Optical Modeling of Fluorine Doped Tin Oxide Films for Spectrally Selective Applications

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Abstract

SnO2: F films are widely used for solar cell applications as the front electrode as well as other applications such as electrochromic and displays. The optical design of these and other applications need knowledge of optical constants. In this study we used the dielectric constant of a combined Drude and Lorentz to model the optical behaviour of SnO2: F using computer code created in MATLAB software. To do this, we used the fitting parameters from existing literature which were inserted into MATLAB code and n and k values were computed. Then, the n and k values were inserted into Fresnel R and T calculator and R and T spectra were computed over the 300nm -2500nm wavelength range using Fresnel’s equations. We plotted n, k, T and R for different values of plasma frequency, ωp and damping parameter, Γ. The films exhibited high visible transmittance of > 60% for all the samples and high infrared reflectance of 81.8% for the highly doped sample. The results implied the possibility of the films to be employed as spectrally selective coating materials.

KEYWORDS: Optical constants, damping parameter, thin-film, Drude-Lorentz model.

1. Introduction

Transparent conductors are materials that possess both good electrical conductivity and optical transparency in the visible portion of the electromagnetic spectrum. A wide bandgap (~>3 eV) is needed for visible transparency. A combination of transparency and conduction can be achieved in two different types of materials (Granqvist & Hultäker, 2002): (1) Extremely thin films of metals especially Ag, Au or Cu on glass or (2) among wide-bandgap oxide semiconductors such as fluorine-doped tin oxide (FTO), antimony-doped tin oxide (ATO), tin-doped indium–oxide (ITO), niobium- doped titanium oxide (TNO) and aluminium-doped zinc oxide (AZO). Wide-band gap oxide semiconductors are in most cases referred to as transparent conducting oxides (TCOs).

TCOs have been employed technologically for more than a half-century in applications requiring both high conductivity and optical transparency. Some TCO applications include transparent electrodes for flat-panel displays (Hecht et al., 2011), liquid crystal displays (LCDs) (Jeong et al., 2006), organic light-emitting diodes (OLEDs) (Weis & Martin., 2015), as coatings for heat-reflective windows i.e. thermal management for window glass (Biswas & Prasanta, 2018), electrochromic (smart) windows (Runnerstrom, et al., 2014), solar cells (Boscarno, et al., 2014), electromagnetic shielding (Angelov, et al., 2015), functional glasses(Karmakar & Basudeb, 2017), electrochemical cells and gas sensors (Shim et al., 2011). TCOs are also applicable to transparent optoelectronics because they have the unique features of optical transparency in the visible region and controllable electrical conductivity, from almost insulating to degenerate semiconducting (~ 10⁴ S/cm) behaviour.

Tin oxide, among the semiconductors, demonstrates special features in chemical inertness (Mishra, et al., 2009), stability to heat treatment and mechanical hardness. Further, tin oxide films are highly transparent in the visible range (Chitra, et al., 1991). It also has a direct bandgap of approximately 3.6eV(Shanting, 2017) which makes it possible to have a wide range of applications in electronic devices. In order to improve its optical and electrical properties, tin oxide films need to be doped with the right dopants such as fluorine, cadmium, molybdenum and

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antimony (Wang ,et al., 2019). Among these dopants, fluorine is found to be the best dopant for tin oxide since the radii of O$^2-$ and F$^2-$ are similar hence there will be no mismatch of lattices during doping (Wang ,et al., 2019).

Thin films of transparent oxide semiconductors, such as F-doped tin oxide, are widely investigated due to their high optical transmission, electrical conduction, and infrared reflection. These properties make these films to find wide applications in optoelectronic devices, hybrid microelectronics, photothermal conversion and direct energy conversion devices particularly in conductor-insulator- semiconductor solar cells. Fluorine-doped tin oxide has a work function of about 4.9eV, electron concentration in the order of $10^{20}$ cm$^{-3}$, an approximate minimum resistivity of about 200 $\mu\Omega$cm and a visible absorption coefficient of about 0.04 (Roy & Gordon, 2000).

