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A model for engineering the electrical conductance at nanoscale

J.A. Leon-Gil [a], J. Alvarez-Quintana [a, b, *]

[a] Centro de Investigación en Materiales Avanzados S. C. Unidad Monterrey, Alianza Norte # 202, Autopista Mty-Aeropuerto Km. 10, Apodaca, Nuevo León C.P. 66600, Mexico
[b] Genes-Group of Embedded Nanomaterials for Energy Scavenging, CIMAV-Unidad Monterrey, Mexico

A B S T R A C T

With the emergence of nanoelectronics faster and denser circuits are being produced, this largely because the aggressive scaling to the nanometer range of the insulating film used as dielectric. Moreover, enhancements of the electrical conductivity of nanofiller based composites can be achieved by the incorporation of conductive nanofillers into polymer matrix. In such systems electron wave-function penetration into the dielectric is important as it leads to undesired or desired leakage currents by tunneling respectively. Therefore, a proper design of the electrical conductance in such structures becomes important in order to control accurately their performance. In this research, a model for engineering the electrical conductance of resistors at nanoscale is presented. The conductance at infinitesimal bias of nanoresistors is modeled within the framework of Landauer's tunneling which results in an exponential integral function for the total electrical conductance. Model takes the effects of azimuthal and inclination angles between nanocontacts into account, as well as the effect of the thickness of the dielectric layer. The model also unveils a U-shaped behavior of the electrical conductance as a function of the azimuthal angle between nanocontacts. As a result, a minimal electrical conductance is predicted when the azimuthal angle reaches $90°$.

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1. Introduction

It is of a great importance from both fundamental and application point of views to understand the behavior of the electrical conductance formed by two electrodes separated by a thin insulating film; in such system if the film is sufficiently thin, electrons can flow between the two electrodes by means of tunnel effect [1]. Ultrahigh frequency diodes or metal—insulator—metal diodes (MIM diodes) might just be the technology that allows electronics achieve the next big leap in processing speed and energy harvesting [2—8]. The reason is that unlike Schottky diodes, MIM diodes are not affected by parasitic capacitances because they work on the basis of electron tunneling. Currently, an aggressive scaling of ultrathin-gate oxide films becomes necessary as metal oxide semiconductor field effect transistors (FETs) approach to nanometer regimes, for ultrathin insulators direct tunneling current will dominate the gate leakage current and therefore the off and on-state of the transistor [9—11]. Additionally, new research on

plastic-based flexible electronics where large volume processing using roll-to-roll, inkjet printing or spray deposition, represent the "electronics everywhere" trend of the future is aimed in understanding electron transport through organic dielectric molecules between metallic electrodes [12—20]. Besides this, nanofiller based composites have attracted research interest because the significant improvement in electrical conductivity due to the addition of small amounts of fillers in polymeric or ceramic host materials [21—25]. In such systems: if the number of nanoscale fillers per unit volume n is large, nanofillers touch each other and the conductance is by percolation [26,27]. Nevertheless, when n is smaller than the percolation threshold n_c, nanofillers are isolated from each other, and the conductance could be due to hopping [28—30] or by tunneling [30—33], depending on the existence or nonexistence of impurity centers inside of the dielectric matrix as well as the thickness of the insulating layer between nanofillers. Previously, satisfactory approximations for charge transfer in metal—insulator—metal structures via tunneling based on perturbation theory or Bardeen approach [34], Non Equilibrium Green Functions [35,36], density functional theory [37,38], local density approximation [39,40], Wentzel—Kramers—Brilliouin approximation [41,42], Airy functions via transfer matrix methods [43,44] and

* Corresponding author. Genes-Group of Embedded Nanomaterials for Energy Scavenging, CIMAV-Unidad Monterrey, Mexico.
E-mail address: jaime.alvarez@cimav.edu.mx (J. Alvarez-Quintana).

Landauer theory [45,46], have so far been modeled; however all those reported derivations have been done considering a single dielectric bridge between the two electrodes ignoring the geometrical aspects of the structure, which are so important in real devices. As a result, such approximations let only predict values of the electrical conductance per unit area making impossible to use them so as to engineer electrical conductance by way of geometrical parameters. Taking into consideration, that although in dielectric gate and MIM diode applications the dielectric nanolayer has a well-defined geometry and thickness; in nanocomposites, the nanofillers are randomly oriented and distributed. Therefore, an accurate modeling of the electrical conductance which considers geometrical parameters such as relative orientation and position between electrodes as well as dielectric thickness gradient to predict and engineer the electrical conductance of nanoresistors is important for nanoelectronics and nanocomposite technology development.

