

Contribution of Drude and Brendel Model Terms to the Dielectric Function; A case of TiO₂:Nb Thin Films

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ABSTRACT

Parametric modeling provides a mean of deeper understanding to the properties of materials. Dielectric function is one of the key parameters which can provide information on the dielectric nature of a thin film or bulk materials. It can be obtained by modeling the material using appropriate existing, new or modified models. In our work, we utilized existing Brendel and Drude models to extract the optical constants from spectrophotometric data of fabricated undoped and niobium doped titanium oxide thin films. The individual contributions by the two models were studied to establish influence on the dielectric function. The effect of dopants on their influences was also analyzed. Results indicate a minimal contribution from the Drude term due to the dielectric nature of the undoped films. However as doping levels increase, the rise in the concentration of free electrons favors the use of Drude model.

Keywords: Brendel Model, Drude Model, Modeling Optical Constants, titanium Oxide

1 Introduction

Oscillator models are of interest to material scientists for the study of atomic and electronic behavior in materials [1]. This is made possible through the electronic or atomic interaction with an electric field [2], [3]. Examples of such models are the Lorentz and Drude models [1], [4], [5]. To the very least, Lorentz assumes electrons are bound by a spring like force while the later considers electrons as being unbound. Despite the simplistic assumption, Drude model has been shown to provide a fair explanation on cases when electrons are considered to have an appreciable interaction with each other and can be used to study the optical properties at energies below the band gap accounting for intraband transitions of the conduction electrons [6]. Several other models have been developed to address materials whose behavior do not fit well in the realm of Lorentz and Drude models. Brendel oscillator model [7] is the one of such models, which is an extension of the simple harmonic oscillator model [8], and is useful in modeling the influence of interband transitions in the band gap region but accounts for local variations in disordered systems.

2 Theoretical Considerations

There is a fundamental connection between electrical and optical properties of matter. They both are governed by the electronic structure and electromagnetic radiation interacts with charges present in the matter. The polarization of charges \mathbf{P} by an applied field \mathbf{E} is a function of the complex dielectric function ε according to

$$\mathbf{P} = \varepsilon_0(\varepsilon - 1)\mathbf{E}, \quad (1)$$

where ϵ_0 is the dielectric constant of free space and-

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega). \quad (2)$$

The optical properties can also be described in terms of the complex index of refraction N as-

$$N(\omega) = n(\omega) + ik(\omega) \quad (3)$$

where n is the real index of refraction and k is the extinction coefficient. Although they have a frequency dependence, they are usually called optical constants. The dielectric function is related to the index of refraction through the equation

$$\epsilon = N^2. \quad (4)$$

The dielectric function can often be divided into several terms, each term represents different excitation mechanism;

$$\epsilon = \epsilon_\infty + \chi_{VE} + \chi_{FC}. \quad (5)$$

where ϵ_∞ high frequency dielectric constant while χ_{VE} and χ_{FC} are the susceptibilities of the valence electrons and the free carriers respectively. The form of the latter parameter is often dictated by the oscillator models.

The free carrier behavior is often investigated by Drude model and χ_{FC} can be expressed as:

$$\chi_{FC} = \frac{\omega_p^2}{\omega^2 + i\omega\Gamma}, \quad (6)$$

Where ω is the radiation frequency, Γ is the damping and ω_p is the plasma frequency of the bound electrons, which depends on the number of electron taking part in the interband or intraband transition, n_e with;

$$\omega_p^2 = \frac{n_e q^2}{\epsilon_0 m_e}. \quad (7)$$

Considering the Brendel Oscillator model [7], χ_{VE} takes the form;

$$\chi_{VE} = \frac{1}{\sqrt{2\pi\sigma_B}} \cdot \int_{-\infty}^{\infty} \exp\left(-\frac{(x-\Omega_o)^2}{2\sigma_B^2}\right) \frac{\Omega_f^2}{x^2 - \omega^2 + i\omega\Gamma} dx \quad (8)$$

where Ω_0 is the resonance frequency, Ω_f is the oscillator strength parameter and σ_B denotes the width of the distribution. The Brendel term is a weighted superposition of an infinite number of Lorentz oscillators and has been found to be applicable to interband absorption in a number of materials [9]. It follows therefore that the expression for the dielectric function in Equation (5) based on Brendel and Drude models herein simply referred to as Brendel-Drude becomes:

$$\epsilon = \epsilon_\infty + \frac{1}{\sqrt{2\pi\sigma_B}} \cdot \int_{-\infty}^{\infty} \exp\left(-\frac{(x-\Omega_o)^2}{2\sigma_B^2}\right) \frac{\Omega_f^2}{x^2 - \omega^2 + i\omega\Gamma} dx + \frac{\omega_p^2}{\omega^2 + i\omega\Gamma} \quad (9)$$

3 Experiment and Modeling

Experimental data used was obtained from thin films of TiO₂:Nb made through dual-target reactive dc magnetron sputtering by following procedures as described elsewhere [10], [11]. A small amount of H₂ was added in order to avoid target poisoning and allow stable sputtering conditions [12], [13]. The film's composition was determined by Rutherford backscattering spectrometry (RBS) technique in the range of atomic weights from 1 (H) to 41 (Nb). Extraction of optical constants was done by fitting spectrophotometric

experimental data to Brendel and Drude models using the Scout software.