Thin-film surface coatings are most widely employed for the efficient conversion of solar radiation into other useful forms, such as thermal energy for heating and cooling applications; and electrical energy by direct conversion using photovoltaic cells. The other current applications of such optical coatings include: transparent heat mirrors (Dobrikov, et al., 2009), antireflection coatings (Ronard & Willey, 2016), architectural coatings (Thelen, 1981), photo-thermal converters (Thelen, 1981), and photocatalysis (Nakata & Fujishima, 2012).

Invar Hamberg (1984) in his thesis(Ivar, 1984), reported that for the material to be used as spectrally selective coating material, it must meet three conditions: (1) should have a significantly wide band gap in order for the material to guarantee the key absorption edge to be below a solar wavelength length of approximately 300nm; (2) a prospect to dope the material to attain a high free carrier concentration leading to a high infrared reflectivity; (3) a limited absorption between the key absorption edge and the plasma wavelength, to guarantee a high luminous transmittance. Also, Maghanga in his thesis (Maghanga, 2009) reported separately that for a material to be used as a spectrally selective reflector (SSR), it must exhibit very high visible transmittance and high infrared reflectance. Furthermore, he suggested that the region of the plasma absorption peak must be positioned in the part of the solar spectrum with photon energies lower than the bandgap of the given solar cell. Spectrally selective films are those films that allow peculiarly selected portions of the light spectrum to pass through a medium while blocking some i.e. their transmission and/or reflection properties are regulated for selected and controlled packages of thermal radiation fluxes (Wanga & Shi, 2017). The conditions aforementioned necessitated the need to investigate a thin film that would meet all the conditions. Thus, the main aim of the study was to optically model fluorine doped tin oxide films for spectrally selective applications.

There are apparently many methods that have been employed to study the optical behaviour of SnO$_2$: F films as it is the case in numerous publications. The appropriate investigation of the optical properties of the films requires the finding of optical constants such as the extinction coefficient, $k$ and refractive index, $n$ over the desired wavelength range. In the present work, we employed the dielectric constant of a combined Drude and Lorentz to investigate the optical properties of SnO$_2$: F films.

### 1.1 Theoretical Background

The absorption and refraction of a medium can be described by a single quantity called complex refractive index (Mark, 2001). This is usually given the symbol $\tilde{n}$ or N and is defined as shown in equation (1).

$$ N = n + ik $$

[1]

The real part of N namely $n$ is the same as the normal refractive index defined in equation (2). The imaginary part of N, namely $k$, is called the extinction coefficient which is related to the absorption coefficient as shown in equation (3).

$$ n = \frac{c}{v} $$

[2]

$$ \alpha = \frac{2\omega k}{c} = \frac{4\pi k}{\lambda} $$

[3]
The complex refractive index of any medium can be related to the complex dielectric constant by using equation (4). This shows that if \( n \) is complex, then \( \varepsilon \) must also be complex.

\[
N^2 = \tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2 \tag{4}
\]

By comparing equations (1) and (4), explicit relationships between the real and imaginary parts of \( N \) and \( \tilde{\varepsilon} \) can be computed and the resulting equations are as shown in equations (5) and (6).

\[
\varepsilon_1 = n^2 - k^2 \tag{5}
\]

\[
\varepsilon_2 = 2nk \tag{6}
\]

Here \( n, k, \varepsilon_1 \) and \( \varepsilon_2 \) are referred to as the optical ‘constants’ of the medium. They are referred to as constants due to historical reasons otherwise they are functions of wavelength. \( \varepsilon_1 \) is related to the polarizability and \( \varepsilon_2 \) to the true optical absorption. These values depend on the photon energy, \( E = \hbar \omega \). Further, these optical constants, for any medium, can be calculated from a Drude-Lorentz model given in equation (7) (Kadi, et al., 2012). The individual Drude and Lorentz models are as given in equations (8) and (9) respectively.

