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Iridium (IV) Oxide (IrO_2) Nanoparticles and Cancers

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Abstract: In the current research, roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations is investigated. The calculation of thickness and optical constants of Iridium (IV) Oxide (IrO_2) roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations produced using sol–gel method over glassy medium through a single reflection spectrum is presented. To obtain an appropriate fit for reflection spectrum, the classic Drude–Lorentz model for parametric di–electric function is used. The best fitting parameters are determined to simulate the reflection spectrum using Lovenberg–Marquardt optimization method. The simulated reflectivity from the derived optical constants and thickness are in good agreement with experimental results. The results of optimization algorithm of Lovenberg–Marquardt with physical model of Drude–Lorentz for determining optical constants of Iridium (IV) Oxide (IrO_2)–roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations produced using sol–gel method through a single reflection spectrum show that higher doping leads to lower reflectivity and reflection coefficient and also, leads to increase in thickness of thin layer.

Keywords: Iridium (IV) Oxide (IrO_2) Nanoparticles, Cancer Nanobiotechnology, Synchrotron and Synchrocyclotron Radiations

1. Introduction

Roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations is investigated. Iridium (IV) Oxide (IrO_2) is a semi–conductor of type n which its 3d level is filling up [1–6] and it belongs to a group of smart materials that reacts to variations of temperature, electrical or magnetic fields and pressure. This oxide can be used as thin films for a wide range of applications including electrical and or optical–thermal switching tools and energy storing covers [7–14]. Therefore, determining optical constants (refractive coefficient, n, and extinction coefficient, k) of Iridium (IV) Oxide (IrO_2) thin films is essential for designing optoelectronical and optical tools for producing optical covers and similar tools such as multilayer covers and filters [15–21]. The measured experimental parameters including optical reflectivity are used as a function of wavelength to determine optical parameters of thin layers [22–27]. For determining optical parameters, various physical models such as Kuschi, Frouhi–Blumber and Tawk–Lorentz have been suggested to calculate refractive coefficient, n, and extinction coefficient, k. for any thin layer, an appropriate optical model should be selected and used for estimation of real and imaginary di–electric function according to its physical condition [28–34]. To do this, an initial guess is needed for parameters of di–electric function and thickness which is defined as a range regarding physical characteristics of thin film and the available results in the literature. Iridium (IV) Oxide (IrO_2)– roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations are produced over glassy medium in sol–gel laboratory, Faculty of Chemistry, BioSpectroscopy Core Research Laboratory and Cancer Research Institute (CRI) at California South University, Irvine, California, USA, under similar conditions. Measurement of thin films are performed on four samples of Iridium (IV) Oxide (IrO_2) as roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations with mole ratio of 0.5, 1 and 1.5% of Iridium (IV) Oxide (IrO_2) [35–40]. Simulation of experimental spectra are performed using a single reflection spectrum of thin films and through Drude–Lorentz physical model in optimization process of Lovenberg–Marquardt. Optical constants such as reflection coefficient, n, extinction coefficient, k, and layer thickness are simultaneously determined at wavelength of 400–1100 (nm).

2. Modeling, Simulation and Calculation Method

A usual method for describing optical constants of thin films is utilizing classic dispersion relationships based on di–electric function. One of the oldest and most applicable dispersion relationships is Drude–Lorentz di–electric equation which is based on the interaction between light and material. This relationship is shown in Eq. (1):

$$\varepsilon = \varepsilon_\infty + \sum_{j=1}^{n} \frac{f_j E_{0j}^2}{E_{0j}^2 - E^2 + i\Gamma_j E} + \frac{E_P^2}{E^2 + iE_\tau E} \qquad (1)$$

where ε_∞, f_j, E_0 and Γ_j are di–electric constant at high frequencies, resonance amplitude, power and resonance width–band which are recognized as the reason for damping. Damping is due to absorption process which includes transition between two states. The third term is related to Drude model. E_p is density of Plasma energy and E_r is incident energy [4]. The complex di–electric function as $\varepsilon=\varepsilon_1 + i\varepsilon_2$ which describes the reaction of material with electromagnetic waves as a function of photon energy, E, or wavelength, λ, has a real part ε_1 and an imaginary part ε_2. Real and imaginary parts of complex reflection coefficient, namely n(λ) and k(λ) are related to di–electric function as Eq. (2) [5]:

$$n(\lambda) = \left(\frac{\varepsilon_1 + \left(\varepsilon_1^2 + \varepsilon_2^2\right)^{1/2}}{2} \right)^{1/2}$$
$$k(\lambda) = \left(\frac{-\varepsilon_1 + \left(\varepsilon_1^2 + \varepsilon_2^2\right)^{1/2}}{2} \right)^{1/2} \qquad (2)$$

Reflection spectrum (R) of samples for normal incident is a function of film thickness d, medium reflection coefficient S, incident light wavelength λ, reflection coefficient n(λ) and extinction coefficient k(λ).

