

Diffusion in Nano-Systems as a Function of Carrier Mass Analyzed with a New Analytical Transport Model

P. Di Sia^{1,2,*}

¹University of Verona, Lungadige Porta Vittoria 17, 37129, Verona, Italy.

²ISEM, Institute for Scientific Methodology, 90011, Palermo, Italy.

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ABSTRACT

Nano-research is considered very promising as basis for micro-nano-systems sector. In micro-nano-devices an important role is played by sensitivity, which can be modified in relation to used materials, so as in relation to the effective mass of the carriers travelling inside the nano-structure. The efforts in designing new devices benefit of theoretical modelling, which continuously tests current experimental data and offers innovation. In this paper an interesting analysis concerning possible ways in the process of performance improvement of micro-nano-systems is considered, in particular in relation to a recently appeared analytical model for transport dynamics. Variations of the carrier mass and the corresponding advantages are considered and analyzed, in relation to the most used nano-materials in this area, as Si, TiO₂, ZnO, GaAs and CNTs.

1. Introduction

Considering the current increase of pollution, the global warming and world crisis, the search for cleaner and renewable energy resources is a human duty for present and for future generations [1, 2]. It is therefore mandatory the exploration of alternative sustainable energy resources, such as biomass/biofuel [3], geothermal power [4], hydrogen energy [5], solar energy [6]. The rapid growth of mobile electronics for applications in communication, environmental monitoring, personal health care, defense, medicine is oriented in the same direction. For these reasons, the development of technologies for powering sensors and micro-nano-systems is one of the primary objective of theoretical and applied science [7].

The development of nano-bio-devices and nano-bio-sensors inevitably passes through their fast operativity and sensitivity; in the case of nano-materials utilization, this leads to the study of diffusion characteristics [1, 8, 9].

In this paper a detailed study concerning the behaviour of diffusion in relation to the effective mass of carriers travelling in a nanostructure is presented, considering some of the most used nano-materials at today. A recent theoretical analytical model, able both to predict new peculiarities and confirm existing experimental data, will be used [10]. It shows that the use of particular materials allows an increase of sensitivity for micro-nano-bio-devices and sensors based on them; the future improvements in this direction are expected to reduce the time scale for real-time detection and their sensitivity.

Simulation of inorganic nanotubes (INT) is based on the same concepts used for carbon nanotubes (CNT) where the nanotubes are assumed to be formed by rolling up of nano sheet (NS) to form a hollow cylinder and can be single or multi walled. For CNT, the basic structural unit is a single atomic layer, known as graphene [18, 19]. Majority of INT are of the form MX₂ (M=transition metal, X= S, Se, O). The basic structural unit of these INT is a triple layer sheet, consisting of a layer of transition metal cations and sandwiched between layers of anions [20]. WS₂ NT was the first MX₂ NT discovered in 1992, soon followed by MoS NT in 1993 and thereafter by others [21].

It should be noted that in NS, two of their dimensions are not confined to nano scale and are extremely thin films with thickness less than 100 nm. They can be deposited on a substrate (nano films), free standing (nano sheets), multi-layer structures (nano laminates) or integrated in a surrounding matrix material. NS can be metallic, ceramic or polymeric and used as single layer or multilayer structures [22].

From information available, theoretical studies of zirconia NS (ZNS) and ZNT are presently lacking or minimal [16]. Therefore, in this study an attempt is made to understand the relation between bulk ZrO₂ and ZNS made from cubic polymorph. More emphasis is on structural properties of sheets cleaved from ZrO₂ bulk in order to obtain details of the geometry of the basic units of ZNS required for simulation of ZrO₂ NT.

2. Experimental Methods

2.1 Analytical Model for Carrier Transport

The Drude-Lorentz model, one of the most utilized models for describing the charge transport in nanostructures [11, 12], gives detailed information about transport parameters, as the velocities correlation function $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_r$, the mean square deviation of position $R^2(t)$ and the diffusion coefficient $D(t)$. Recently it has appeared a generalization of this model [10], which works in the time domain and has the interesting characteristic to be an analytical treatment; in these years the classical version has been generalized at quantum [13] and relativistic level [14].