\[
\varepsilon = \varepsilon_\infty - \frac{\omega_D^2}{\omega^2 + i\Gamma_D \omega} + \frac{\omega_L^2}{\left(\omega_0^2 - \omega^2\right) - i\omega \Gamma_L} \tag{7}
\]

\[
\varepsilon_1(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \Gamma^2}, \quad \varepsilon_2(\omega) = \frac{\Gamma/\omega}{\omega^2 + \Gamma^2} \tag{8}
\]

\[
\tilde{\varepsilon} = 1 + \frac{Ne^2}{\varepsilon_0 m \left(\omega_0^2 - \omega^2\right) - i\omega \Gamma} \tag{9}
\]

The Fresnel equations that are usually used to work out the transmittance and reflectance of the films are as shown in equations 10-19 (Ribbing, 2002).

\[
t_p = \frac{2N_1 \cos \theta_1}{N_1 \cos \theta_2 + N_2 \cos \theta_1} \tag{10}
\]

\[
t_s = \frac{2N_1 \cos \theta_1}{N_1 \cos \theta_2 + N_2 \cos \theta_1} \tag{11}
\]

\[
r_p = \frac{N_2 \cos \theta_1 - N_1 \cos \theta_2}{N_2 \cos \theta_1 + N_1 \cos \theta_2} \tag{12}
\]

\[
r_s = \frac{N_1 \cos \theta_1 - N_2 \cos \theta_2}{N_1 \cos \theta_1 + N_2 \cos \theta_2} \tag{13}
\]

And at normal incidence the equations become:

\[
r_1 = \frac{N_2 - N_1}{N_2 + N_1}, \quad r_2 = \frac{N_3 - N_2}{N_3 + N_2} \tag{14}
\]
\[
\begin{align*}
t_1 &= \frac{2}{N_1 + N_2}, \quad t_2 = \frac{2N_2}{N_2 + N_3} \\
\end{align*}
\]

Hence, \( r \) and \( t \) can be found according to:

\[
\begin{align*}
r &= \frac{r_1 + r_2 e^{-2i\varphi}}{1 + r_1 r_2 e^{-2i\varphi}} & [16] \\
t &= \frac{t_1 t_2 e^{-i\varphi}}{1 + r_1 r_2 e^{-2i\varphi}} & [17]
\end{align*}
\]

where the phase shift, \( \varphi \), is given by

\[
\varphi = -\frac{2\pi N_2 d \cos \theta}{\lambda}, \text{ which for normal incidence becomes: } \varphi = -\frac{2\pi N_2 d}{\lambda} & [18]
\]

and \( r_1 \) and \( t_1 \) are the Fresnel coefficients for the boundary between air and film and \( r_2 \) and \( t_2 \) are the corresponding coefficients for the boundary between film and substrate.

With the Fresnel equations above, the intensity reflectance, \( R \), and the intensity transmittance, \( T \), can be calculated according to:

\[
\begin{align*}
R &= r r^* \quad \text{and} \quad T = \text{Re}\left(\frac{N_3}{N_1}\right) t t^* & [19]
\end{align*}
\]

where \( r^* \) is the conjugate of the amplitude reflectance and \( t^* \) is the conjugate of the amplitude transmittance.

2. The Simulation Method.

The Drude–Lorentz modelling of optical spectra of \( \text{SnO}_2 : \text{F} \) films were simulated using equation (7) which was implemented in a computer code that was created in MATLAB software. To do this, we used the fitting parameters from literature shown in table (1) which were inserted into the MATLAB code from which \( n \) and \( k \) values, as well as the real part \( (\varepsilon_1) \) and imaginary part \( (\varepsilon_2) \) were computed. Then, each pair of \( n \) and \( k \) values were inserted into Fresnel equation R & T calculator together with Fresnel’s equations (equations 10-19), which is MATLAB code created in MATLAB software, to compute R- and T- spectra of \( \text{SnO}_2 : \text{F} \) films at different film thicknesses, \( d \) and for the various doping concentrations, \( n_e \) over 300 – 2500nm wavelength range. Different values of plasma frequencies, \( \omega_p \left(\text{s}^{-1}\right) \), were used as shown in table 2. All the simulation was done by using the MATLAB codes created in MATLAB software.

