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ANALYTICAL MODELLING FOR SENSITIVITY IMPROVEMENT OF NANO-BIO-DEVICES

Paolo Di Sia

University of Padova, School of Science, School of Engineering, Department of Neurosciences, Padova, Italy & Primordial Dynamic Space Research, Verona, Italy

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Abstract:

The nano-bio-device/sensoristic sector is one of the mainstreams of nanotechnology and requires careful information for constant improvement of the nanodevice performance. The sensing/sensitivity plays a peculiar role, is a determinant characteristics, able to cause a great improvement of the device quality. The paper provides a detailed analysis on the casuistry for increasing the performance of nano-systems through enhanced diffusion, studied with the use of a recent analytical transport model, able to accommodate previously not completely understood behaviours and to predict new interesting features at nanoscale.

Key Words: Nano-Bio-Materials, Nanophysics, Devices Performance, Diffusion, Sensitivity, Modelling, DS Model, Modern Education.

1. Introduction:

The ability to manipulate the matter, together with advances in synthesis and assembly of structures at the nanoscale, is nowadays carrying to important advances in scientific and technological areas. We can think to the discovery and controlled preparation of carbon nanotubes [1], the ability to put engineered molecules on appropriate electrical contacts for measuring the transport characteristics through molecules [2], the availability of proximal probe techniques for the manipulation of matter [3], the development of chemical synthetic methods for preparing nanocrystals [4], the introduction of biomolecules and supermolecular structures for nanodevices [5], the isolation of biological motors and their incorporation into non-biological environments [6].

New devices are created in microelectronics and telecommunications industries, relying on nanoscale phenomena and based on film layers with thickness in the nano-range; they are categorized as nanodevices by their main feature at nanoscale [7]. For a profound understanding of nanoscale phenomena, a severe knowledge of electronic, magnetic and photonic interactions at this scale is needed, achieved through experiments, theory and modelling [8]. The development of nanoscale objects is bringing to the same results currently obtained with scanning tunneling microscopy (STM) and atomic force microscopy (AFM), so as the integration of nanoscale control electronics onto micromachines [9]. This is based on the theoretical comprehension of transport properties at nanoscale [10], with the new peculiarities discovered by theoretical modelling.

In these years it has been performed a new generalization of the Drude-Lorentz model, based on the complete Fourier transform of the frequency-dependent complex conductivity of a system, that relies on analytical expressions of the most important quantities related to transport phenomena, i.e. the velocities correlation function at the temperature T, the mean squared deviation of position and the diffusion [11-13]. The model is useful both "a priori", for searching new characteristics and peculiarities at nano-level, and "a posteriori", for testing existing experimental data. The comparison with existing used models, as Drude-Lorentz and Smith models, has demonstrated a very good fit and is giving also interesting information about new behaviours at nanoscale [14,15]. Nanowires-based devices are a powerful class of ultrasensitive devices utilized in many environments as biological, chemical, medical ones, and in many areas of healthcare and life sciences. Given the high demand of growingly compact and powerful systems, there is a strong interest in the development of nanoscale devices with new functions and enhanced performance. The careful control of key nanomaterial parameters, which determine the electronic and optoelectronic properties, is decisive for the desired result, and modelling helps in this regard.

2. Nanowire-Based Electronics:

Nanowires-based devices are a powerful class of ultrasensitive devices for utilization at chemical, biological, environmental, medical level, covering areas of life sciences and healthcare [16,17]. They represent a detection platform for a broad range of biological and chemical species in solution, with a high number of key features, including direct, label-free, real-time electrical signal transduction, ultrahigh sensitivity, fine selectivity [18,19]. These devices are powerful in the detection of proteins, viruses, DNA, and have the potential to notably impact on disease diagnosis, genetic screening, drug discovery. Advances in assembling complex nanowire sensor arrays and integrating them with conventional and nanoscale electronics is leading to powerful sensor systems, that help to enable personalized medicine [20]. These nanowire sensors transduce chemical/biological binding events into electronic/digital signals; the potential for a sophisticated interface between nanoelectronics and biological information processing systems is aimed.

Electronic and optoelectronic devices impact many areas of society, from household appliances and multimedia systems to communications, computing and instrumentation. Given the strong demand of compact and powerful systems, there is high interest in the development of nanoscale devices with enhanced performance and new functions. Semiconductor nanowires and carbon nanotubes offer many opportunities for the creation of nanoscale devices and nanowire-based nanosystems. The control of key nanomaterial parameters is a central point, including chemical composition, structure, size, morphology, doping, determining electronic and optoelectronic properties.