The general calculation is performed via contour integration [15] and the integral is determined by the poles of the real part $Re \sigma(\omega)$ of the complex conductivity $\sigma(\omega)$ in the complex plane. The analytical expression of the velocities correlation function $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_r$ allows the analytical calculation of the mean square deviation of position:

$$R^2(t) = 2 \int_0^t dt' (t-t') \langle \vec{v}(t') \cdot \vec{v}(0) \rangle \quad (1)$$

and the diffusion coefficient [10,13,14]:

$$D = \frac{1}{2} \frac{d}{dt} R^2(t) \quad (2)$$

The behaviour of diffusion has been analysed as a function of the carriers mass travelling inside a nanostructure, electrons in this case, but we wish to underline that the model holds also in consideration of different charged carriers, as ions. The expressions of the diffusion coefficient D in the classical case are two [10]:

*Corresponding Author

Email Address: paolo.disia@gmail.com (P. Di Sia)

$$D = 2 \left(\frac{K_B T}{m_{eff}} \right) \left(\frac{\tau}{\alpha_R} \right) \sin \left(\frac{\alpha_R t}{2 \tau} \right) \exp \left(-\frac{t}{2 \tau} \right), \quad (3)$$

$$D = \left(\frac{K_B T}{m_{eff}} \right) \left(\frac{\tau}{\alpha_I} \right) \left(\exp \left(-\frac{1 - \alpha_I t}{2 \tau} \right) - \exp \left(-\frac{1 + \alpha_I t}{2 \tau} \right) \right) \quad (4)$$

where K_B is the Boltzmann constant and $T = 300$ K is the fixed temperature of the system. In Eqs. (3), (4) two parameters of the model α_R and α_I appear, defined as:

$$\alpha_R = \sqrt{4 \tau^2 \omega^2 - 1}, \quad (5)$$

positive real number, and:

$$\alpha_I = \sqrt{1 - 4 \tau^2 \omega^2}, \quad (6)$$

real number such as $0 < \alpha_I < 1$, with τ and ω relaxation time and frequency respectively.

3. Results and Discussion

The following nano-materials have been considered: Si, TiO₂, ZnO, CNTs, GaAs. With experimental data from literature (Table 1), it is possible to calculate the values of α_R and α_I (Table 2) and therefore to study the behaviour of diffusion in time.

Table 1 Values of effective mass m_{eff} and relaxation time τ for the considered nano-materials; m_e is the mass of the electron.

Nanomaterial	m_{eff}	τ (s)
Si [16]	$1.08 m_e$	0.5×10^{-13}
TiO ₂ [17]	$6 m_e$	0.1×10^{-13}
ZnO [18]	$0.24 m_e$	0.84×10^{-13}
CTN [19]	$0.5 m_e$	0.17×10^{-13}
GaAs [20-22]	$0.067 m_e$	3.24×10^{-13}

From Ref. [22], the value $\mu_e = 8500 \text{ cm}^2 / (\text{Vs})$ for the calculation of τ has been used.

Table 2 Values of α_I and α_R (Eqs (3), (4)) calculated considering two fixed values of ω (see text) and values of τ from Table 1.

Nanomaterial	$\alpha_I(\omega_1)$	$\alpha_R(\omega_2)$
Si	0.995	9.950
TiO ₂	0.999	1.732
ZnO	0.986	16.770
CTN	0.940	33.985
GaAs	0.760	64.800

Two values of ω have been fixed, deliberately far, covering a wide range in frequency: $\omega_1 = 10^{12}$ Hz, $\omega_2 = 10^{14}$ Hz. Figures 1, 2, 3 illustrate the behaviour of diffusion versus time t for the considered nano-materials, increasing gradually the scale of diffusion for a detailed view of the found diffusion values. The first fixed value of frequency $\omega_1 = 10^{12}$ Hz led to $\alpha < 1$ values. The involved relation is therefore Eq. (4), a superposition of two exponentials, as functions of t , τ and $\alpha(\tau, \omega)$.

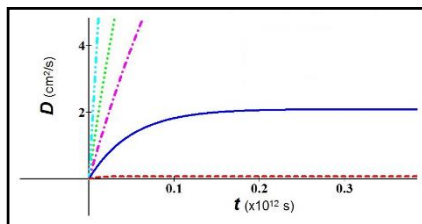


Fig. 1 Behaviour of D (in the range $(0, 4) \text{ cm}^2/\text{s}$) vs time for the considered nano-materials; TiO₂: red dashed line; Si: blue solid line; CNT: violet dot-dashed line; ZnO: green dots line; GaAs: light blue double dot-dashed line. For the other parameters see text and Tables 1, 2.

