*International Journal of Applied and Advanced Scientific Research (IJAASR)*
*Impact Factor: 5.655, ISSN (Online): 2456 - 3080*
*(www.dvpublication.com) Volume 3, Issue 2, 2018*

# ON SURFACE ELECTRON MOBILITY OF NANOMATERIALS FOR CANCER NANOTECHNOLOGY

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**Cite This Article:** Paolo Di Sia, "On Surface Electron Mobility of Nanomaterials for Cancer Nanotechnology", International Journal of Applied and Advanced Scientific Research, Volume 3, Issue 2, Page Number 46-50, 2018.

**Abstract:**

Nanometer-sized particles have optical, magnetic, chemical and structural properties that set them apart from bulk solids, with fruitful potential applications in nanomedicine. The intrinsic limitations of conventional cancer therapies have led to the development and application of nanotechnology for more effective and safer cancer treatment, Mobility, correlated to carrier diffusion, plays a very important role in the dynamics of processes that take place at this scale. Interesting details about surface electronic diffusion for nanomaterials used in nanomedicine are given in this paper thanks to a recent analytical "time-domain" model for classical and quantum transport in nano-systems, which is demonstrating high generality and good fitting with available experimental data of literature and last models.

**Key Words:** Nanomedicine, Nanomaterials, Diffusion, Mobility, Cancer, Mathematical Modelling & Analytical Modelling

## 1. Introduction:

The intrinsic limitations of conventional cancer therapies, limited to surgery, radiation and chemotherapy, have progressively led to the development and application of nanotechnology for a more effective and safer cancer treatment (cancer nanomedicine). Significant technological breakthroughs have been achieved in this field, although many obstacles remain due to the complexity and heterogeneity of tumor biology, a still incomplete understanding of nano-bio interactions and challenges related to clinical translation and marketing. The growing understanding of nano-bio interactions is allowing the development of more effective nano-drugs for cancer patients.

Significant progress has been made in the sector of targeted drug delivery technologies; the targeted drug delivery, mediated by nanoparticles, allows to significantly reduce the dosage, optimize release properties, increase specificity and bioavailability, improve shelf life and minimize adverse effects on healthy cells. Some nano-drugs are able to overcome the blood-brain barrier that is an obstacle to the treatment of brain tumors.
Nanoscale objects are used autonomously or as part of larger systems containing multiple objects at the nanoscale. Nanoparticles are mainly used as nanocarriers to provide cytotoxic drugs to tumor tissue. Nanomedicine is also used to dose multiple drugs at the same time for better cytotoxic effect.

The theranostics perspective is to simultaneously perform diagnosis and treatment, identifying the single tumor particles. This is possible thanks to magnetic nanoparticles, multi-functional entities coated by a polymer, vehiculated to the place of interest by an external magnetic field. The appropriate polymeric coating allows to combine the particle with chemotherapy drugs that, once reached the tumor area, can be released over time, thus allowing a lower dose and a more targeted action compared to the classic treatments [1-3]. It is equally important the knowledge of nanoparticles charge mobility, which is related to the carrier diffusion, for obtaining more information on their localization and activation in the desired parts of the human body.

## 2. On the Most Used Nanomedicine Nanomaterials:

The most commonly used materials for the synthesis of nanoparticles are iron oxides and gold (often used, together with silver, as a coating), but also diamond nanocrystals and fullerenes [4]. Iron oxide nanoparticles have been widely studied because iron oxide is a strongly ferromagnetic material and because they are not toxic. Among iron oxides, magnetite ($Fe_3O_4$) is one of the most used.

By appropriately combining the size, composition, shape and surface of nanoparticles, the cellular absorption of drug in the cell and molecular imaging can be improved. Gold nanoparticles (AuNPs) have been widely used as targeted delivery vectors of drug, as sensors and as contrast agents for the molecular imaging of tumor cells, due to their stability, their ability to bind to biomolecules, their characteristics of plasmonic absorption of the surface and their optical properties [5]. It has been prepared teranostic agents based on gold nanoparticles bound to the surface with anti-cancer receptors such as paclitaxel (PTX) [6]. This agent has been evaluated on the basis of its efficacy for the diagnosis and treatment of tumors as HeLa (of human breast), A549 (of human lung) and MG63 (of human osteosarcoma). To evaluate the effect of functionalized AuNPs, their intracellular assumptions and their cytotoxicity were studied.

There are several non-invasive imaging techniques used to visualize the real-time distribution of nanoparticles; the most common are Magnetic Resonance Imaging (MRI), X-ray Computed Tomography (CT), Positron-Emission Tomography (PET), Single-Photon Emission Computed Tomography (SPECT), Ultrasound

Computer Tomography (UCT), Fluorescence Molecular Tomography (FMT), Photoacoustic Tomography (PAT) [7].

Nanocrystals are quantum dots of order of the volume of a protein, with the property of emitting fluorescence in nearly all colors; they can be used as probes for highlighting focused reactions in cells, are available in an almost unlimited range of colors, customized by changing the particle size or composition.