3. Technical Details:

In the mainstream of modelling, a generalization of the Drude-Lorentz model, based on the complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$ of a system, is based on analytical expressions of 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*(*t*). It has been performed its classical, quantum and relativistic version [11-13].

The classical version has been deeply tested during years and fits very well with existing experimental data; it gives also explanations of the ultra-short times and of high mobility, with which the charges spread in mesoporous systems, of large interest in photocatalitic and photovoltaic systems [21-24]. It demonstrates high generality and is useful even in the study of ions, like mass transfer, and solutions, so as in nanobiosystems, with significant results with porous and cellular materials, so as for biological, medical and nanopiezotronic devices.

In detail, we focus on the expressions of the diffusion coefficient, of great importance for its link with the sensitivity of nano-bio-devices.

(I) *Classical case*

$$D=2\left(\frac{K_B T}{m^*}\right)\left[\frac{\tau}{\alpha_R}\sin\left(\frac{\alpha_R}{2}\frac{t}{\tau}\right)\exp\left(-\frac{t}{2\tau}\right)\right] \tag{1}$$

with: $\alpha_R=\sqrt{4\tau^2\omega_0{}^2-1}\ \in\Re^+$

$$D(t)=\left(\frac{k_B T}{m^*}\right)\left(\frac{\tau}{\alpha_I}\right)\left[\exp\left(-\frac{(1-\alpha_I)}{2}\frac{t}{\tau}\right)-\exp\left(-\frac{(1+\alpha_I)}{2}\frac{t}{\tau}\right)\right] \tag{2}$$

with: $\alpha_I=\sqrt{1-4\tau^2\omega_0{}^2}\ \in(0,1)\subset\Re$

(II) *Quantum case*

$$D=2\left(\frac{K_B T}{m^*}\right)\sum_{i=0}^{n}\left(\left[\frac{f_i\tau_i}{\alpha_{iR}}\sin\left(\frac{\alpha_{iR}}{2}\frac{t}{\tau_i}\right)\exp\left(-\frac{t}{2\tau_i}\right)\right]\right) \tag{3}$$

with: $\alpha_{iR}=\sqrt{4\tau_i^2\omega_i^2-1}\ \in\Re^+$

$$D(t)=\left(\frac{k_B T}{m^*}\right)\sum_{i=0}^{n}\left(\left(\frac{f_i\tau_i}{\alpha_{iI}}\right)\left[\exp\left(-\frac{(1-\alpha_{iI})}{2}\frac{t}{\tau_i}\right)-\exp\left(-\frac{(1+\alpha_{iI})}{2}\frac{t}{\tau_i}\right)\right]\right) \tag{4}$$

with: $\alpha_{iI}=\sqrt{1-4\tau_i^2\omega_i^2}\ \in(0,1)\subset\Re$

(III) *Relativistic case*

$$D(t)=2\left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma}\right)\left(\frac{\tau}{\alpha_{R_{rel}}}\right)\left[\sin\left(\frac{\alpha_{R_{rel}}}{2\rho}\frac{t}{\tau}\right)\exp\left(-\frac{t}{2\tau\rho}\right)\right] \tag{5}$$

with: $\alpha_{R_{rel}}=\sqrt{4\gamma\omega_0^2\tau^2-1}\ \in\Re^+$

$$D(t)=\left(\frac{k_B T}{m_0}\right)(\tau)\left(\frac{1}{\gamma}\right)\left(\frac{1}{\alpha_{I_{rel}}}\right)\left[\exp\left(-\frac{(1-\alpha_{I_{rel}})}{2\rho}\frac{t}{\tau}\right)-\exp\left(-\frac{(1+\alpha_{I_{rel}})}{2\rho}\frac{t}{\tau}\right)\right] \tag{6}$$

with: $\alpha_{I_{rel}}=\sqrt{1-4\gamma\omega_0^2\tau^2}\ \in(0,1)\subset\Re$

It also holds:

$$\alpha_{I_{rel}}=\sqrt{\Delta_{I_{rel}}},\quad \alpha_{R_{rel}}=\sqrt{\Delta_{R_{rel}}},\quad \gamma=1\Big/\sqrt{1-\beta^2},\quad \beta=v/c,\quad \rho=\gamma^2. \tag{7}$$

v is the speed of carriers, c the speed of light, 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.