Simulation of the measured reflection data using optimization of objective function, which is the square of difference between the measured reflection spectrum and the calculated one, is defined as:

$$O = \left(\varepsilon_\infty, f, \Gamma, E_0, E_P, E_\tau, d\right) = \sum \left(R_{meas} - R_{calc}\right)^2 \qquad (3)$$

where, R_{meas} and R_{calc} are the measured and theoretical reflection spectrum, respectively. using the fitting parameters obtained from minimization of objective function, dispersion curves of reflection and extinction coefficients can be estimated.

3. Results and Discussion

The measured and simulated reflection spectra with fitting parameters of Iridium (IV) Oxide (IrO_2)–roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations at various concentrations of 0.5, 1 and 1.5%, named as a, b, and c, and roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations sample, named as p, are shown in Figure 1 in wavelength range of 400–1100 (nm) (visible regions close to infrared) using Drude–Lorentz model for air, film, medium, air system.

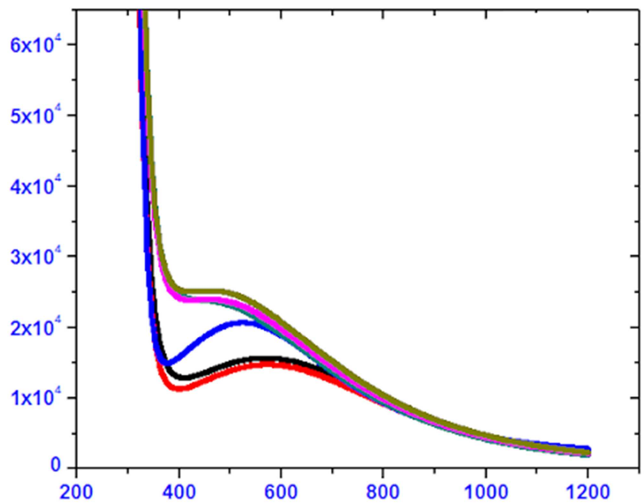

Figure 1. *Results of simulating the reflection spectrum for Iridium (IV) Oxide (IrO_2)–roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations at concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) non–doped.*

Comparison of the results were shown that the sample containing 0.5% of Ir (sample a) has shown more reflectivity than samples containing 1% and 1.5% of Iridium (IV) Oxide (IrO_2) (samples b and c). As can be seen in Figure 1, the reflection of thin films is decreased by increase in mole concentration of Ir to Iridium (IV) Oxide (IrO_2). This reduction can be attributed to various reasons such as increasing roughness, increasing thickness and increasing the concentration of contaminant. The results of investigation about surface roughness using AFM method confirms the increasing of roughness by increasing the concentration of Ir. Therefore, dispersion of incident light is increased in thin films. Variation of thickness of thin film by increasing the percentage of Ir is effective in variation of reflectivity of thin films which is due to sol viscosity. Changing the crystalline structure and chemical composition of thin films induced by penetration of Ir ions into the crystalline lattice of Iridium (IV) Oxide (IrO_2) is another effective factor which leads to changing the reflection spectrum. The results of structural analysis using XRD confirms the tendency to be amorphous by increasing the concentration of contaminant.

The best fitting parameters obtained from optimization process and experimental data fitting are listed in Table 1.