Nanodiamonds can carry drugs, preventing the release of healthy cells and limiting toxic effects. Fullerenes are "in vivo" a powerful antioxidant with no acute toxicity, with a protective activity on neurons [8]. Chemical sensors are created using nanotubes for the measure of various properties of molecules.

**3. Study of Electron Diffusion for the Indicated Nanomaterials:**

Informations about transport processes in solid state physics and soft condensed matter are obtainable through Drude-Lorentz-like models; they give results on the most important quantities related to the transport processes, i.e. the velocities correlation function, by which we get the velocity of carriers at time *t*, the mean squared deviation of position, by which we get their position, and the diffusion coefficient *D*, which gives interesting information about the carriers propagation in time and space [9-13].

We use in this paper a recent analytical model, which is gaining success for its fit with previous models and its power of predictivity. In the classical case (non-relativistic velocities and negligible quantum effects), the expression for the carrier diffusion are as follows:

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

with:

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

and:

$$D(t)=2\left(\frac{k_B T}{m^*}\right)\left(\frac{\tau}{\alpha_R}\right)\left[\sin\left(\frac{\alpha_R}{2}\frac{t}{\tau}\right)\exp\left(-\frac{t}{2\tau}\right)\right] \quad (3)$$

with:

$$\alpha_R=\sqrt{4\tau^2\omega_0^2-1} \quad (\alpha_R \in \Re^+). \quad (4)$$

$k_B$ is the Boltzmann's constant, $T$ the temperature of the system, $m^*$ the effective mass of carriers, $\tau$ the relaxation time, $\alpha_I$ and $\alpha_R$ parameters of the model, $\omega_0$ center frequency [13]. Eqs (2) and (4) are 3-variables relations, therefore the knowledge of two of them allows to get the third one; the two parameters can be then found by calculation or *a priori* fixed.

**4. Results and Discussion:**

We studied the behaviour of diffusion of the indicated nanomaterials (CNTs, Au, Ag, C). The fixed parameters are: the temperature $T$ = 310 K, three values of parameters (0.1, 0.9, 2), an average relaxation time $\tau_{av} = 10^{-13}$ *s* and values of $m^*$ as in Table 1.

| Nanomaterial | $m^*$ |
|---|---|
| CNTs | 0.5 $m_e$ |
| Au | 1.1 $m_e$ |
| Ag | 1.15 $m_e$ |
| C | 1.66 $m_e$ |

Table 1: Values of effective masses for the indicated nanomaterials ($m_e$ = electron mass) [14-17].

The behaviour of diffusion $D$ in time is resumed in figures 1-4. We note how the variation of parameters brings not only to variations of diffusion values, but also to that of the shape of curves, because of appearance of $\alpha_{I/R}$ in the arguments of exponentials of equations (1) and (3). This is important and peculiar, because these equations are different; the first is a superposition of two exponentials, the second one is a damped oscillation in time.

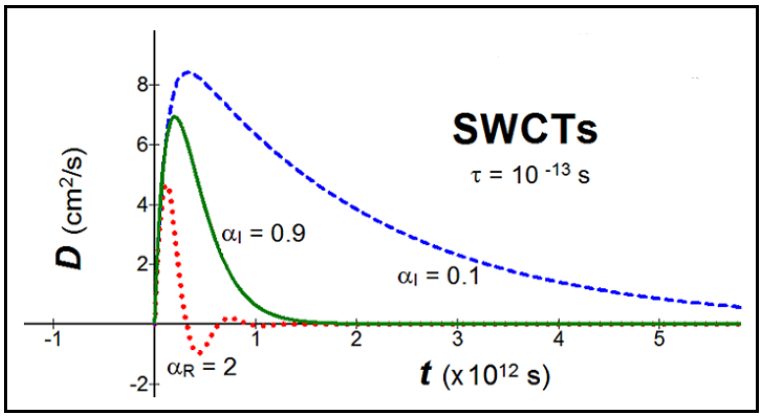


Figure 1: *D* vs *t* for CNTs; for further details see text.

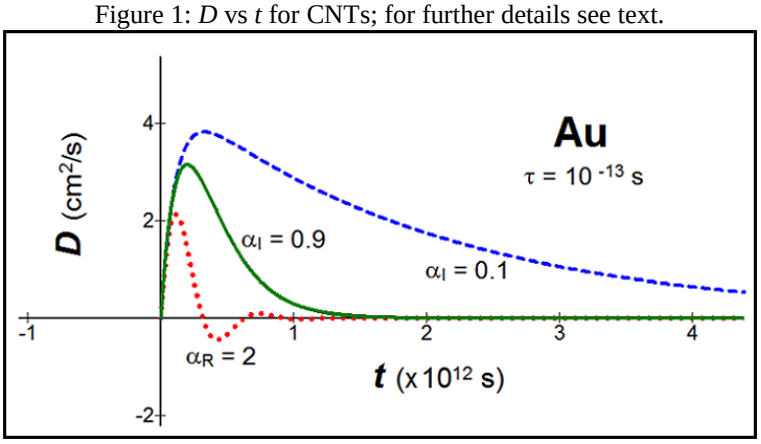


Figure 2: *D* vs *t* for Au; for further details see text.

