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A new theoretical model for the dynamical analysis of Nano-Bio-Structures

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Abstract. The conversion of mechanical energy into electrical energy at nanoscale using piezoelectric nanowire arrays has been in detail shown by deflection of nanowires. Recently it has performed an analytical model, both at classical and at quantum level, for describing the most important quantities concerning transport phenomena; the model predicts interesting peculiarities, as high initial charge diffusion in nanodevices constituting by nanowires and permits also in particular to deduce interesting informations about the devices sensitivity, focusing on the correlation between sensitivity and high initial diffusivity of these materials at nanometric level.

Keywords: theoretical modelling; transport processes; nanophysics; nanodevices; nanosensoristics; diffusion

1. Introduction

The world of nanosystems has increased of importance in these last years in relation to a lot of applications, going from realtime and implantable biosensing systems to personal electronics, environmental monitoring and electromechanical systems (Patolsky 2006, Patolsky 2007). For powering a nanosystem it is possible to use a battery, but it reveals some problems concerning its lifetime, the small size, the weight; moreover, for example for biomedical applications, the toxicity of the materials, that compose batteries, has to be considered with attention. Another way is to harvest energy from the environment by converting mechanical, chemical and thermal energy into electricity (Paradiso 2005). Approaches have been developed in the generation of energy using thermoelectrics (Sales 1996), piezoelectrics (Roundy 2005), bacterial organisms (Bond 2002) and solar cells (Huynh 2002). One of the basic principles is to use piezoelectric and semiconducting coupled ZnO nanowires for converting mechanical energy into electricity (Wang 2006). The research involves the integration of multifunctional nanodevices in a nanosystem, so that it can work as a "living element", i.e., with sensorial, controlling, communication, and answer/action abilities. In parallel with these technological efforts, the theorists try to refine the existing theories and to create new models, in order to confirm the experimental data and to discover new nanoscale aspects. Recently it has been proposed a new model, which generalizes the class of the Drude-

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Lorentz-like models and describes the conductors in nanostructured form. This model permits a complete analytical calculation of the most important quantities concerning transport phenomena, i.e. the velocities correlation function, the mean square deviation of position and the diffusion coefficient (Di Sia 2011, 2012). The model has been tested and is still testing in relation to the most commonly used and studied materials at today in this sector, i.e., zinc oxide (ZnO), titanium dioxide (TiO_2), gallium arsenide (GaAs), silicon (Si) and carbon nanotubes. In this paper it will focus in particular about results regarding the zinc oxide.

2. ZnO nanowires and nanobelts

At nanotechnological level, among the most representative studied 1-D nanostructures, we find carbon nanotubes, Si nanowires and ZnO nanowires/nanobelts. Zinc oxide (ZnO) is one of the dominant materials at nanoscale; the number of publications and citations of areas concerning ZnO nanostructures is remarkable and important as for example quantum computing, carbon nanotubes, semiconductor thin films, dark matter.

ZnO is a semiconductor material with a large window of applications, going from optics, optoelectronics, sensoristics, to actuatoristics, energetics, biomedical sciences and spintronics (Zhou 2008).

The ZnO nanowire-based technology offers a lot of advantages:

1) the nanowires/nanobelts can be submitted to extremely great elastic deformations without possible fractures and have a big resistance to the strain;

2) these elements can be easily bent, therefore they are sensitive to small mechanical stresses;

3) ZnO nanowire arrays can easily be grown via chemical synthesis (at 80 °C) and they have a good integration with technologically important materials, like silicon or polymers;

4) ZnO exhibits both semiconducting and piezoelectric properties, which forms the basis for electromechanically coupled sensors and transducers;

5) ZnO is a not toxic material, is biocompatible and degradable and has a wide range of applications, from medicine to cosmetics;

6) ZnO exhibits the most diverse and abundant configurations of known nanostructures, such as nanowires, nanobelts, nanosprings, nanorings, nanobows, nanohelices (Wang 2008).

The piezoelectricity is an intrinsic ZnO property, which demonstrates that this material is of great interest for applications in the nanosensoristic sector. The stress-based sensors created with nanowires of piezoelectric ZnO can be built with a not complex and reliable technique, and to accessible costs (Fig. 1).