Table 1. *Fitting parameters of di–electric function of DL model.*

Parameter	Pure	% 0.5 Iridium (IV) Oxide (IrO_2)	1% 1 Iridium (IV) Oxide (IrO_2)	% 1.5 Iridium (IV) Oxide (IrO_2)
ε_∞	0.85	0.75	0.65	0.55
E_P	9.85	8.75	7.65	6.55
E_τ	5.45	5.4	5.35	5.25
f	3.35	3.25	3.15	3.05
E_0	5.5	5.4	5.3	5.2
Γ	4.5	4.4	4.3	4.2
$d(nm)$	225	335	445	655

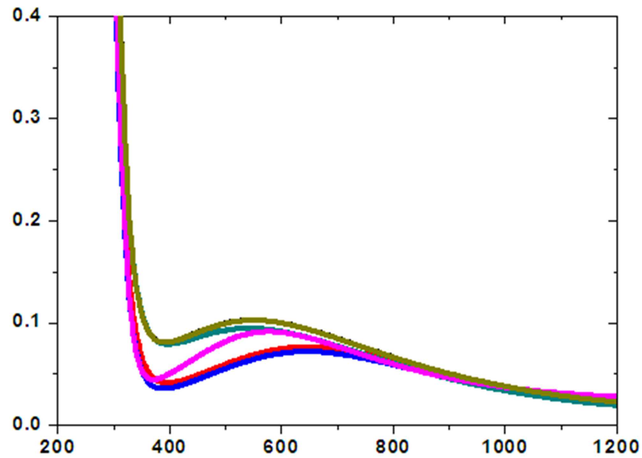

Figure 2. *Reflection coefficient of Iridium (IV) Oxide (IrO_2) thin films with Ir concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) pure sample.*

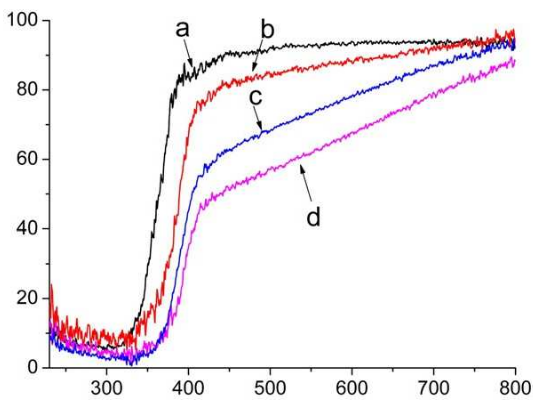

Figure 3. *Extinction coefficient of Iridium (IV) Oxide (IrO_2) thin films with Ir concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) pure sample.*

As cab be seen in Table 1, more increase in Ir leads to increase in Γ, f, E_0 and d and decrease in other parameters as crystalline structure and inter–atom distance changes in lattice of Iridium (IV) Oxide (IrO_2) thin film. According to A. Heidari [7], E0 in the range of 2.9–3.1 (eV) shows optical transition capacity band to displaced state of conducting band which according to the data of Table 1, it can be concluded that optical transition energy (gaff energy) increases with increase in Ir concentration. The calculation results of optical constants including reflection coefficient and extinction coefficient using the parameters of obtained di–electric function from the optimization process of thin films at various concentrations of Iridium (IV) Oxide (IrO_2) as 0.5% (sample a), 1% (sample b) and 1.5% (sample c) are shown in Figures 2 and 3, respectively.

As can be seen in Figure 3, reflection coefficient of samples at 500–1100 (nm) are the same and are decreased by increasing wavelength. By increasing the concentration of Ir, reflection coefficient is totally reduced which is in good agreement with the results related to variations of reflectivity in Figure 2 in which, increasing roughness leads to increase in dispersion and hence, reducing the amount of reflection spectrum. It can be seen in Figure 3 that k(λ) for two samples of p and a are of increasing rate at wavelength range of 400–500 (nm). Further, all samples are of decreasing rate at the range of 500–800 (nm). Totally, k(λ) is reduced by increase in Ir concentration. In other words, optical absorption is reduced in this range and the emerged peaks at extinction coefficient are in agreement with parameters of Drude–Lorentz obtained from the optimization algorithm.

4. Conclusions, Summary, Recommendations, Perspectives, Useful Suggestions and Future Studies

The results of optimization algorithm of Lovenberg–Marquardt with physical model of Drude–Lorentz for determining optical constants of Iridium (IV) Oxide (IrO_2)–roles and applications of Iridium (IV) Oxide (IrO_2) nanoparticles in cancer nanobiotechnology using synchrotron and synchrocyclotron radiations produced using sol–gel method through a single reflection spectrum show that higher doping leads to lower reflectivity and reflection coefficient and also, leads to increase in thickness of thin layer.

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