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Effects on Diffusion by Relativistic Motion in Nanomaterials

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***Abstract* — considering the results of experimental research, theoretical modelling brings continuously new details in the knowledge of matter at nanoscale. It has been recently appeared a new "time-domain" Drude-Lorentz-like model for classical and quantum transport in nanosystems, demonstrating high generality and good fitting with experimental literature data. The extension of this model to relativistic particles travelling in nanostructures offers interesting new details, in particular in relation to a variation in diffusion of charges travelling in nanomaterials. This peculiarity has current crucial importance in the sector of applications, for example in the biological and medical sectors, so as for nano-bio-devices fabrication. After a brief introduction, new technical details and examples of application for nano-diffusion at relativistic velocity are presented.**

Index Terms **— Diffusion, Nano-bio-materials, Nanofabrication, Nano-bio-devices, Theoretical modelling, Relativistic velocity.**

I. INTRODUCTION

In modern industry we assist to a progressive miniaturization of used devices and systems, having progressively reached the nanoscale domain. In particular the nanofabrication aims at building nanoscale structures able to act as components, devices, systems, hopefully in large quantities and at low cost. All nanotechnology fields draw advantage by nanofabrication, especially for the realization of nano devices involving the traditional areas across engineering and science [1]. The conventional technologies consider the emerging techniques developed for next generation lithography, while the non-conventional include scanning probe microscopy lithography, self-assembly and imprint lithography, so as distinctly developed techniques for realizing carbon tubes and molecular devices [2]. The nanofabrication is crucial for the realization of possible conceivable benefits in the field of electronics, bioengineering and material science. Of increasing importance are for example the advantages of ultra-high resolution capability, the use of tip-based nanofabrication technology as proper tool in the nanoscale structures manufacturing, so as single-probe tip technologies, multiple-probe tip methodology, 3-D modelling with tip-based nanofabrication and imaging technology [3], [4]. A great variety of nanodevices for electronic, optoelectronic, photonic, bio-mechanical applications have been created through the fast development of materials and fabrication technology. Further developments in this direction deeply depend on the state-of-art knowledge of science and technology at nanoscale, in particular by modalities to vary the response of nanodevices, which depends strongly by diffusion of charges inside nanostructures [5]. Improvements in the knowledge of diffusion peculiarities can benefit implantable, ultrasensitive, chemical and molecular bio-sensoristics, so as medical science, nano-robotics, micro-(nano)-opto-electro-mechanical systems (M(N)OEMS), remote and mobile environmental sensors, portable and resistant personal electronics, electro-mechanical coupled devices, manipulation processes at nano-molecular level [6], [7]. Aamong the most commonly studied, promising and used nanomaterials, we have nowadays Silicon (Si), Zinc Oxide (ZnO), Titanium Dioxide (TiO_2), Gallium Arsenide (GaAs) and Carbon Nanotubes (CNTs). The theoretical detailed understanding of the behaviour of transport processes in these nanomaterials is therefore crucial for indicating new application ideas and new streams in nanofabrication. One of them concerns the study of the implications of relativistic motion in nanostructures [8]. After a technical introduction of the relativistic expression of diffusion through a new analytical model, interesting examples of application will be presented, where it is possible to check that ultra-fast injections of charges in a nanostructure offers the possibility to vary the initial peak in diffusion and the value of diffusion in time, through a modulation of the carriers velocity.

II. RELATIVISTIC EXPRESSION OF DIFFUSION THROUGH A NEW ANALYTICAL MODEL

Recently it has been appeared a new analytical model, which generalizes the Drude-Lorentz model, based on the complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$ of a system. It provides analytical time-dependent expressions of the most important quantities related to the transport processes, i.e. the

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velocities correlation function $<\vec{v}(t)\cdot\vec{v}(0)>_T$ at temperature *T*, the mean squared deviation of position $R^2(t)=\left\langle[\vec{R}(t)-\vec{R}(0)]^2\right\rangle$ and the diffusion coefficient *D* of a system [7], [9], [10]. Considering literature data, it is possible both to fit and confirm experimental results and to find new characteristics and details for experimental confirmation and for the fabrication of nano-bio-devices with desired characteristics [11]-[15]. The model was performed in classical and quantum way; the complete relativistic version is under construction [16]. In this paper new results regarding the relativistic analytical expression of diffusion are introduced.
Considering the motion equation of a particle travelling in a nanostructure, the starting point is the dynamics law:

