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Advances in Analytical Modelling for Nano-Bio-Technology

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Abstract

Nano-bio-technology is one of the most important mainstreams of current world research; improvements in creation and increase of nano-devices performance are a primary objective of pure research and applied technology. The devices sensitivity is an essential characteristic, for determining a great increase of their quality; various ideas and techniques are considered in this direction. A new appeared theoretical analytical model for the study of transport dynamics is able to accommodate previously not completely understood behaviours and indicates precise ways for calibrate and improve the device performance.

Keywords: Nano-technology, Nano-bio-materials, Nano-bio-devices, Diffusion, Sensitivity, Analytical Modelling, Mathematical Modelling.

In last years the increased ability to manipulate matter, combined with advances and discoveries in the synthesis and assembly of structures at nanoscale, brought to interesting advances in scientific and technological areas. For explaining the nanoscale phenomena, a deep understanding of electronic, magnetic and photonic interactions at this size scale is desiderable, through experiments, theory and mathematical modelling [1,2].

Nanomaterial-based devices are a powerful class of ultrasensitive devices for direct utilization at biological, chemical, medical, environmental level, in many areas of healthcare and life sciences. Considered the strong current demand of increasingly compact and powerful systems, there is a great interest in the development of nanoscale devices with new functions and enhanced performance. Central for this realization is the rational control of key nanomaterial parameters, determining electronic and optoelectronic properties [3-7].

Recently it has appeared a new generalization of the Drude-Lorentz model, based on the complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$ of the system, which presents analytical expressions for the most important quantities related to transport phenomena, i.e. the velocities correlation function $<\vec{v}(t)\cdot\vec{v}(0)>_T$ at the temperature T, the mean squared deviation of position $R^2(t)=\langle[\vec{R}(t)-\vec{R}(0)]^2\rangle$ and the diffusion coefficient D [8]. It avoids time-consuming numerical and/or simulation procedures, is mathematically very elegant and useful both for the study of new devices with desired characteristics and for testing and/or obtaining new values by existing experimental data. It considers also quantum [9] and relativistic [10] effects, the quantum relativistic step is in progress [11]. The comparison with existing utilized models, as Drude-Lorentz and Smith models [12] and the utilization of existing experimental data have demonstrated a very good fit with current knowledge [13-19] (Figure 1).

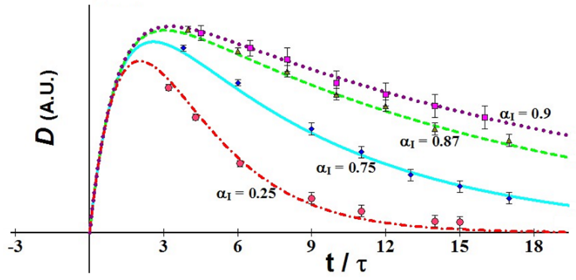

Figure 1: Diffusion behaviour vs time for some values of α_I (see text) as prediction of the model. Dots are experimental data from THz spectroscopy [23], with distribution represented by error bars

The peculiarities of its mathematical structure are giving also interesting informations about previsions of new behaviours at nanoscale [20-22] (Figure 2).

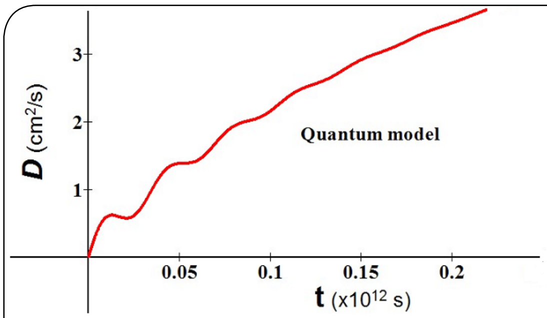

Figure 2: Initial oscillation in diffusion, appeared using the quantum version and considering data from literature [24]

The sensitivity of a nano-bio-device is connected to the increase and rapidity of detection, i.e. to the charge transport inside a device and therefore to the values and variations of its diffusion.

The quantum and relativistic diffusion coefficients D present the following analytical expressions respectively:

$$D(t)=\left(\frac{k_B T}{m^*}\right)\sum_{i=0}^{n}\left(\left(\frac{f_i \tau_i}{\alpha_{iI}}\right)\left[\exp\left(-\frac{(1-\alpha_{iI})}{2}\frac{t}{\tau_i}\right)-\exp\left(-\frac{(1+\alpha_{iI})}{2}\frac{t}{\tau_i}\right)\right]\right) \quad (1)$$

$$D(t)=\left(\frac{k_B T}{m_0}\right)(\tau)\left(\frac{1}{\gamma}\right)\left(\frac{1}{\alpha_{I_{rel}}}\right)\left[\exp\left(-\frac{(1-\alpha_{I_{rel}})}{2\rho}\frac{t}{\tau}\right)-\exp\left(-\frac{(1+\alpha_{I_{rel}})}{2\rho}\frac{t}{\tau}\right)\right] \quad (2)$$

with k_B the Boltzmann's constant, T the temperature of the system, m_0 and m* rest and effective mass respectively, τ_i and ω_i relaxation time and frequency of the i-th state respectively, ω_0 center frequency, $\alpha_I \in (0,1) \subset$ ¯¯ parameter of the model with the following definitions:

$$\alpha_{iI}=\sqrt{1-4\tau_i^2\,\omega_i^2} \quad (3)$$

$$\alpha_{I_{rel}}=\sqrt{1-4\gamma\,\omega_0^2\,\tau^2} \quad (4)$$

with $\gamma=1/\sqrt{1-\beta^2}$, $\beta=v/c$, $\rho=1+\beta^2\gamma^2=\gamma^2$ [9,10]. The model contains also another parameter $\alpha_R \in$ ¯¯+, which keeps into account of damped oscillating behaviour of diffusion, and it works from sub-pico-level to macro-level. Current results concern the nano-level.

Many variables can influence the diffusion and therefore the sensitivity of a nano-bio-device; considering Eqs. (1) and (2):

1) the temperature T of the system;

2) the parameter $\alpha_I=\alpha_I(\tau_i,\omega_i)$, i.e. the values of τ_i and ω_i;

3) the variation of the effective mass m*, linked to the physical and chemical treatments on materials, like doping [25,26];

4) the variations of the chiral vector inscribed in (n,m) indices [27];

5) the quantum weights of each mode and the variation of carrier density N [9];

6) the possibility to vary the initial peak in diffusion and the value of diffusion in time through a modulation of the carriers velocity [10].

In conclusion, being the diffusion strictly connected to the sensitivity and therefore to the performance of nano-bio-devices, it is possible to determine the peculiar characteristics of a nanomaterial-based device, considering parameters such as the temperature of the system, the variation of the effective mass, frequencies and relaxation times, weights of each mode, variation of carrier density, the possibility to relativistic-like carriers velocities for ultrashort times. The new predictions could be properly confirmed considering powerful experimental time-resolved techniques, like TRTS [28-33].

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