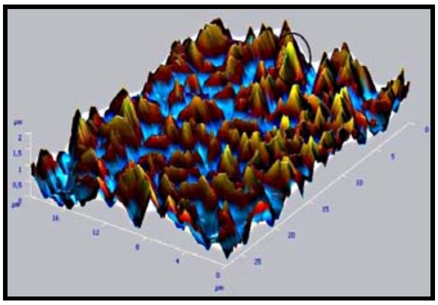

Fig. 1 AFM image of the microstructure of ZnO (in the circle the characteristic pyramidal shape). The pyramides tops exhibit negative and positive potential at opposite sides under deflection

3. Nanodevices with high initial diffusivity: theoretical aspects of an interesting new model

One of the most important feature of a nanosensor is the sensitivity, resulting in the ability to detect in very high modality. This aspect is connected to the charge transport and assumes different characteristics with respect to those of bulk. Among the most utilized models for describing experimental transport data there is the Drude-Lorentz model (Ziman 1979). An extension of this model was proposed by Smith (2001) and successfully applied to fit the conductivity in a large variety of systems. Other interesting models are the effective medium theories (EMTs); the commonly used EMTs include the Maxwell-Garnett (MG) model and the Bruggeman (BR) model (Han 2007).

The new cited model is based on a complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$ of the system. The conductivity $\sigma(\omega)$ is in general a complex function of the frequency ω, which can be deduced from linear response theory (Green-Kubo formula)

$$\sigma_{\beta\alpha}(\omega) = \frac{e^2}{\hbar V}\int_0^\infty dt e^{i\omega t}\int_0^\beta d\lambda < \vec{v}^{\alpha}(t-i\lambda)\vec{v}^{\beta}(0) > \tag{1}$$

where $\beta = 1/KT$, K is the Boltzmann's constant, V the volume of the system, T the temperature.

By inversion of Eq. (1), it is possible to find the velocities correlation function $<\vec{v}(t)\cdot\vec{v}(0)>_T$ inside the integral. However, the presence of an integration from 0 to ∞ in Eq. (1) is a problem for inversion, which can be overcame evaluating the integral on the entire time axis (-∞, +∞). Considering the real part of the complex conductivity in Eq. (1), the extension to the entire time axis is possible and a complete Fourier transform can be performed, obtaining real velocities.

After this step, it is possible to obtain the analytical form of the mean square deviation of position $R^2(t) = \left\langle [\vec{R}(t) - \vec{R}(0)]^2 \right\rangle$, writable, by means of a transformation of coordinates relative to the region of integration, in the form

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

The diffusion coefficient D is defined in the usual way as

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

Eqs. (1),(2),(3) offer the most important informations related to the dynamical analysis of the system. One of the most interesting peculiarities of the model is the “time domain” approach used, not previously found in such a contest, contrarily to the existing theoretical approaches recoverable in literature, which are “frequency domain” treatments and/or numerical methods (Di Sia 2011, 2012).

4. Results and discussion

A lot of nanostructures realized with the most used materials in this sector have found useful applications in the sector of nano-bio-sensoristics. It has experimentally been determined that the times required to the charges for traversing the nanoparticles inside a nanostructure are very small; this fact is detectable with a higher current with respect to that expected (Di Sia 2012). The experimental data show that the carriers inside nanoparticles deviate from their Drude-type behaviour.

It has been compared the velocities correlation function and the diffusion coefficient, calculated through the new model, with the relative data found by experiments (Baxter 2006). In Fig. 2 it is plotted the mean square deviation of position $R^2(t)$ vs t/τ for ZnO nanostructures in the form of nanoparticles, annealed and not annealed nanowires, annealed and not annealed films, with an average value of τ calculated through the experimental data (Baxter 2006).

From Fig. 2 it is possible to observe that the R value, obtainable as the square root of the value in vertical axis, which offers directly the distance in "10^{-7} cm" units, i.e., in nanometers, may become greater than the dimension of the nanoparticles composing the structure (Sridevi 2009); this fact indicates moreover an increased mobility of the carriers in short times, of order of few τ, contrarily to the expected behaviour, i.e., a low mobility in the desordered structure. In Fig. 3 it is presented the diffusion coefficient vs t/τ considering a ZnO nanostructure as possible basic element of a nanosensor with a relaxation time $\tau \cong 0.7 \cdot 10^{-13}\, s$, for different values of the parameter α_I (Di Sia 2011, 2012).

