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Enhanced Diffusion for Nano-Systems: Interesting Details by a New Analytical Drude-Lorentz-Like Model

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***Abstract* – The nano-systems sector is today very important and requires advances for the increase of nanodevices performance. Among the most important characteristics required to nano-systems, the sensitivity plays a peculiar role, determining significant improvements of their quality. The paper offers an interesting analysis on the opportunity to increase the performance of nano-systems through a new appeared analytical model for the study of transport dynamics, which is able to accommodate previously not completely understood behaviours and predicts new interesting features at nanoscale.**

***Keywords* – Nano-Systems, Diffusion, Nano-Bio-Materials, Sensitivity, Analytical Theoretical Modelling.**

I. INTRODUCTION

Currently the ability to manipulate the matter, combined with advances in synthesis and assembly of structures at nanoscale, is carrying to interesting advances in scientific and technological areas. Peculiar examples can be done:

1) The discovery and controlled preparation of carbon nanotubes, with appropriate use for the fabrication of individual electronic devices [1], [2];
2) The increasing ability to put engineered individual molecules onto appropriate electrical contacts and to measure the transport characteristics through molecules [3], [4];
3) The availability of proximal probe techniques for the manipulation of matter and for the fabrication of nanostructures [5]-[7];
4) The development of chemical synthetic methods for preparing nanocrystals and methods for assembling them into a variety of larger organized structures [8];
5) The introduction of biomolecules and supermolecular structures in the field of nanodevices [9], [10];
6) The isolation of biological motors and their incorporation into non-biological environments [11], [12].

We assist to an increase of new devices creation in microelectronics and telecommunications industries, which rely on nanoscale phenomena for their operation, also based on thin film layers with thicknesses in the nano-range. These kinds of systems are categorized as nanodevices by their main feature at nanoscale, rather than by their large-scale dimensions [13].

For a deep understanding of nanoscale phenomena, a rigorous knowledge of the electronic, magnetic and photonic interactions at this size scale is needed; this is achieved through experiments, theory and modelling [14]. Nanoelectronic devices, nanoprobes and sensors measure and control the nanoworld, in which properties are different with respect to that of the ordinary macroworld. The development of nanoscale objects, which manipulate and perform work on other nanoscale objects in efficient way, is bringing to the same results currently obtained with scanning tunneling microscopy (STM) and atomic force microscopy (AFM) [15], so as the integration of nanoscale control electronics onto micromachines [16]. All this is based on the theoretical comprehension of transport properties at nanoscale [14] and is addressed by the new peculiarities that theoretical modelling finds. In this paper interesting details related to diffusion in nanosystems, determined through a new analytical theoretical model, will be done.

II. NANOWIRE-BASED ELECTRONICS

Nanowires-based devices are a powerful class of ultrasensitive devices for the useful utilization at chemical, biological, environmental, medical level, covering many areas of life sciences and healthcare, by diagnosing diseases to discovery and screening of new drug molecules [17]-[19]. Nanowire field-effect devices, also modified with specific surface receptors, represent a powerful detection platform for a broad range of biological and chemical species in solution; they have a great number of key features, including direct, label-free, real-time electrical signal transduction, ultrahigh sensitivity, fine selectivity [20]-[23]. These devices have unique capabilities in the detection of proteins, viruses, DNA for the analysis of small organic molecule binding to proteins, with the potential to significantly impact on disease diagnosis, genetic screening, drug discovery, as well as powerful new tools for research in many biology areas [24]. Advances in this direction can be developed at commercial level in simple nanowire devices, representing a clear application of nanotechnology and a substantial human benefit. Progress in capabilities for assembling larger and more complex nanowire sensor arrays and integrating them with first conventional and later nanoscale electronics for processing, is leading to powerful sensor systems, that help to enable the future dream of personalized medicine [25]. Considering that these nanowire sensors transduce chemical/biological binding events into electronic/digital signals, the potential for a highly sophisticated interface between nanoelectronics and biological information processing systems is suggested [26]. Electronic and optoelectronic devices impact many areas of society, from simple household appliances and multimedia systems to communications, computing and instrumentation. Given the strong demand of compact and powerful systems, there is growing interest in the development of nanoscale devices with new functions and enhanced performance [27].