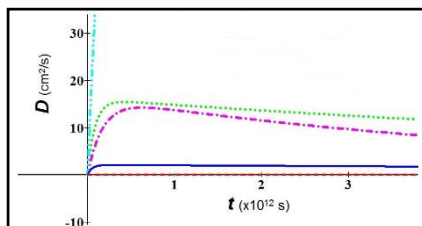


Fig. 2 Behaviour of D (in the range $(0, 30) \text{ cm}^2/\text{s}$) vs time for the considered nano-materials; TiO₂: red dashed line; Si: blue solid line; CNT: violet dot-dashed line; ZnO: green dots line; GaAs: light blue double dot-dashed line. For the other parameters see text and Tables 1, 2.

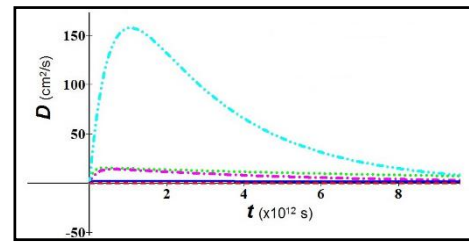


Fig. 3 Behaviour of D (in the range $(0, 150) \text{ cm}^2/\text{s}$) vs time for the considered nano-materials; TiO₂: red dashed line; Si: blue solid line; CNT: violet dot-dashed line; ZnO: green dots line; GaAs: light blue double dot-dashed line. For the other parameters see text and Tables 1, 2.

Figures 1-3 underline the importance of having small effective mass of nanomaterials for the increase of diffusion. Another interesting factor to keep in due consideration is also the rapidity to reach the maximum value of diffusion, important feature in building micro-nano-devices (-sensors), and dependent by their specific use.

Figures 4 and 5 illustrate the behaviour of the diffusion D versus time t , considering the second fixed value of frequency $\omega_2 = 10^{14}$ Hz. In this case we find $\alpha > 1$ values, therefore the involved relation is Eq. (3), a product of a sinusoidal function times an exponential, doing a damped oscillatory behaviour.

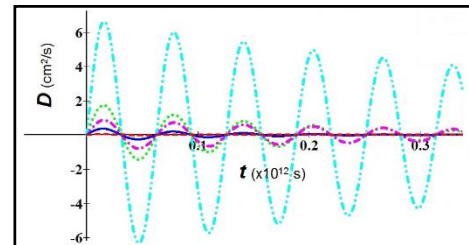


Fig. 4 Behaviour of D (in the range $(-6, 6) \text{ cm}^2/\text{s}$) vs time for the considered nano-materials; TiO₂: red dashed line; Si: blue solid line; CNT: violet dot-dashed line; ZnO: green dots line; GaAs: light blue double dot-dashed line. For the other parameters see text and Tables 1, 2.

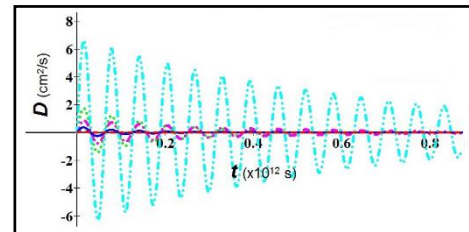


Fig. 5 Behaviour of D (in the range $(-6, 8) \text{ cm}^2/\text{s}$) vs time for the considered nano-materials; TiO₂: red dashed line; Si: blue solid line; CNT: violet dot-dashed line; ZnO: green dots line; GaAs: light blue double dot-dashed line. For the other parameters see text and Tables 1, 2.

In this second case we have both the possibility of having high values of diffusion and rapidity to reach the maximum D -value in short times. These are important characteristics for micro-nano-sensors, independently by their peculiar use [8].

4. Conclusion

In this paper the application of a new model for transport processes has been attempted, which is a new formulation of the Drude-Lorentz model, for studying the electron diffusion inside a micro-nano-structure. The study focused on the dependence of diffusion by values of effective mass of carriers inside currently used nano-materials, i.e. silicon, titanium dioxide, zinc oxide, carbon nanotubes and gallium arsenide. CNTs, ZnO and GaAs show interesting high values of diffusion; they are therefore to be taken into due consideration in the creation process of micro-nano-devices (-sensors) with particular characteristics of high sensitivity.

Searching for good performance values of diffusion and rapidity to reach the extreme values in the range of diffusion allowed by the specific nano-material, the variation of effective masses can be usefully complemented by the variation of the temperature of the system, the relaxation time and the frequency. Eqs. (3) and (4) show that the diffusion is a function of temperature, relaxation time and frequency too: $D = f(T, m_{eff}, \tau, \omega)$, with $\alpha_{R/I} = \alpha(\tau, \omega)$; it is however noteworthy the study of each variable separately by the others, for a better understanding of their specific role in the overall context.

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