We get the classical expressions of diffusion with $f_i = 1$, $\tau_i = \tau$ and $\omega_i = \omega_0 =$ center frequency.

Equations governed by the parameter α_I are a superposition of exponentials; the behaviour of curves is similar to typical Drude-Lorentz behaviour. Equations governed by the parameter α_R are a product of an exponential with a sinusoidal function, with typical damped oscillation in time. The model, called DS model, includes also a gauge factor, which allows its use from sub-pico-level to macro-level. Interesting applications have been performed also for economics, neuro-science, brain processes, nano-medicine [25,26]. The sensitivity, connected to the increase and rapidity of detection, is one of the most important characteristic of a nano-bio-device, and is linked to values and variation of diffusion.

4. Discussion and Results:

Among the most studied nanomaterials to date we recognize 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). If we consider a nanowire as basis element of a nanobiosystem (device), we can perform an interesting analysis related to the diffusion, obtaining results that allow both to confirm experimental known data and to provide intriguing previsions, useful in the improvement of new high efficiency nanobiosystems, nanobiosensors and nanobiodevices. About the variables influencing the diffusion and therefore the sensitivity of a nanobiosystem, we have:

a) the temperature T of the system, which is directly proportional to D;

b) the parameters α_I, α_R, i.e. the values of τ and ω_0; they appear in the arguments of the exp/sin functions in equations, therefore their variation affects also with the shape of the diffusion curves;

c) the variation of the effective mass m^*, which is connected to the physical and chemical treatment of materials, like doping; electronic, optical, photochemical, photoelectrochemical, photocatalytic and photoexcited properties can be tuned by dopants selection for materials engineering [27,28];

d) the variation of the chiral vector inscribed in (n,m) indices, reflecting in a variation of m^* [29];

e) at quantum level, the possibility to evaluate the weights of each mode and to vary the carrier density N, as it holds $\omega_{p_i}{}^2 = \frac{4\pi N e^2}{m} f_i$, with ω_{p_i} plasma frequencies;

f) at relativistic level, the possibility to act on the initial peak in diffusion through a variation of the carriers velocity.

We consider below some examples of application, considering the classic case for simplicity. The analysis starts considering the behaviour of D for two values of τ and near to the boundary values of the interval of α_I. We consider the environmental temperature $T = 300K$, but it is also possible to study the behaviour as a function of T.

Figure 1 represents the behaviour of the diffusion in time for Silicon. The considered values are: $\alpha_{I1} = 0.1$, $\alpha_{I2} = 0.9$, $\tau_1 = 10^{-12}s$, $\tau_2 = 10^{-13}s$ [30].

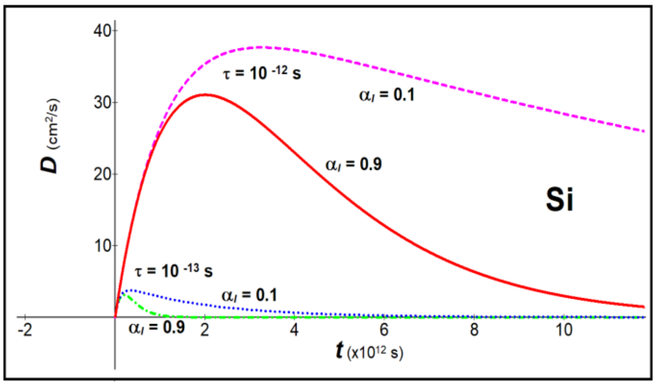

Figure 1: D vs t for Si ($T = 300K$; $m^*_{Si} = 1.08 m_e$).

We note how the increase of τ, corresponding to a decrease of ω_0 for constant α_I, helps the increase in diffusion; for τ constant, the variation of α_I brings to a variation in diffusion. The parameter α_I changes also the form of curves, reflecting in a variation of the D curve shape.

It follows the same study for ZnO [31] (Figure 2).