Semiconductor nanowires emerged as a powerful class of materials that, through controlled growth and organization, are opening up interesting opportunities for novel nanoscale photonic and electronic devices. Semiconductor nanowires and carbon nanotubes offer many opportunities for the assembly of nanoscale devices and nanowire-based nanosystems. The rational control of key nanomaterial parameters is therefore a central point, including chemical composition, structure, size, morphology, doping; these parameters determine electronic and optoelectronic properties for predicting present and new devices functionalities. The rational control of these key parameters passes therefore through a deep understanding at theoretical level, with adequate mathematical modelling [28]. The increase of the parameters control for single nanowire-based nanodevices and basic NWs building blocks makes possible and will increase the key advantages of nanowires in electronics and photonics, compared with the current conventional technologies.

II. CONFIRMATIONS AND NEW INFORMATIONS FROM A NEW ANALYTICAL DRUDE-LORENTZ LIKE MODEL

In 2011 it has been appeared a new generalization of the Drude-Lorentz model, based on the complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$ of a system, able to offer 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 $R^2(t)=\left\langle[\vec{R}(t)-\vec{R}(0)]^2\right\rangle$ and the diffusion coefficient *D* [29], avoiding numerical and/or simulation procedures. The model is useful both "a priori", for the study of new devices with desired characteristics and "a posteriori", for testing and/or obtaining new parameters values by existing experimental data. It has been performed the classical and the quantum version of the model [29], [30] and started the complete relativistic version [31], [32].

The classical version of the model has been deeply tested in last years; it fit very well with existing experimental data [14], [23], [33], [34]-[45] and gives also explanations of the ultra-short times and of high mobilities, with which the charges spread in mesoporous systems, of large interest in photocatalitic and photovoltaic systems [46]-[48]. It is in agreement with important existing models, such as the Smith model [49], successfully applied to fit the conductivity in a variety of systems in the frequency domain, but also criticized for the presence of a parameter with not clear meaning, related to the backscattering mechanism; it arises in a natural way in this new model, without further assumption on successive scattering events.

The quantum version of the model comprehends the oscillator strength weights, related to the various energy levels. It demonstrated high generality and offered perspectives even in the study of ions, like mass transfer, and solutions, so as in nanobiosystems. It allows significant applications for the diffusion in nanostructured, porous and cellular materials, so as for biological, medical and nanopiezotronic devices [50]-[52].

III. DISCUSSION AND RESULTS

The sensitivity is one of the most interesting feature for a nanobiosystem; it 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 diffusion.

Among the most promising nanomaterials, studied at today at theoretical and experimental level, we find Silicon (Si), Zinc Oxide (ZnO), Titanium Dioxide (TiO_2), Gallium Arsenide (GaAs), Carbon Nanotubes (CNTs), Cadmium Telluride (CdTe), Cadmium Sulfide (CdS), Copper Indium Selenide (CIS), Copper Indium Gallium Selenide (CIGS).

Considering a nanowire as the basis element of a nanobiosystem (device), an interesting analysis related to the diffusion of some indicated materials has been done. The obtained results permit both to confirm experimental existing results and also to offer interesting previsions, which could be of great interest in the development and improvement of new high efficiency nanobiosystems, nanobiosensors and nanobiodevices .