The figures shown below represent the modelled optical data for the different samples i.e. \( S_A, S_B, S_C, S_D, S_E, S_F \) and \( S_G \). \( S_A \) is the undoped sample whereas \( S_G \) is the heavily doped sample. The dopant concentration was increased gradually by varying the value of \( \omega_p \left(\text{s}^{-1}\right) \) as depicted in table 2.

<table>
<thead>
<tr>
<th>( \varepsilon_\infty )</th>
<th>( \omega_p \left(\times 10^{14} \text{s}^{-1}\right) )</th>
<th>( \Gamma_D ) ( \text{(eV)} )</th>
<th>( \omega_p ) ( \left(\text{s}^{-1}\right) )</th>
<th>( \Gamma_L ) ( \text{(eV)} )</th>
<th>( \omega ) ( \left(\text{s}^{-1}\right) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{SnO}_2 )</td>
<td>4.0</td>
<td>-</td>
<td>-</td>
<td>1.56 ( \times 10^{14} )</td>
<td>0.5064</td>
</tr>
</tbody>
</table>
Table 2: Values of plasma frequencies, $\omega_p \left( \text{s}^{-1} \right)$ used to calculate the optical constants in a combined Drude and Lorentz model.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$S_A$</th>
<th>$S_B$</th>
<th>$S_C$</th>
<th>$S_D$</th>
<th>$S_E$</th>
<th>$S_F$</th>
<th>$S_G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\omega_p \left( \times 10^{14} \text{s}^{-1} \right)$</td>
<td>0</td>
<td>1.43</td>
<td>2.02</td>
<td>2.85</td>
<td>3.49</td>
<td>4.03</td>
<td>5.71</td>
</tr>
</tbody>
</table>

3. Results and Discussion
3.1 Optical Studies
In order to compare the reflectance and transmittance of SnO$_2$ thin films with various F-doping levels, the optical R- and T-spectra in the UV-VIS-NIR region of the samples were computed and the results are shown in Figures 1 (a), (b), (c) and (d). The various film thicknesses shown in figures 1 (a), (b) and (c) are meant to magnify the optical properties of the graphs in the near IR for easy comparison.
It is clearly noted from the figures 1 (a), (b) and (c) that the films exhibit high transmittance in the visible region but in near IR region the transmittance starts to decrease with increase in F-doping concentration. The decrease in transmittance is due to reflection by the free electron in the highly F-doped SnO$_2$. This further illustrates that although doping improves the free carrier concentration thus the conductivity, it jeopardizes the transmittance of the films. Thus, there is a demand that a compromise between the optical properties and electrical properties should be attained for TCOs. On the other hand, reflectance increases in the near-infrared region with increasing F doping concentration to a maximum of 81.8% for the highly doped sample. The reduction of transmittance and the rise of reflectance at near-infrared indicate that the samples start to conduct. These observations are perfectly in agreement with other already reported work (Shadia, et al., 2008). The transmittance and reflectance behaviour of the films at various F-doping levels illustrates that doping improves the optical properties as well as conductivity of the films to a significant degree.

The shifts in the transmittance and reflectance fringes of the doped samples propose that doping leads to a slight change in the thickness and in the refractive index of the films. This can be verified by using the number of
interference fringes as given in equation 20(Swinepoxes, 1983) and by Swanepoel formula given in equation 21(Theiss & Teiss, 2001) respectively.

\[ d = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_1 - \lambda_2 n_2)} \]  

where \( n_1 \) and \( n_2 \) are refractive indices at two adjacent maxima (or minima) at \( \lambda_1 \) and \( \lambda_2 \) respectively.

\[ n = \sqrt{N + \sqrt{N^2 - S^2}} \]  

where

\[ N = 2S \frac{T_M - T_m}{T_M T_m} + \frac{S^2 + 1}{2} \]  

where \( S \) is the refractive index of the substrate, \( T_M \) and \( T_m \) represent the maximum and minimum transmittance envelopes at the fringes.