2. The proposed model

It is instructive to consider a system of two nanostructures (i.e. two carbon nanotubes, nanorods, nanoribbons etc.) randomly dispersed in an insulating continuum media. Fig. 1a and b shows this situation by mean of two nanotubes overlapped and separated a distance d respectively. Same figures also show the inclination (α) and azimuthal (θ) angles between nanotubes. Therefore, if the distance between them is the order of some nanometers, then through the overlapping area is accomplished the charge transfer by tunneling between fillers. In general, the thermal conductance of a piece of material with cross section A, length d and conductivity σ is given by

$$K = \frac{\sigma A}{d} \quad (1)$$

For the tunneling conductivity σ, we use the Landauer formalism $\sigma = (2e^2/h)T/R$ [45,46]. Evidently, la formula has the ratio of the transmission probability divided by the reflection

Fig. 1. a) and b) Two nanotubes overlapped and rotated via the azimuthal (θ) and the slant (α) angles respectively, c) infinitesimal conductances filling the space between nanocontacts, and d) real overlapped nanorods.

probability; the factor $1/R$ arises from the reflected electrons changing the chemical potential of the reservoirs. However, during tunneling the transmission probabilities are very small [46] and the reflection probabilities are very near to the unity, thus the tunneling conductivity normally appears as $\sigma = (2e^2/h)T$, where the first term is described often as the quantum unit of the electrical conductance, and T is the transmission probability given by $T = \gamma e^{(-2\kappa d)}$; here k is the characteristic wave vector for tunneling or the inverse decay tunneling length, d is the separation between contacts and γ is determined by the characteristics of the electrodes. By applying these statements then the tunneling conductance for an infinitesimal slide of material according to equation (1) is given by

$$dK = \gamma\left(\frac{2e^2}{h}\right)\left(\frac{e^{-2kd}}{d}\right)(-2d)Adk \quad (2)$$

When electron tunneling is described in terms of a single evanescent state in the insulator layer we can write the vector k in terms of the decay rate of the wave function k_0 for $k_{\parallel} = 0$ in the barrier region in the form of $k^2 = k_0^2 + k_{\parallel}^2$, therefore by integrating over $k_{\parallel}$ the total tunneling conductance is given by

$$K = \frac{\gamma k_0}{4\pi}\left(\frac{2e^2}{h}\right)\left(\frac{e^{-2k_0 d}}{d}\right)A \quad (3)$$

Nonetheless, in the engineering context it is important to control the electrical conductance starting from easy access parameters during microfabrication process such as the geometrical parameters d and A. At nanoscale, to control the parameter d could be tedious and impractical because it implies to control the dielectric film thickness below of the minimal distance between contacts to keep the tunneling in order to obtain different conductance values. On the other hand, to control the cross section A by increasing or decreasing the contacts width will induce angular tunneling due to edge effects on the electric field distribution. Therefore, the only way to engineer the electrical conductance in equation (3) is by altering the cross section A via the azimuthal angle between contacts, this action will keep the contacts width avoiding edge effects but will change the cross section; as a result, the electrical conductance will be altered. Base on the above statements, in the present analysis in order to calculate the total electrical conductance it is considered that a set of infinitesimal shunt electrical conductances fill the space between electrodes (a shunt set of single dielectric channels), as shown in Fig. 1c. Therefore, the electrical conductance of one infinitesimal resistor is given by $dK = \frac{\sigma}{d}dA$, where by analogy with equation (3), the tunneling conductivity is $\sigma = \frac{\gamma k_0}{4\pi}\left(\frac{2e^2}{h}\right)e^{-2k_0 d}$.

It can be observed that the cross section A and the separation between electrodes d are not constants, rather depend on the azimuthal angle θ and inclination angle α. Therefore, $d = Tan(\alpha)x + b$ and $A = Dx$, here D is the nanofiller size (i.e. nanotube diameter, electrode width, etc.), $x = D/Sin\theta$ and b the minimal distance between nanostructures or electrodes to start the tunneling. After applying some mathematical artifices and by integrating $dK = \frac{\sigma}{d}dA$ in terms of the x variable, the total thermal conductance is given by

$$K = \frac{\gamma k_0 D}{4\pi Tan(\alpha)}\left(\frac{2e^2}{h}\right)\int_0^{x_0}\frac{e^{-2k_0[Tan(\alpha)x+b]}[2k_0 Tan(\alpha)]}{2k_0[Tan(\alpha)x+b]}dx \quad (4)$$

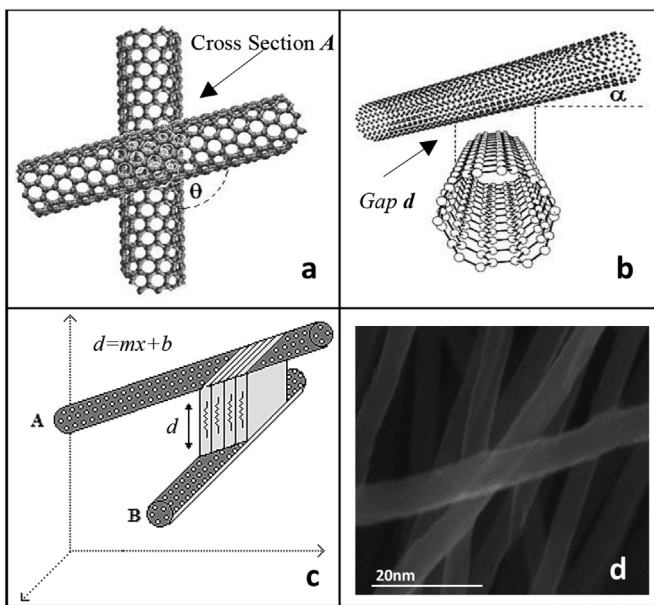Equation (4) is the main result of the present research and it