TEMPERATURE DEPENDENCE OF ELECTRICAL CONDUCTION THROUGH 1, 4-DITHIOLBENZENE MOLECULAR ASSEMBLY (PART II)

Kuek Chian Shiun and Aissa Boudjella
Faculty of Science, Engineering and Technology, University Tunku Abdul Rahman, Jalan University, Bandar Barat, 31900 Kampar, Perak, Malaysia

e-mail: kuekcs@mail.utar.edu.my e-mail:aissab@mail.utar.edu.my

Abstract

Numerical simulations have been performed to investigate the effect of the temperature on the electronic transport through molecular assembly system (MAS). The model involves 1,4-dithiolbenzene (DTB) molecules stacked in (1D) ordered structure. The MAS can contain up to two DTB molecules packed in the parallel geometrical arrangement.[1)] With the Fermi level E_f located in the middle of the HOMO-LUMO gap (HLG), [2, 3)] the electronic transport through a single or two DTB molecular units connected in parallel between two metallic contact is presented. The calculations were performed into two steps. First, the energy levels HOMO (the highest occupied molecular orbital) and LUMO (the lowest unoccupied molecular orbital) were obtained using an approach based on Landauer formalism with the density functional theory Kohn-Sham.[4, 5)] Then, the current-voltage (*I-V*) as well as the conductance-voltage (*G-V*) characteristics were calculated using the molecular conduction toy (MolCtoy).[2, 6)] These calculations were carried out for various temperature T=50~325K and intermolecular distances d=3.3~6.9 $\mathring{A}$. The charging energy $U=1$ *eV*, and the molecule–metal coupling strength $\sigma_1=\sigma_2=\sigma_i=0.1$ *eV* are kept constant. The influences of the electrical and physical parameters such as HOMO-LUMO gap (HLG), π-orbital and the intermolecular distance between two adjacent molecular units on the electron transport of MAS are analyzed.

Figure 1 represents a molecular assembly of DTB molecules in the parallel geometrical arrangement connected between two metallic electrodes. The temperature related current-voltage *I(V,T)* and conductance-voltage *G(V, T)* characteristics of MAS containing two DTB molecular units with $d=6.9$ and 3.3 $\mathring{A}$ are illustrated in figures 2 and 3, respectively. For the *I-V* curves, there are three distinct regions of operation of molecular assembly: 1) the conductance gap region, in this region the current is zero. The molecular system behaves as open circuit with an absence of temperature dependence; 2) above a certain threshold voltage, the current starts to increase linearly. This region exhibits a little temperature dependence; 3) finally; a point will be reached on the *I-V* curve at which the current becomes saturated. In this saturation region, the current is not affected by the variation of the temperature. For the *G-V* characteristics, while the conductance increases as the temperature increases, the magnitude of the maximum peaks decreases. In this molecular configuration, we can expect a significant π-coupling for sufficient a small distance *d* between two DTB adjacent molecular units. When *d* changes from 6.9 to 3.3 Å, the HLG decreases by 34.32%. The author[1)] reported the variation of the HOMO, LUMO, and HLG as a function of the intermolecular distances *d* of molecular structure containing two DTB molecular units. Therefore, it is important to associate the temperature related *I-V* characteristics with HLG. The shorter HLG, the smaller threshold voltage is observed for the variation of *I (V, T)* characteristics.

To conclude, the electron conduction in our molecular system model may be explained by two distinct mechanisms: 1) the direct tunneling, the main transport mechanism with the absence of temperature dependence and 2) the thermionic conduction with little temperature effect which can not be ignored. The prediction by Moore's law, the number of transistor integrated on a chip would grow exponential with time. Therefore, the heat dissipation is a critical issue in circuit design, because the huge device density in modern VLSI circuits. To predict the functionality of this a new generation molecular electronic assembly devices that can be implemented on a chip, the temperature rise effect caused by the power consumption devices on I-V characteristics may need to be considered.

References:

1) A. Boudjella et al.. Will be published in Japanese journal of applied physics Vol. 47, No 6, 2008.
2) F. Zahid, M. Paulsson, and S. Datta: in Semiconductors and Organic Nano-tecniques, ed. H. Morkov (Academic Press, New York, 2003).
3) S. N. Yaliraki, M. Kemp, and M. A. Ratner: J. Am. Chem. Soc. 121 (1999) 3428.
4) M. Buttiker, Y. Imry, R. Landauer, and S. Pinhas: Phys. Rev. B 31(1985) 6207.
5) S. Datta: Electronic Transport in Mesoscopic (Cambridge University Press, Cambridge, U.K., 1995), p. 57.
6) www.nanohub.org