It is also noted from the figures that there is the cross over between R and T curves which shifts towards the visible range with increasing fluorine doping. These cross over show the position of the plasma wavelength. The plasma frequency \( \omega_p \), which according to classical Drude is as given in equation 23, is used to characterize the reflection by the free carriers. Using equation 23 we computed the carrier concentration, \( n_e \) of the samples and their corresponding values were recorded as shown in tables 3 and 4.

\[ \omega_p = \left( \frac{n_e e^2}{\varepsilon_0 \varepsilon_\infty m^*} \right)^{\frac{1}{2}} \]  

where \( \varepsilon_0 \) is the permittivity of free space, \( \varepsilon_\infty \) the high-frequency dielectric constant and \( m^* \) the effective conduction -band mass. In this paper, we assumed the value of \( m^* = 0.25m_e \) (Kulkarnia, Kirk, Schultz, Khan, & Lima, 1999) where \( m_e \) is the free electron mass.

The optical constants i.e. spectral refractive index \( n(\lambda) \), extinction coefficient \( k(\lambda) \), real \( (\varepsilon_1) \) and imaginary \( (\varepsilon_2) \) parts of the dielectric constant for SnO\(_2\) and SnO\(_2\) : F films are reported as shown in figures 2, 3, and 4 respectively. From figure 2 it was clear that the undoped film shows a dielectric behaviour with \( n = 2 \) over the 300nm -2500nm wavelength range. This value is well comparable with 1.98 already reported(Shamala., 2004). This refractive index value makes the transparent semiconducting tin oxide suited to be employed as an inherent antireflection coating on silicon(Maudes & Rodrigues, 1980).

From figures 3 and 2 it is clearly noted that \( k(\lambda) \) increases with an increase in wavelength whereas \( n(\lambda) \) shows a decrease towards higher wavelengths. These effects are more pronounced with increasing F-doping concentration. This behaviour was as expected for the case of metallic materials (Mageto, et al., 2015) and it may be associated to both shift of the plasma edge as well as the Burstein- Moss shift of the band edge(Mergel & Qiao, 2002).
Figures 4 show that $\varepsilon_1$ decreases with increasing fluorine doping concentrations while $\varepsilon_2$ shows an increase. It is also clearly noticed that the real dielectric constant, $\varepsilon_1$, is substantially negative in the wavelength range of high reflectance. This can be understood to mean that high negative values of $\varepsilon_1$ match with a phase relationship between the light and polarization. This relation aligns the polarization in the opposite direction to the incoming electromagnetic wave and hence high reflectance.

![Figure 2. Spectral refractive index, $n(\lambda)$ for the SnO$_2$ and SnO$_2$: F for various levels of F-doping concentration.](image)

Comparing figures 2 and 4(a), it is clearly noted that the real refractive index, $n$, is small over the region where $\varepsilon_1$ is negative. This makes the material to be optically metal-like (Mageto, et al., 2012). This further informs us that when $\varepsilon_1$ is negative, the optical constants are $n \approx 0$ and $k = \sqrt{-\varepsilon}$ corresponding to an exponentially damped field without energy loss, $\varepsilon_2 = 0$ (Wooten, 1972).