$$\frac{d}{dt}(m_{part}\,\vec{v})=\sum_i \vec{F}_i\,. \quad (1)$$

About forces acting on particle, it has been considered an outer passive elastic-type force of the form $F_{el}=K\,x$, with $K=m_0\,\omega_0{}^2$, a passive outer friction-type force of the form $F_{fr}=\lambda\,\dot{x}$, with $\lambda=m_0\,\gamma/\tau$, and an outer oscillating electric field $E=e\,E_0\,e^{-i\omega t}$.
thinking the motion along an *x*-axis and in the fixed ground reference frame, with the same procedure utilized for the performed classical and the quantum case [9], [10], the equation becomes:

$$m_0\,a\,\gamma\left(1+(\beta\gamma)^2\right)=\sum_i \vec{F}_i\,, \quad (2)$$

with $\beta=v/c$ and $\gamma=1\Big/\sqrt{1-\beta^2}$.
The diffusion coefficient is defined as $D(t)=1/2\left(dR^2(t)/dt\right)$; it is possible also to write it as a function of the velocities correlation function:

$$D(t)=\frac{1}{2}\frac{dR^2(t)}{dt}=\int_0^t dt'\left\langle\vec{v}(t')\cdot\vec{v}(0)\right\rangle. \quad (3)$$

Having the relativistic analytical expression of $<\vec{v}(t)\cdot\vec{v}(0)>_T$ [16], the time-dependent form of the diffusion coefficient *D* is as follows:

$$D=\left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma}\right)\left(\frac{\tau}{\alpha_{I_{rel}}}\right)\left(\exp\left(-\frac{1-\alpha_{I_{rel}}}{2\rho}\frac{t}{\tau}\right)-\exp\left(-\frac{1+\alpha_{I_{rel}}}{2\rho}\frac{t}{\tau}\right)\right), \quad (4)$$

where k_B is the Boltzmann's constant, T the temperature of the system, m_0 the rest mass of the carrier, τ the classical relaxation time. The parameter $\alpha_{I_{rel}}$ is a parameter of the model; it is defined in this way:

$$\alpha_{I_{rel}}=\sqrt{1-\frac{4\rho\,\omega_0^2\,\tau^2}{\gamma}}=\sqrt{1-4\gamma\,\omega_0^2\,\tau^2}\,, \quad (5)$$

with $\rho=1+\beta^2\gamma^2=\gamma^2$ and ω_0 classical center frequency [7], [9], [10], [17].

III. RESULTS AND DISCUSSION

It has been considered the effects of relativistic velocities of carriers in relation to the behavior of *D* for the previously indicated nanomaterials, considering in all cases the room temperature $T=300K$, the parameter of the model $\alpha_{I_{rel}}=0.5$ ($\alpha_{I_{rel}}\in[0,1]\subset\mathbb{R}$) and values of m and τ as resumed in Table 1.

Nanomaterial	m^*	$\tau(s)$
CTN [18], [19]	$0.5\,m_e$	$0.17\cdot10^{-12}$
Si [20]	$1.08\,m_e$	$0.5\cdot10^{-13}$
TiO_2 [21]	$6\,m_e$	$0.1\cdot10^{-13}$

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ZnO [22]	0.24 m_e	$0.84 \cdot 10^{-13}$
GaAs [23], [24]	0.067 m_e	10^{-12}

Table 1. Values of effective masses m^* and relaxation times τ for the indicated nanomaterials (m_e = electron mass at classical "Drude" velocity $v = 10^7\ cm/s$, which is equal to the rest mass of electron with an error less than $1/10^7$) [18]-[24].

In Fig. 1 the variation of the diffusion in time for CNTs is presented, starting by non-relativistic velocity of the carriers moving in a nanostructure and considering then relativistic velocities. The increase in carriers velocity implies a marked variation of the initial peak of diffusion, so as a substantial change in the process of diffusion decrease.

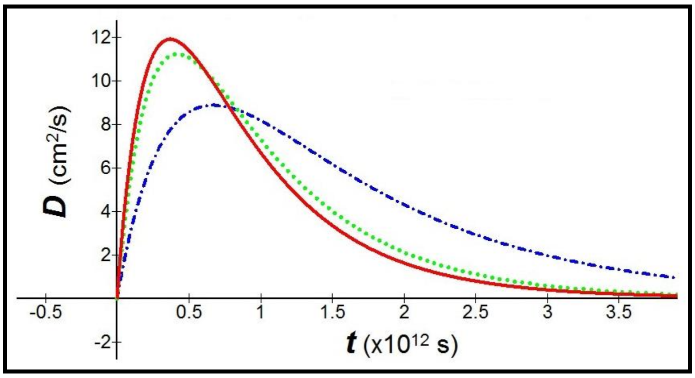

Fig. 1. *D* vs *t* for CNTs at three different velocities of the carriers (red solid line: $v_e = 10^7\ cm/s$; green dashed line: $v_e = 10^{10}\ cm/s$; blue dot-dashed line: $v_e = 2 \cdot 10^{10}\ cm/s$). The considered value of the parameter $\alpha_{I_{rel}}$ is: $\alpha_{I_{rel}} = 0.5$ [18], [19].