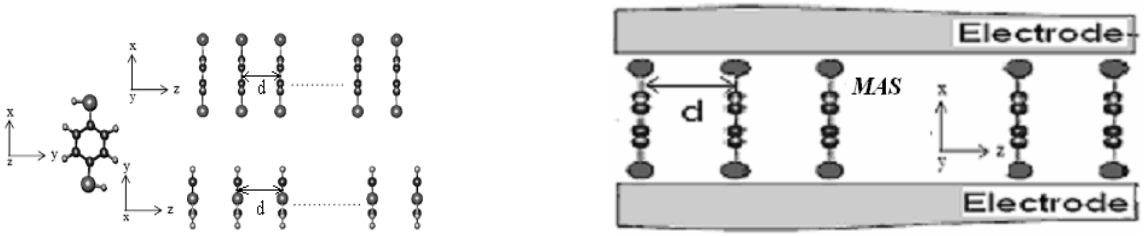
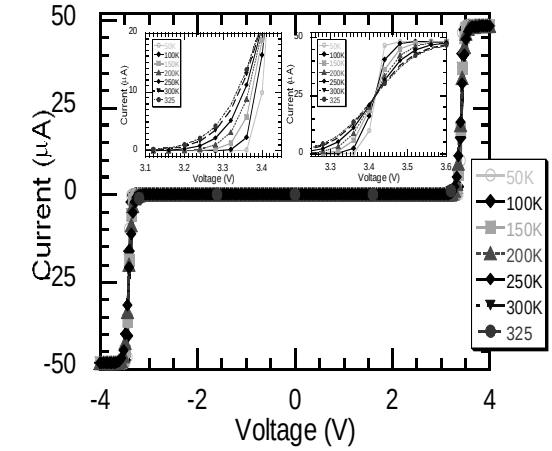
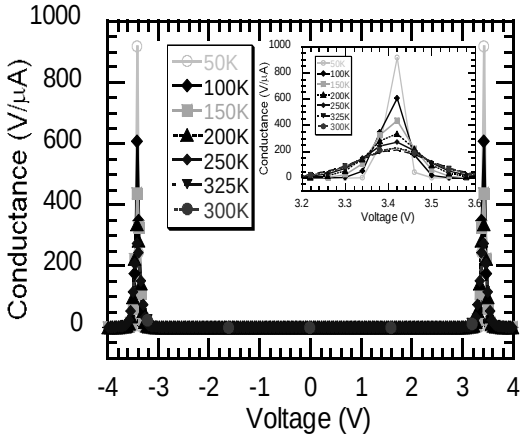


Fig. 1. Structure of MAS connected between two metallic electrodes.

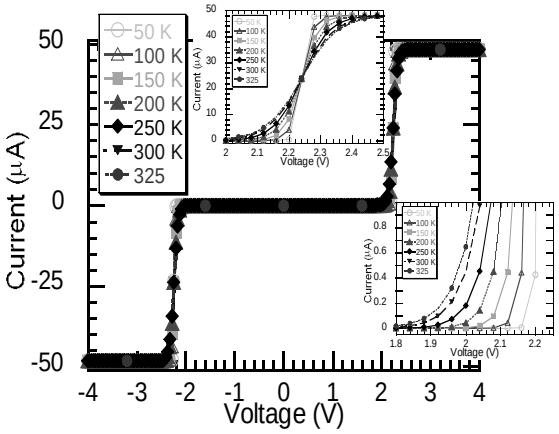


(a)

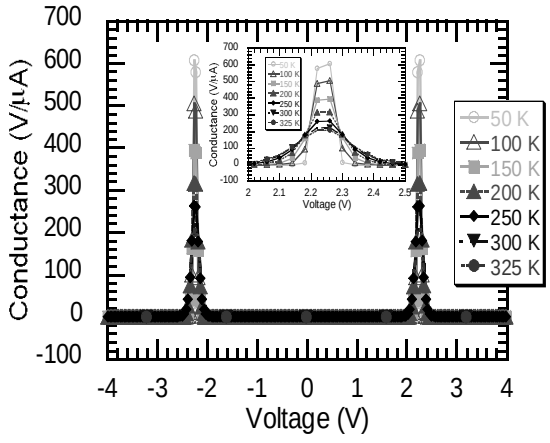


(b)

Fig. 2.The *I-V* (a) and *G-V* (b) characteristics For *N=2, HLG=3.411 eV, d =6.9 Å, U=1* eV, and $\sigma_1=\sigma_2=\sigma_i=0.1$ *eV*.



(a)



(b)

Fig. 3. The *I-V* (a) and *G-V* (b) characteristics For *N=2, HLG= 2.240 eV, d =3.3 Å, U=1 eV*, and $\sigma_1=\sigma_2=\sigma_i=0.1$ *eV*.