![Figure 3. Spectral extinction coefficient, $k(\lambda)$ for the SnO$_2$ and SnO$_2$: F showing values of k calculated from (a) Drude-Lorentz model and (b) Hong’s formula at d = 350nm.](image)
Figures 3 show a comparison of the spectral extinction coefficient, $k(\lambda)$, between the various values of $k$ computed from the Drude-Lorentz model and that from Hong's formula. Hong’s formula that was used to compute the $k$ values is as shown in equation 24 (Hong, 1989). The slight difference observed may be due approximation and assumption nature of the formulae.

$$\frac{1 - R}{T} = \exp\left(\frac{4\pi kd}{\lambda}\right)$$  \[24\]

![Graphs showing comparison between spectral extinction coefficients](image)

- **Figure 4. The real part of dielectric constant, $\varepsilon_1$, and the complex dielectric constant, $\varepsilon_2$, versus wavelength.**

<table>
<thead>
<tr>
<th>Sample</th>
<th>Plasma frequency, $\omega_p$ ($\times 10^{15}$ s$^{-1}$)</th>
<th>Plasma wavelength, $\lambda_p$ (nm)</th>
<th>Carrier concentration, $n_e$ ($\times 10^{20}$ cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_D$</td>
<td>0.81916</td>
<td>2301.08</td>
<td>1.6817</td>
</tr>
<tr>
<td>$S_E$</td>
<td>1.0422</td>
<td>1808.60</td>
<td>2.7223</td>
</tr>
<tr>
<td>$S_F$</td>
<td>1.2354</td>
<td>1525.81</td>
<td>3.8249</td>
</tr>
<tr>
<td>$S_G$</td>
<td>1.7870</td>
<td>1054.84</td>
<td>8.0029</td>
</tr>
</tbody>
</table>

**Table 3: Carrier concentration, $n_e$ values at different plasma frequencies for the samples at $d = 350$nm**

<table>
<thead>
<tr>
<th>Thickness $d$(nm)</th>
<th>Sample</th>
<th>Plasma frequency, $\omega_p$ ($\times 10^{15}$ s$^{-1}$)</th>
<th>Plasma wavelength, $\lambda_p$ (nm)</th>
<th>Carrier concentration, $n_e$ ($\times 10^{20}$ cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>$S_D$</td>
<td>1.3043</td>
<td>1445.16</td>
<td>4.2637</td>
</tr>
<tr>
<td>200</td>
<td>$S_E$</td>
<td>1.6905</td>
<td>1115.05</td>
<td>7.1619</td>
</tr>
<tr>
<td>350</td>
<td>$S_F$</td>
<td>1.7870</td>
<td>1054.84</td>
<td>8.0029</td>
</tr>
<tr>
<td>600</td>
<td>$S_G$</td>
<td>1.8166</td>
<td>1037.63</td>
<td>8.2705</td>
</tr>
</tbody>
</table>

**Table 4: Carrier concentration, $n_e$ values at different film thickness.**

Using values in tables 3 and 4 we drew the graphs of carrier concentration, $n_e$ as a function of plasma frequency, $\omega_p$. The graphs are as shown in figures 5. It is clearly noted from the figures that the carrier concentration of all the
samples increases linearly with increasing plasma frequency, $\omega_p$. This further makes it clear that it is the carrier concentration that shifts the plasma edges towards the visible range as was shown in figures 1.

![Graph showing carrier concentration against plasma frequency](a) ![Graph showing carrier concentration against plasma frequency](b)

**Figure 5.** Carrier concentration against wavelength showing (a) various plasma frequencies of the samples and (b) various film thicknesses of the samples.

The optical bandgap $E_g$ was evaluated from the standard expression (Granqvist C., 1995).

$$\alpha \ h \nu \ \propto \ (h \nu - E_g)^m \tag{25}$$

where $h$ is Planck’s constant, $\nu$ is the frequency and hence $h \nu$ is the photon energy in electron-volts (eV) and $\alpha = \frac{2\pi k}{\lambda}$ is the absorption coefficient. The constant $m$ depends on the optical transition mode having the values as listed in Table 4.

The Plots of $(\alpha h \nu)^2$ versus photon energy, $h \nu$, in the high absorption region, and extrapolation of the curve to $h \nu$ axis gives the indirect band gap. Similarly, $(\alpha h \nu)^2$ versus $h \nu$ and extrapolating to the $h \nu$ axis gives a direct bandgap. Tin oxide is a direct bandgap material (Shanthi, Dutta, Banerjee, & Chopra, 1980).
Figure 6. \((\alpha h\nu)^2\) Verses \(h\nu\) plots for determining the optical direct band gap of SnO\(_2\) and SnO\(_2\): F.