In Fig. 2 the *D* behavior of Si is considered.

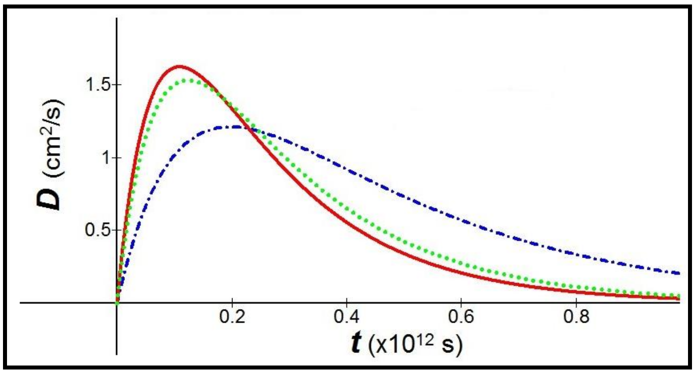

Fig. 2. *D* vs *t* for Si at three different velocities of the carriers (red solid line: $v_e = 10^7\ cm/s$; green dashed line: $v_e = 10^{10}\ cm/s$; blue dot-dashed line: $v_e = 2 \cdot 10^{10}\ cm/s$) [20].

In Figs. 3-5 the same procedure has been applied for TiO_2, ZnO and GaAs respectively. For direct comparison, the curves related to all considered nanomaterials are reported in Fig. 6, in the case of non-relativistic involved carriers velocities.

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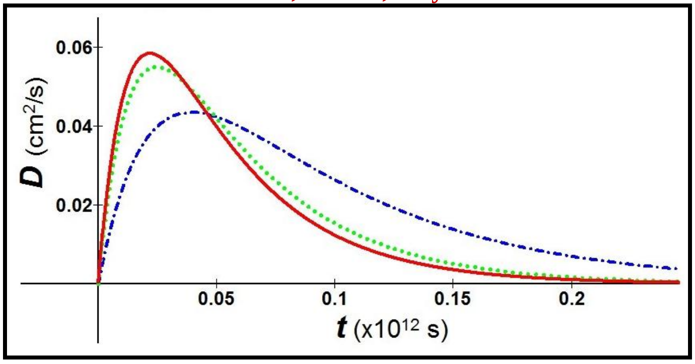

Fig. 3. ***D*** **vs** ***t*** **for** TiO_2 **at three different velocities of the carriers (red solid line:** $v_e = 10^7\ cm/s$ **; green dashed line:** $v_e = 10^{10}\ cm/s$ **; blue dot-dashed line:** $v_e = 2 \cdot 10^{10}\ cm/s$ **) [21].**

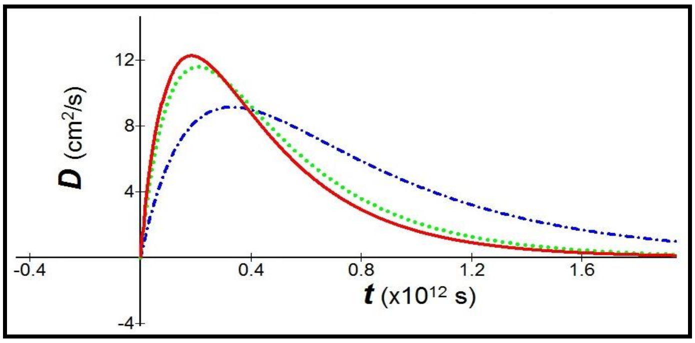

Fig. 4. ***D*** **vs** ***t*** **for ZnO at three different velocities of the carriers (red solid line:** $v_e = 10^7\ cm/s$ **; green dashed line:** $v_e = 10^{10}\ cm/s$ **; blue dot-dashed line:** $v_e = 2 \cdot 10^{10}\ cm/s$ **) [22].**