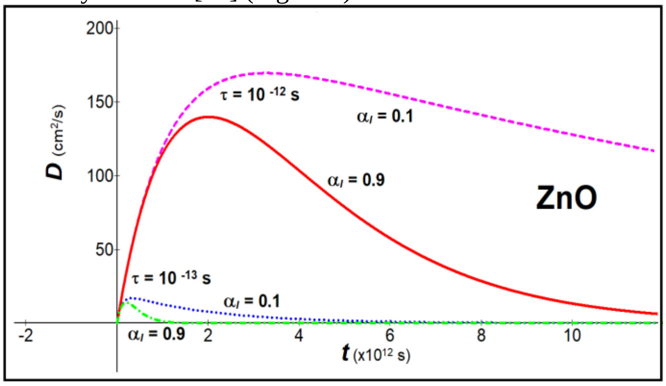

Figure 2: D vs t for ZnO ($T = 300 K$; $m^*_{ZnO} = 0.24 m_e$)

Figures 3-5 refer the same study for CdS, CdTe and GaAs respectively, considering the same values of T , τ and α_I [32-36].

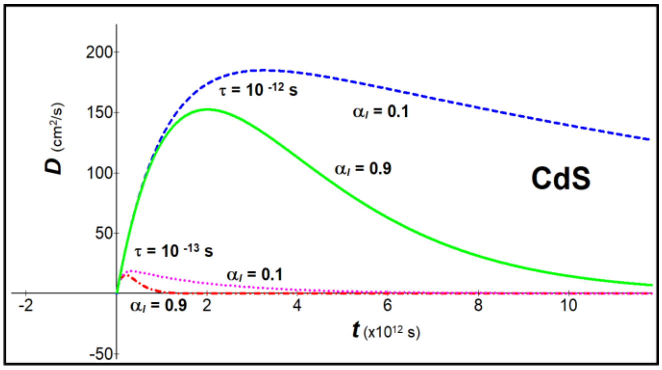

Figure 3: D vs t for CdS ($T = 300 K$; $m^*_{CdS} = 0.22 m_e$)

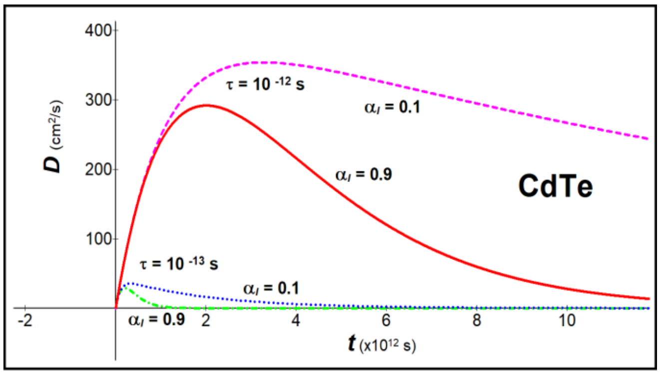

Figure 4: D vs t for CdTe ($T = 300 K$; $m^*_{CdTe} = 0.115 m_e$)

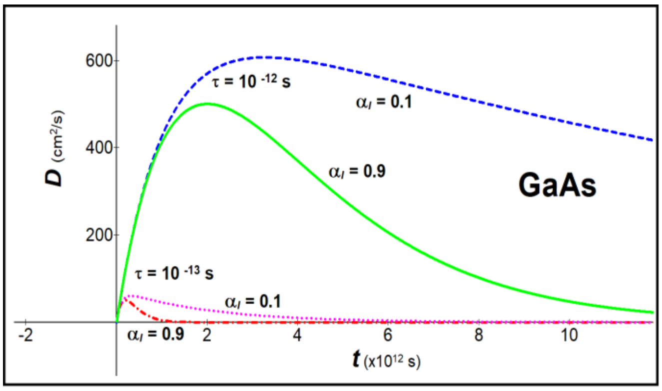

Figure 5: D vs t for GaAs ($T = 300 K$; $m^*_{GaAs} = 0.067 m_e$)

Figure 6 illustrates the behaviour of diffusion for CNTs with variation of the system temperature; it is $m^* = 0.5 m_e$ [29] (m_e is the electron mass), $\tau = 0.17 \cdot 10^{-12} s$ [37,38] and $\alpha_I = 0.5$.