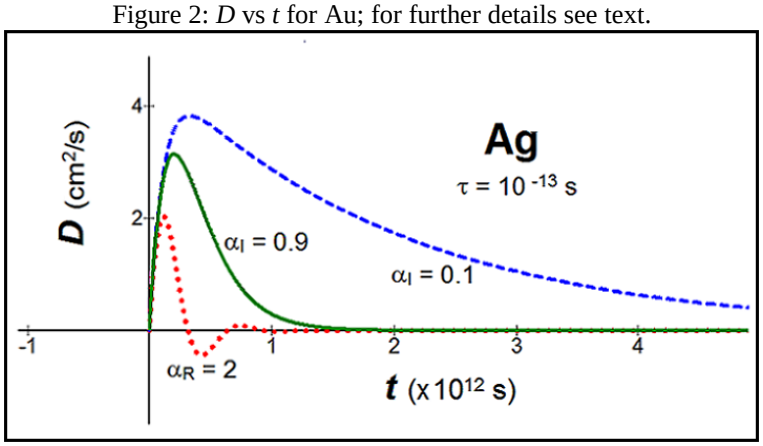


Figure 3: *D* vs *t* for Ag; for further details see text.

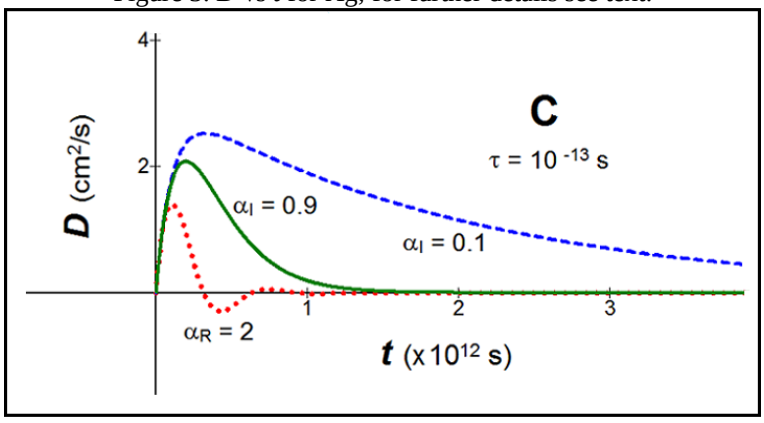


Figure 4: *D* vs *t* for C; for further details see text.

Table 2 resumes the peak values of diffusion with the necessary time, as determinable by figures, for the chosen values of $\alpha_I$ and $\alpha_R$ .

| Nanomaterial | $D$ (cm$^2$/s) (at $t$ (ps)) $\alpha_I = 0.1$ | $D$ (cm$^2$/s) (at $t$ (ps)) $\alpha_I = 0.9$ | $D$ (cm$^2$/s) (at $t$ (ps)) $\alpha_R = 2$ |
|---|---|---|---|
| CNT | 6.950 (0.192) | 8.440 (0.323) | 4.630 (0.087) |
| Au | 3.142 (0.198) | 3.849 (0.318) | 2.162 (0.106) |
| Ag | 3.143 (0.199) | 3.825 (0.328) | 2.048 (0.112) |
| C | 2.091 (0.192) | 2.569 (0.321) | 1.374 (0.116) |

Table 2: Values of peaks in diffusion and respective times for the considered nanomaterials

As indicated above, the two parameters $\alpha_{I(R)}$ are functions of the two variables $\tau$ and $\omega_0$, but by a mathematical point of view, relations (2) and (4), as implicit functions, depend on three variables. They can therefore be used both *a priori* and *a posteriori*. In the first case we choose the value of $\alpha_{I(R)}$ and through the knowledge of $\tau$, we calculate $\omega_0$ and vice versa. In the second case, the values of $\tau$ and $\omega_0$ will give us the value of $\alpha_{I(R)}$ and therefore they will determine if the diffusion behaviour will be of damped oscillating type, or a superposition of two exponential functions. These characteristics are certainly important in relation to the particular kind of action that will be done within the patient's survey.

**5. Conclusions:**

Theranostics is a relatively recent discipline, but in the last few years it is developing incredibly fast. Researchers have created various nanoparticle-based systems that can be used for therapy, such as for hyperthermia or radiotherapy treatment, drug delivery for targeted delivery of chemotherapeutic drugs, and for diagnosis (use of nanoparticles as contrast agents for imaging). To control therapy and response at the cellular level, the use of fluorescent agents, such as fluorescent organic dyes or quantum dots, allows the achievement of high resolution images, with the definition of different organelles even within the cell. These processes are related to the surface electronic (carrier) mobility of nanoparticles, therefore the knowledge of charge diffusion is of extreme interest. The particular choice of nanomaterial brings to a variation of the carrier diffusion in time and therefore to a variation of its peak; in this direction we can consider also the variation of temperature $T$ [18], the variation of the effective mass through doping and related to the chiral vector [19], so as the targeted choice of the two parameters of the model. The rapidity of answer and the potentiality of drugs activation for nanomaterials travelling in the human body is very important and often decisive for a rapid diagnosis and implementation of possible resolution strategies.

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