4 Results and Discussion

Figure 1 shows composition results for the undoped and Niobium doped titanium films which confirmed that undoped film had no niobium and one of the doped film sample had 3.7% niobium (at.%).

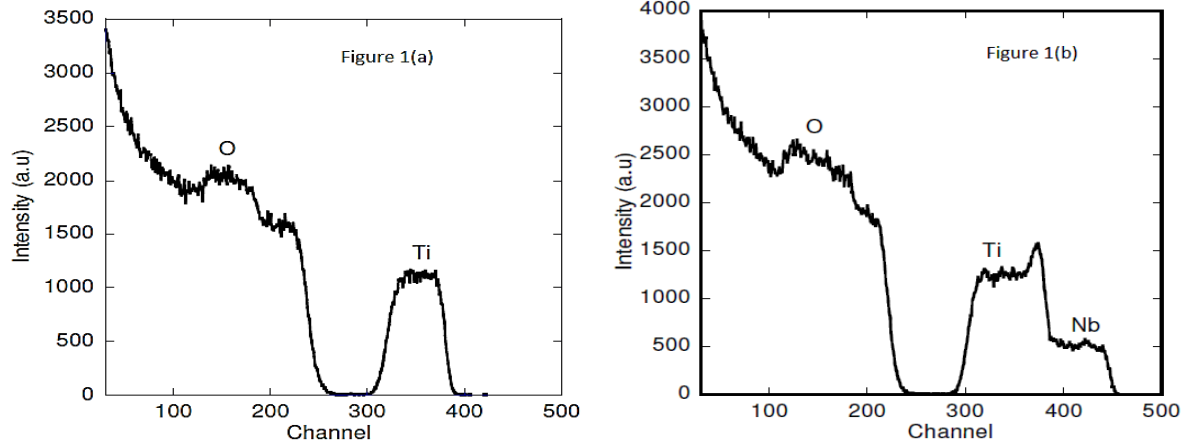


Figure 1: RBS spectra for (a) Undoped TiO_2 and (b) Nb doped TiO_2 with 3.7 at. % Nb. The elements are marked

The optical properties of the materials were determined from the best fit between computed and experimental data, using SCOUT commercial software [14]. The extensive data obtained contained optical parameters from Intraband, interband and dielectric background contributions. Figure 2 is a sample fit for a 3.7 at. % TiO_2 : Nb film. The fit utilized Brendel and Drude models.

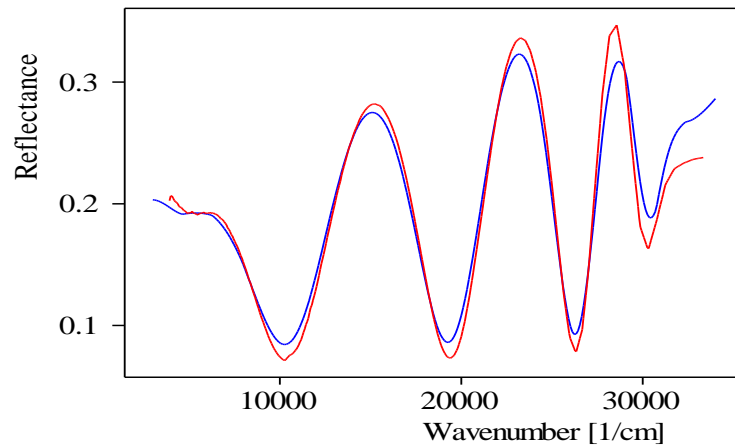


Figure 2: Simulated (blue) and experimental (red) spectra for Nb: TiO_2 film with 3.7 at.% Nb and thickness 228 nm. The sample was annealed in vacuum for 30 minutes at 450 °C

Table 1 shows electrical resistivity and carrier concentration for two films. The values were computed using well-known expressions;

$$\text{Resistivity: } \rho = \frac{\Omega_r}{2\pi\epsilon_o\epsilon_o\omega_p^2} \quad (10)$$

$$\text{Mobility: } \mu = \frac{e}{mc\omega_p^2} \quad (11)$$

The undoped film were insulating with resistivity in the order of 10^2 ohm-cm while niobium doping introduced

free carriers into the film and improved conductivity. From theory, good conductors respond well to Drude model as a result of interaction between the free electrons and the electric field [1], [4]. Undoped films are therefore expected to respond poorly to Drude model while attempting to utilize the model to extract the optical constants (n and k).

