{\text{subb}}} \frac{1}{e^{|E_i - E_f|/k_B T} + 1} \quad (1)$$

which is also the number of channels N involved in conduction and can be approximated by counting the number of states crossing the Fermi energy. N_{subb} is the number of subbands. As the wire of our interest is in the nanometer scale, electronic transport, may be treated as ballistic [16, 24] to a first approximation. According to Landauer Büttiker formalism [25], conductance of a nanowire through a single channel is

$$g(v) = \frac{2e^2}{h} [\eta \tau(\mu_1) + (1 - \eta) \tau(\mu_2)] \quad (2)$$

where η is the voltage division factor which describes how the electrostatic potential difference v is divided between the two junctions. μ_1 and μ_2 correspond to the electrochemical potentials of the two contacts, and τ is the transmission function. Assuming that $\eta = 0$, the conductance spectrum is proportional to the transmission function, and

$$g(v) = \frac{2e^2}{h} \tau(E_f) \quad (3)$$

where $\tau(E_f)$ is the transmission function at Fermi level. Therefore, electronic transport through the wire which has N number of channels is given by $g = G_0 \sum_{n=1}^N \tau_n$, where $G_0 = 2e^2/h$ and τ_n is the transmission probability of the n th channel of the nanowire [16]. In an infinite periodic wire, the transmission probability of the states is unity, hence the conductance of one such wire with N number of channels is $G = NG_0$.

3. Results and discussion

The electronic band structure of the Cu (5×4) nanowire is shown in figure 2. It can be seen from the band structure that

there are 5 channels and based on the Landauer formalism described above, the total conductance of the wire is $5G_0$. Similarly, the conductance for (9×4) wire is $8G_0$ and that of (12×9) wire is found to be $10G_0$.

The total number of channels N , for Cu nanowires of different cross sectional areas were calculated in a similar manner and are plotted in figure 3. The number of channels increases linearly with area, as can be seen from figure 3 and follows the relation

$$N = a \times \text{area} + c \quad (4)$$

where $a = 0.111 \text{ (nm)}^{-2}$ and $c = 3.036$. The mean free path of electrons (λ_0) in bulk copper is 40 nm at room temperature and the length of the nanowire considered is of the order of λ_0 , the electron transport is considered to be ballistic and hence the resistance is independent of the length. Since we have considered copper nanowires, the mean free path of the electron will be smaller than that of bulk copper wires, due to scattering at the surface. Therefore, 40 nm represents an upper limit for the mean free path of electrons in copper nanowires. The resistance of nanowires whose length L is larger than the mean free path λ_0 is given by [24]

$$R = \frac{h}{2e^2 N} \frac{L}{\lambda_0}. \quad (5)$$

The above equation can be modified further by taking into account the linear dependence of the number of channels to the cross section area of the wire and hence can be rewritten as

$$R = \frac{h}{2e^2(a \times \text{area} + c)} \frac{L}{\lambda_0} \approx \rho \frac{L}{A}. \quad (6)$$

(The constant c can be neglected when the area is large. This additional scattering resistance would appear as a distributed resistance per unit length to account for resistive losses.) ρ in equation (6) is the equivalent resistivity and A is the cross section area. The calculated value of resistivity ρ is $2.91 \times 10^{-8} \Omega \text{ m}$, whereas the resistivity of Cu in experiments [18] is $1.68 \times 10^{-8} \Omega \text{ m}$. Note that both the experimental and the calculated resistivity for Cu are of the same order. However, if we take into account the surface scattering and

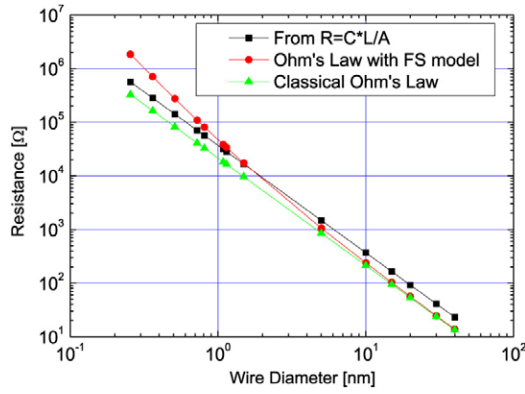


Figure 4. Resistance versus area plot of the copper nanowire. (FS model: Fuchs–Sondheimer model).