The diffusion coefficient *D* related to the new model in the classical version has two analytical expressions, in relation to two parameters of the model. The expression, that does the best results in relation to experimental existing data is as follows:

$$D=\left(\frac{KT}{m*}\right)(\tau)\left(\frac{1}{\alpha_I}\right)\times\times\left(\exp\left(-\frac{1-\alpha_I}{2}\frac{t}{\tau}\right)-\exp\left(-\frac{1+\alpha_I}{2}\frac{t}{\tau}\right)\right) \tag{1}$$

with K the Boltzmann's constant, T the temperature of the system, m^* the effective mass and τ the relaxation time. $\alpha_I\in[0,1]$ is a parameter of the model, a real number with the following definition:

$$\alpha_I=\sqrt{1-4\tau^2\omega_0^2} \tag{2}$$

Many variables can influence the diffusion and therefore the sensitivity of a nanobiosystem; considering (1):

1) The temperature *T* of the system, directly proportional to *D*;

2) The parameter $\alpha_I=\alpha_I(\tau,\omega_0)$, i.e. the values of τ and ω_0; we note that $\alpha_I(\tau,\omega_0)$ appears also in the arguments of the exponentials in (1), therefore its variation affects also with the form of the diffusion curves;

3) The variation of the effective mass m^*, related to the physical and chemical treatments on materials, like doping. Doped nanomaterials provides a flexible way to tune to the properties of the materials; the electronic, optical, photochemical, photoelectrochemical, photocatalytic and photoexcited properties can be tuned

towards the desired direction by doping different elements. Materials can be engineered towards specific applications, through accurate dopants selection [53], [54];

4) The variation of the chiral vector inscribed in (*n*,*m*) indices, which reflects in a variation of m^* [37];

5) For the quantum version of the model, the possibility to consider the weights of each mode and to vary the carrier density *N*, considering that it holds:

$$\omega_{p_i}^{2} = \frac{4\pi N e^2}{m} f_i \qquad (3)$$

with ω_{p_i} plasma frequencies [30];

6) For the relativistic version of the model, the possibility to vary the initial peak in diffusion and the value of diffusion in time, through a modulation of the carriers velocity [31], [32].

It has been considered the behaviour of *D* in relation to some of the previously indicated nanomaterials, for two different values of τ and near to the boundary values of the definition interval of α_I. Equation (2) contains three variables, so the knowledge of two of them permits the determination of the third one. It has been considered the environmental temperature *T* = 300 K for all considered situations, but it is possible to study also the behaviour as a function of *T*. In general (see (1)) the temperature helps the diffusion.

Fig. 1 represents the behaviour of the diffusion in time for Silicon. The considered values are $\alpha_{I1} = 0.1$, $\alpha_{I2} = 0.9$, $\tau_1 = 10^{-12}\,s$, $\tau_2 = 10^{-13}\,s$, with the respective effective mass value [39].

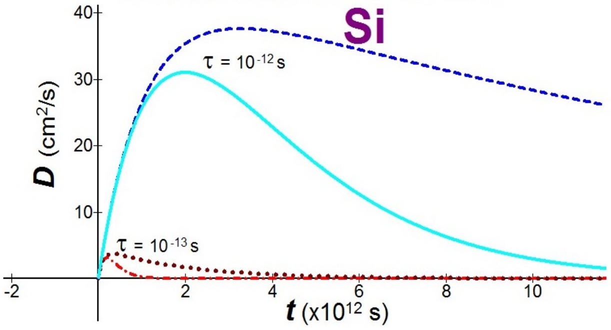

Fig.1. *D* vs *t* for Si at *T* = 300 K considering two different values of τ and α_I (see text); $m^*_{Si} = 1.08\, m_e$.

We note how the increase of τ, corresponding to a decrease of ω_0 for constant α_I (see (2)) helps the increase in diffusion; moreover, for τ constant, the variation of α_I brings to a variation in diffusion. The parameter α_I changes also the form of curves, because it appears in the arguments of the exponentials (see (1)), reflecting in a variation of the *D* curve shape.

It has been considered the same study for ZnO [41] (Fig. 2).