Table 1: Electrical and carrier concentration for undoped and doped $Nb:TiO_2$

Description of annealed Samples of $Nb:TiO_2$	Resistivity $\Omega - cm$	Carrier concentration cm^{-3}
Undoped $Nb:TiO_2$	3.31×10^2	9.13×10^{15}
$Nb:TiO_2$ with 3.7 at.% Nb	3.46×10^{-3}	1.25×10^{21}

Figure 3 clearly shows minimal Drude model contribution which is attributed to the insulating nature of the films. Intraband transitions dominate which is clearly demonstrated by the Brendel model. As carrier concentration rises due to doping, both Drude and Brendel models are expected to play a role due existence of both intraband [15] and interband transitions as is evident in Figure 4. The presence of free carriers is well illustrated in Figure 4. Drude model is expected to have a greater contribution to the k values for the conducting films which is indeed the case.

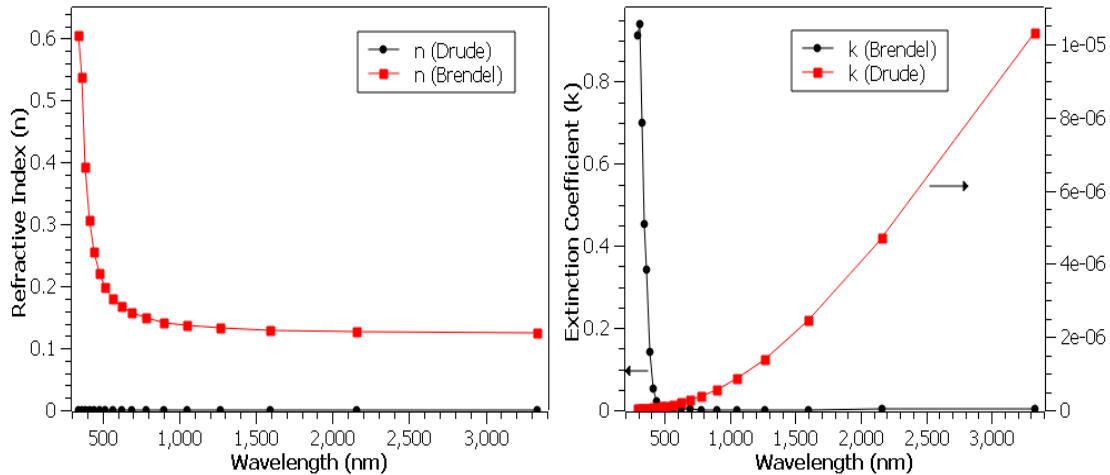


Figure 3: Individual contributions to optical constants n and k due to Drude and Brendel Models for undoped TiO_2 film. The dielectric background for refractive index is 2.026.

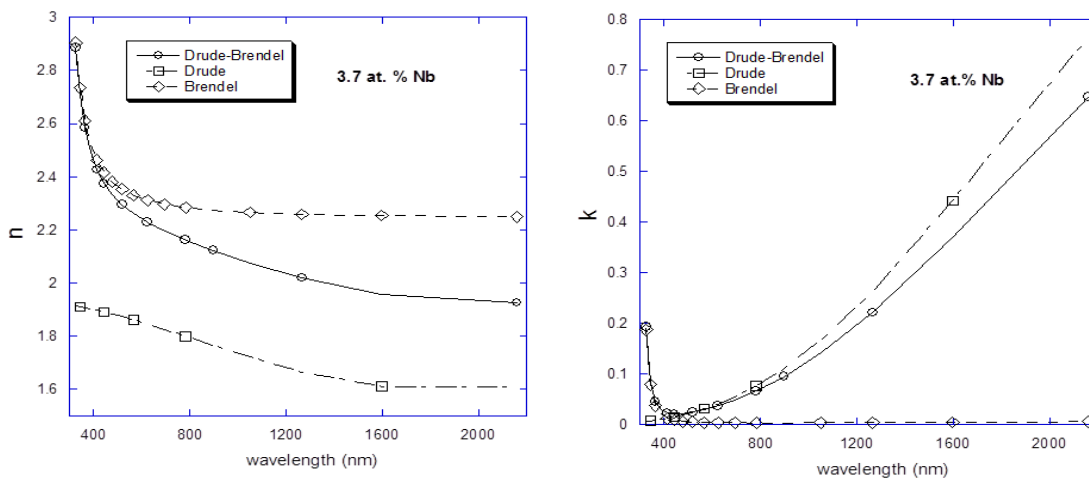


Figure 4: Individual contributions to optical constants n and k due to Drude and Brendel Models for doped TiO_2 film

5 Conclusion

The objective of the work was to demonstrate the versatility of the parametric modeling in the study of materials. The paper has showed individual contributions by Brendel and Drude models and how they relate to the nature of the films and provides a mean for deeper understanding of the materials. Interband transitions in the semiconductors require high energies. In these energy ranges, a model that responds to high frequencies is expected to be useful. Energies below the band gap do not favor interband transitions. Instead transitions are limited to conduction or valence bands and these effects can be investigated fairly well by the Drude model.

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