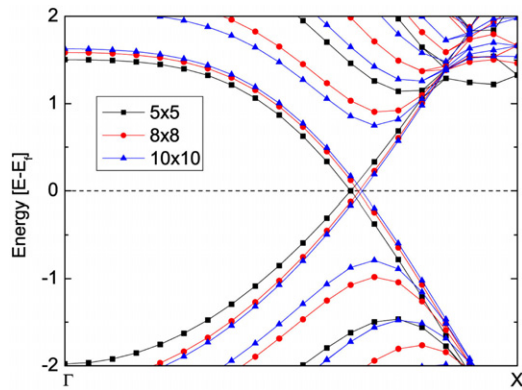


Figure 5. Electronic band structure of single walled carbon nanotubes (5, 5), (8, 8), and (10, 10).

grain boundary scattering effects [14], the resistivity increases in the nanoscale regime as given by the semi-classical Fuchs–Sondheimer model.

The electronic band structure was calculated for Cu nanowires up to an area of 175 \AA^2 (the length of all wires were kept constant i.e., $1 \mu\text{m}$). The number of channels for larger systems were calculated using equation (4). Furthermore, these data were used to calculate the resistivity using equation (6). In figure 4, we plot the resistance obtained using Ohm’s law, Fuchs–Sondheimer model, as well as data obtained from equation (6) for the Cu nanowire as a function of area. Figure 4 shows that the resistance of the Cu nanowire calculated using three different methods and predicts that Ohm’s law represents the lower limit for the resistance at the nanoscale.

Using a similar approach we have computed band structures of metallic single walled carbon nanotubes (SWCNTs) with chirality (5, 5), (8, 8), and (10, 10). The band structure diagram, figure 5, shows that only two bands cross at the Fermi level for all these SWCNTs and hence the total number of channels of these systems near the Fermi energy is two [26].

To optimize the usage of single walled carbon nanotubes, we compare a bundle of SWCNTs with the same radius as that of the copper nanowire. In this way, the number of channels for conduction of the CNT bundle will depend on the total number of carbon nanotubes. We use a SWCNT of small

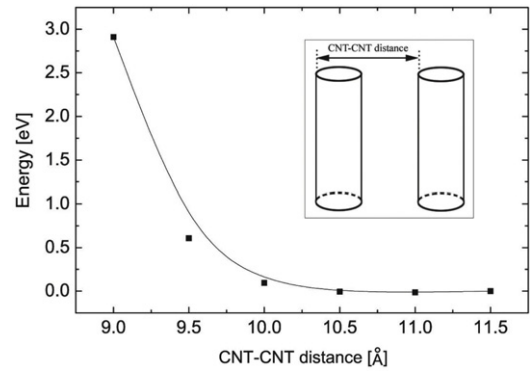


Figure 6. Energy of the system (two SWCNTs) as a function of their inter distance.

diameter, namely (5, 5), to form the bundle in the given area. However, using dense bundles of SWCNTs may not give $2N$ channels, as the interactions between the tubes will alter the band structure. A sparse bundle of SWCNTs with an optimized distance between them is a better choice as it will minimize the interaction between the tubes [2]. We have carried out total energy calculations as a function of distance between the two CNTs and the energy plot is shown in figure 6. From figure 6, we find that the equilibrium distance between the two tubes is 3.5 \AA , which is in agreement with earlier studies [27, 28]. Beyond this value for the inter tube distance, the energy curve reaches a constant value suggesting that the electronic structure is not modified due to the tube–tube interaction. Hence in our calculations, we have assumed that in every 1 nm^2 (from figure 6) square space, there is a single SWCNT (5, 5), whose radius is 3.366 \AA .

The typical mean free path of electrons in CNT is about 1 nm for defect free nanotubes and next generation interconnects will employ 40 nm wires. We have considered a $40 \text{ nm} \times 40 \text{ nm}$ Cu wire and compared its resistance to a CNT bundle of the same radius. There are $40 \times 40 = 1600$ CNTs in this bundle, and hence the number of conducting channels is 3200. Resistance of CNT bundles calculated by the above mentioned method gives $R = h/2e^2/3200 = 12.9 \text{ k}\Omega/3200 \approx 4 \Omega$. The resistance of comparably sized copper is 14Ω (from equation (6)), and becomes even higher when the surface scattering is considered (to 53Ω). This value is one order of magnitude larger than CNTs bundle and hence in effect CNTs is a better material for future interconnects.

In summary, we have studied the resistivity of Cu nanowires up to a thickness of 175 \AA^2 and our results are comparable to the experimentally obtained values. We have compared the resistance of copper and bundles of single walled carbon nanotubes and our results suggest that CNTs provide an alternate material for future interconnects, particularly below the 60 nm length scale. It will be interesting to study the effect of defects and impurities on the transport properties of these systems.

Acknowledgments

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