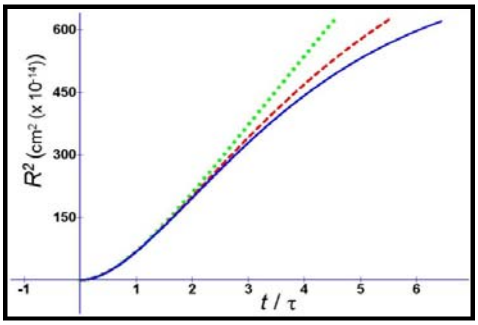

Fig. 2 $R^2(t)$ vs t/τ for three different values of the parameter $\alpha_I = \sqrt{1 - 4\tau^2 \omega_0^2}$ of the model (Di Sia 2011, 2012) (α_I = 0.1 for continuous blue line, 0.5 for dashed red line, 0.9 for dots green line) with the average value $\tau \cong 0.7 \cdot 10^{-13}\, s$

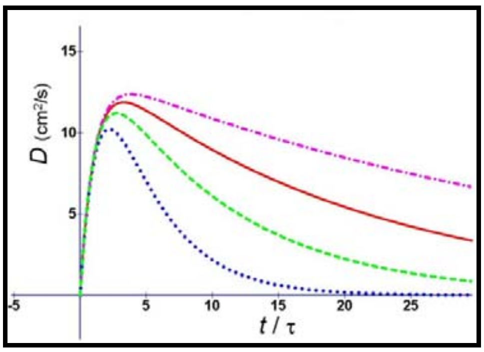

Fig. 3 Diffusion coefficient D vs t/τ for α_I running in the interval (0,1), with $\tau \cong 0.7 \cdot 10^{-13}\, s$

The different lines in Fig. 3 represent the variation of the diffusion coefficient *D* in relation to the variation of the parameter α_I of the model, referred to τ and ω_0 by $\alpha_I = \sqrt{1-4\tau^2\omega_0^2}$. We can note, as attended by theory and experimental results, that the diffusion tends to zero increasing the time. About the beginning of the process, the diffusion coefficient remains finite and it passes from zero to 10÷13 times its initial value. There is therefore a high initial diffusivity, which can adequately support the sensitivity of a nanosensor based on a ZnO nanostructure. Such important result, deriving from the application of the new model, is meaningfully in accordance with results and conclusions obtained through THz spectroscopy (TRTS) (Beard 2001).

The model was tested also for Gallium Arsenide (GaAs), Cadmium Telluride (CdTe), Cadmium Sulfide (CdS), Copper Indium Selenide (CIS), Copper Indium Gallium Selenide (CIGS) in relation to high-efficiency photovoltaics nanomaterials (Di Sia 2013) and other interesting testing applications are scheduled in the near future.

5. Conclusions

The possibility of a rapid answer for the carriers transport is a very important peculiarity concerning nano-bio-sensoristic devices. One of the direct and meaningful consequences results the increased efficiency of devices based on such systems. Such high initial mobility, for fixed ω_0, is detectable in the nanostructures of the most used materials in this field, for a nanoparticle nanostructured system, so as for a single nanotube. The enhanced transport times for nanostructured systems and films may be the basis for single nanotube nanosensors, where enhanced currents arising from piezoelectric charges have been shown to occur independently from the semiconducting nature of ZnO. The work is in progress for testing the model with other important materials at nanolevel, for a complete and detailed description of the behaviour of matter, hopefully in the best agreement with data of experimental research.

References

Baxter, J.B. and Schmuttenmaer, C.A. (2006), “Conductivity of ZnO Nanowires, Nanoparticles, and Thin Films Using Time-Resolved Terahertz Spectroscopy”, *J. Phys. Chem. B*, **110**, 25229-25239.

Beard, M.C., Turner, G.M. and Schmuttenmaer, C.A. (2001), “Subpicosecond carrier dynamics in low-temperature grown GaAs as measured by time-resolved terahertz spectroscopy”, *J. Appl. Phys.*, **90**, 5915-5923.