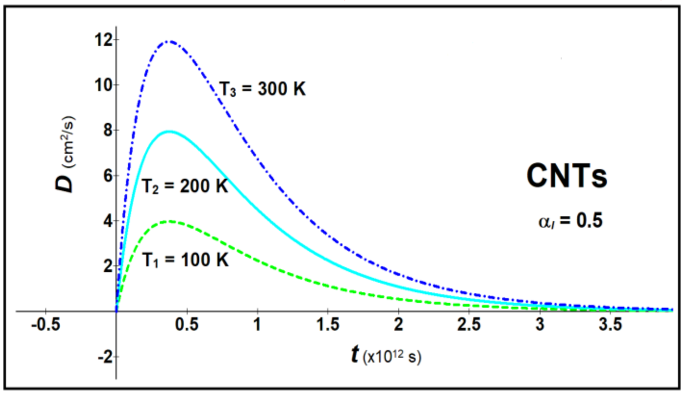

Figure 6: D vs t for CTNs with three different temperatures.

In Figure7 we compare the value of diffusion of three nanomaterials: CNTs, Si and ZnO.

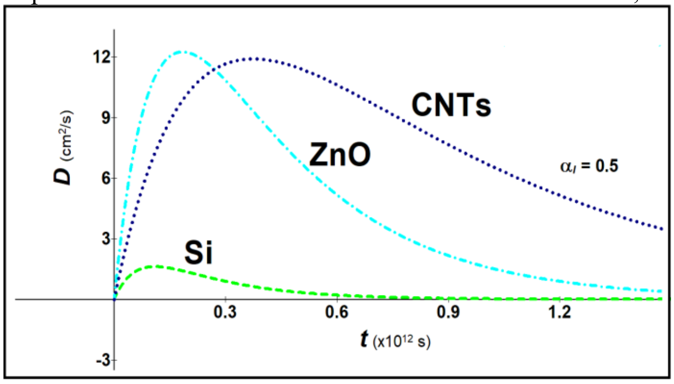

Figure 7: D vs t for three different nanomaterials.

In Figure 8 we focus on the diffusion behaviour of CNTs considering the change of the effective mass as variation of the chiral vector $C_h = (n, m)$. We consider CNTs with (n, m) indices equal to (3,1), (4,2) and (9,2). As expected considering the theory, the decrease of the effective mass involves a raise in diffusion.

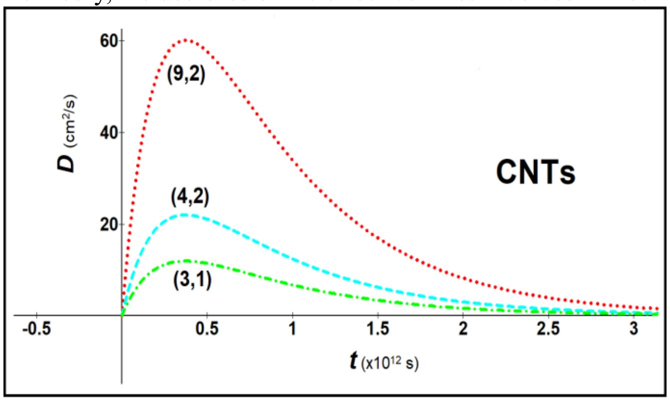

Figure 8: D vs t for CTNs with three different values of chiral vector $C_h = (n, m)$.

We note how the parameter α changes the form of curves, bringing to a shape variation of the diffusion curve [39].

5. Conclusion:

In this work we have considered a fruitful analysis related to the possibility of varying the carriers diffusion inside a nanostructure. The diffusion is strictly connected to the sensitivity and then to the performance of a nano-bio-system, implying the possibility to get, through a theoretical study, the peculiar characteristics of a nanobiomaterial-based device.

Modelling helps in this direction, giving detailed information about the dynamics of carrier transport from sub-pico-level to macro-level. Acting on chemical, physical, structural and model-intrinsic parameters, i.e the temperature T of the system, the model intrinsic parameters, the values of τ_i and ω_i, the variation of the effective mass m^*, the variation of the chiral vector $C_h = (n, m)$, the quantum weights of each mode in the quantum case, the carrier density N, the velocity of carriers,it is possible to carry out an accurate fine tuning of the transport dynamics and thus to assess the performance of a nano-bio-device. Modelling gives new newsworthy innovative information, precious both for operating devices and in the design phase of planned nano-bio-devices. The considered nanomaterials can fulfill, through appropriate combinations of the indicated parameters, a high spectrum of practical and technological needs.

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Conflicts of Interest:

The author declares no conflict of interest.

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