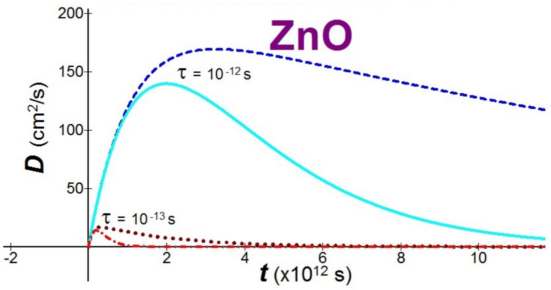

Fig.2. *D* vs *t* for ZnO at *T* = 300 K considering two different values of τ and of α_I (see text); $m^*_{ZnO} = 0.24\, m_e$.

Considering also the smaller effective mass of ZnO with respect to Si, we have in this case greater *D* values. In Figs 3-5 the same study for CdS [55], [56], CdTe [55], [57] and GaAs [55], [58], with decreasing m^* and the same values of *T*, τ and α_I, has been considered.

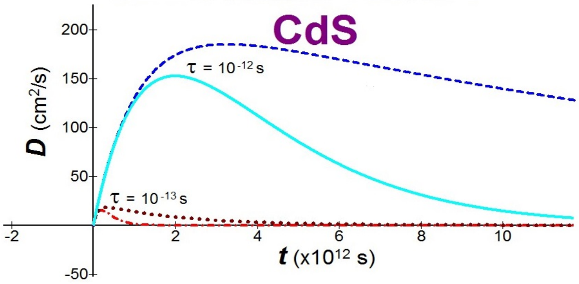

Fig.3. *D* vs *t* for CdS at *T* = 300 K considering two different values of τ and of α_I (see text); $m^*_{CdS} = 0.22\, m_e$.

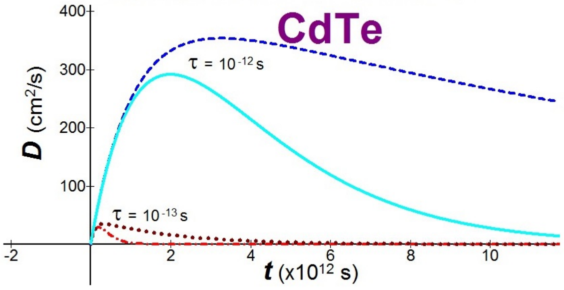

Fig.4. *D* vs *t* for CdTe at *T* = 300 K considering two different values of τ and of α_I (see text); $m^*_{CdTe} = 0.115\, m_e$.

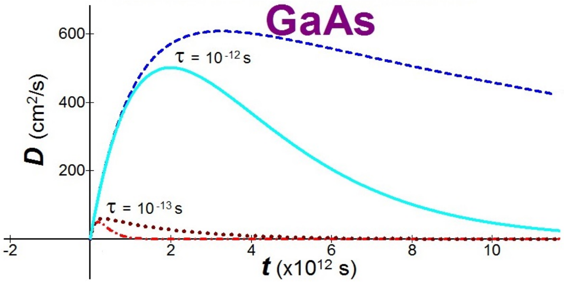

Fig.5. *D* vs *t* for GaAs at *T* = 300 K considering two different values of τ and of α_I (see text); $m^*_{GaAs} = 0.067\, m_e$.

IV. CONCLUSION

In this work it has been considered an interesting analysis about the possibilities of varying the diffusion of carriers inside a nanostructure. Being the diffusion strictly connected to the sensitivity and therefore to the performance of nanobiosystems, this implies the possibility to determine, through a theoretical study, the peculiar characteristics of a nanomaterial-based device. In this direction a new recently appeared theoretical analytical model can help, through the possibility of determining the most important functions related to the charge transport. As parameters for a variation of the device performance, the analysis indicates the temperature of the system, the variation of the effective mass, the variation of the parameter α_I of the model, which is referred to the frequency and the relaxation time, the possibility to consider the weights of each mode and to vary the carrier density N if a quantum treatment is considered, the possibility to consider relativistic velocities of the carriers, also for ultrashort times. The considered nanomaterials can meet, through appropriate combinations of the indicated parameters, a large spectrum of practical and technological needs.

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