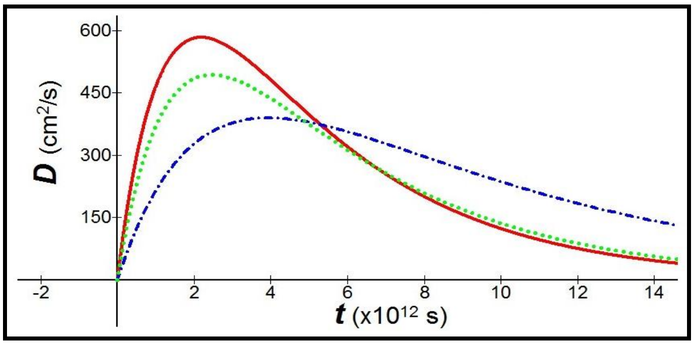

Fig. 5. ***D*** **vs** ***t*** **for GaAs at three different velocities of the carriers (red solid line:** $v_e = 10^7\ cm/s$ **; green dashed line:** $v_e = 10^{10}\ cm/s$ **; blue dot-dashed line:** $v_e = 2 \cdot 10^{10}\ cm/s$ **) [23], [24].**

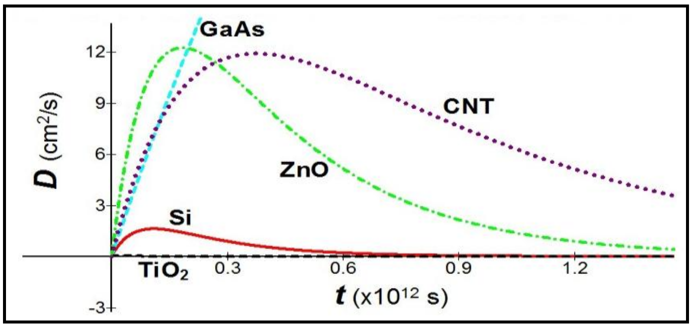

Fig. 6. Variation of ***D*** **in time for the considered nanomaterials, with classical "Drude" velocity of the carriers [18]-[24].**

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Table 2 resumes the peak values of diffusion, as determinable by figures, concerning the variation by classical to relativistic velocities of carriers.

Nanomaterial	D_1 (cm^2/s)	D_2 (cm^2/s)	D_3 (cm^2/s)
CTN	11.96	11.26	8.96
Si	1.63	1.53	1.21
TiO_2	0.06	0.05	0.04
ZnO	12.3	11.63	9.2
GaAs	587.1	495.4	392.9

Table 2. Peaks in diffusion with $v_{carrier} = 10^7\ cm/s$ (D_1), $v_{carrier} = 10^{10}\ cm/s$ (D_2) and $v_{carrier} = 2 \cdot 10^{10}\ cm/s$ (D_3), related to the considered nanomaterials [18]-[24].

Some considerable points are to be noted concerning the obtained results:

1) The possibility of a relativistic motion in a nanostructure brings in general to a decrease of the peak in diffusion, but increases the diffusion in time;

2) This behaviour is one of the modalities with which it is possible to act for varying the diffusion in nanomaterial-based nanodevices;

3) other possibilities have been studied, as the variation of temperature of the system [14], the variation of the effective mass through the doping and in connection to the chiral vector [18], [25], the variation of the parameter $\alpha_{I_{rel}}$ of the model [9], [10], [16], which is referred to the frequency and the relaxation times;

4) The importance of the study of these parameters at nanofabrication level;

5) The model is useful in both ways:

a) For creating new devices with the desired characteristics;

b) For testing and/or obtaining new parameters values by existing experimental data.

IV. CONCLUSIONS

In this work it has been considered the application of relativistic results concerning the diffusion of a new recently appeared theoretical model [7], [9], [10], [16] related to the evolution of the diffusion in time for five among the most important materials currently utilized at nano-bio-level [7], [11]-[15]. The carried analysis showed that the possibility of a variation in velocity for the carriers travelling inside a nanostructure (electrons in this case, but the model holds for charged particles in general) represents one of the possibilities to be considered in the fabrication of nano-bio-devices with precise and well determined characteristics. The model is able to meet, through appropriate combinations of these parameters, a large spectrum of practical and technological needs, particularly in the nano-bio-devices sector and at nano-bio-sensoristic level. The possibility of a rapid answer for the carriers transport is a very considerable peculiarity concerning nano-bio-devices, nano-energy systems, nano-technologies sector, nano-medicine. The ability to obtain different peak values and decay times for diffusion may be the basis for the ideation and fabrication of new particular nano-bio-devices, well adapted to the required characteristics.

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