Bond, D.R., Holmes, D.E., Tender, L.M. and Lovley, D. R. (2002), “Electrode-Reducing Microorganisms That Harvest Energy from Marine Sediments”, *Science,* **295**(5554), 483-485.

Di Sia, P. (2011), “Oscillating velocity and enhanced diffusivity of nanosystems from a new quantum transport model”, *J. Nano Res.*, **16**, 49-54.

Di Sia, P. (2011), **“**Classical and quantum transport processes in nano-bio-structures: a new theoretical model and applications”, PhD Thesis, Faculty of Science, Verona University, Italy.

Di Sia, P. (2011), “An analytical transport model for nanomaterials” *J. Comput. Theor. Nanosci.*, **8**, 84-89.

Di Sia, P. (2012), “An analytical transport model for nanomaterials: the quantum version”, *J. Comput. Theor. Nanosci.*, **9**, 31-34.

Di Sia, P. (2013), “Characteristics in diffusion for high-efficiency photovoltaics nanomaterials: an interesting analysis”, *J. Green Sci. Technol.* (under revision)

Han, J., Zhang, W., Chen, W., Ray, S., Zhang, J., He, M., Azad, A.K. and Zhu, Z. (2007), “Terahertz dielectric properties and low-frequency phonon resonances of ZnO nanostructures”, *J. Phys. Chem. C*, **11**, 13000-13006.

Huynh, W.U., Dittmer, J.J. and Alivisatos, A.P. (2002), “Hybrid nanorod-polymer solar cells”, *Science*, **295**(5564), 2425-2427.

Paradiso, J.A. and Starner, T. (2005), “Energy scavenging for mobile and wireless electronics”, *Per. Computer.*, **05**, 18-27.

Patolsky, F., Timko, B.P., Zheng, G. and Lieber, C.M. (2007), “Nanowire-based nanoelectronic devices in the life sciences”, *MRS Bull.*, **32**, 142-149.

Patolsky, F., Timko, B.P., Yu, G., Fang, Y., Greytak, A.B., Zheng, G. and Lieber, C.M. (2006), “Detection, stimulation, and inhibition of neuronal signals with high-density nanowire transistor arrays”, *Science*, **313**(5790), 1100-1104.

Roundy, S., Leland, E.S., Baker, J., Carleton, E., Beilly, E., Lai, E., Otis, B.J., Rabaey, M., Wright, P.K. and Sundararajan, V. (2005), “Improving power output for vibration-based energy scavengers”, *IEEE Pervasive Computing Journal on Mobile and Ubiquitous Computing*, **4**(1), 28-36.

Sales, B.C., Mandrus, D. and Williams, R.K. (1996), “Filled skutterudite antimonides: a new class of thermoelectric materials”, *Science*, **272**(5266), 1325-1328.

Smith, N.V. (2001), “Classical generalization of the Drude formula for the optical conductivity”, *Phys. Rev. B*, **64**(15), 155106-155111.

Sridevi, D. and Rajendran, K.V. (2009), “Preparation of ZnO nanoparticles and nanorods by using CTAB assisted hydrothermal method”, *Int. J. Nanotech. Appl.*, **3**(2), 43-48.

Wang, Z.L. (2008), “Towards self-powered nanosystems: from nanogenerators to nanopiezotronics”, *Adv. Funct. Mater.*, 18, 3553-3567.

Wang, Z.L. and Song, J.H. (2006), “Piezoelectric nanogenerators based on Zinc Oxide nanowire arrays”, *Science*, **312**(5771), 242-246.

Wang, Z.L., Wang, X., Song, J., Liu, J. and Gao, Y. (2008), “Piezoelectric nanogenerators for self-powered nanodevices”, *IEEE Perv. Comp.*, **7**, 49-55.

Zhou, J., Gu, Y., Fei, P., Mai, W., Gao, Y., Yang, R., Bao, G. and Wang, Z.L. (2008), “Flexible piezotronic strain sensor”, *Nano Letters*, **8**(9), 3035–3040.

Ziman, M. (1979), *Principles of the Theory of Solids*, Cambridge University Press, New York.

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