Figure 6 shows plots of \((\alpha h\nu)^2\) versus photon energy, \(h\nu\) in high absorption region. Extrapolation of the curves to \(h\nu = 0\) gave the direct band of SnO\(_2\) and SnO\(_2\): F films in the range 3.55eV – 3.81eV for the undoped and heavily doped films. It was found out that the direct band gap for SnO\(_2\) to be 3.55 eV which compares well with 3.6eV as already reported (Zhang, 2017).

Further, it is noted that there is a widening of bandgap with increase of fluorine doping concentration. This widening of the bandgap can be understood on the basis of Burstein–Moss shift, which occurs due to filling up of low-lying energy levels by the conduction electrons (Hamberg & Granqvist). According to this well-known Burstein-Moss (BM) shift, above the Mott critical density the partial filling of the conduction band causes a blocking of the lowest states and thus a widening of the optically observed bandgap. Further, above the Mott critical density, the valence and conduction bands are shifted in energy as a result of electron-electron and electron-impurity scattering (Ivar, 1984). In SnO\(_2\) these incline to partially compensate the BM shift.

Now, assuming the function of electron-electron and electron-impurity scattering, the energy gap for direct transitions in the doped material is given in terms of the unperturbed bands as shown in equation 26 (Ivar, 1984).

\[
E^o_g = E^o_c (k_F) - E^o_v (k_F)
\]  

[26]

Alternatively, equation (26) may be expressed as shown in equation (27)

\[
E^o_g = E^o_o + \Delta E^BM_g
\]  

[27]

where the BM shift is given by equation (28)

\[
\Delta E^BM_g = \frac{\hbar^2}{2m^*_{vc}} \left(3\pi^2n_c^*\right)^{2/3}
\]  

[28]

with the reduced effective mass according to equation (29)

\[
\frac{1}{m^*_{vc}} = \frac{1}{m^*_v} + \frac{1}{m^*_c}
\]  

[29]
Equation (29) predicts an energy gap shift proportional to $n_e^{2/3}$. Using equation (28) the values of BM of the samples $S_D$, $S_E$, $S_F$ and $S_G$. were computed. The computed values were $2.7736 \times 10^{18}$ eV, $3.8238 \times 10^{18}$ eV, $4.7968 \times 10^{18}$ eV and $7.8470 \times 10^{18}$ eV respectively. From the values, it is clear that the optical bandgap should increase.

### Table 4: Values of the exponent m for Equation 25 for different band gap transition modes.

<table>
<thead>
<tr>
<th>Transition mode</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct allowed</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>Direct forbidden</td>
<td>$\frac{3}{2}$</td>
</tr>
<tr>
<td>Indirect allowed</td>
<td>2</td>
</tr>
<tr>
<td>Indirect forbidden</td>
<td>3</td>
</tr>
</tbody>
</table>

Figure 7 shows absorption spectra over the wavelength range 300 – 2500nm for the samples in figure 1(c). The absorption for each sample was calculated from the relation in equation (30). It was noted that almost all the samples have an absorption peak which shifts towards the visible wavelength range with increase in fluorine doping concentration. The shift of the position of the absorption edge can be associated with the varying bandgap.

$$T + R + A = 1$$  \[30\]

where $T$ is the transmittance, $R$ is the reflectance and $A$ is the absorption.

![Absorption spectra](image)

**Figure 7.** Spectral absorptance $A = 1-(R+T)$ for the samples in figure 1.0 (c).

### 3.2 Electrical Studies.

The relationship between electrical conductivity and the optical constants is as given in equation (31) (Wooten, 1972).

$$\frac{\sigma_1}{c} = \frac{n k}{\lambda_{\text{ce}}},$$  \[31\]
where \( \lambda_0 = \frac{2\pi c}{\omega_0} = 12,850 \text{nm} \).

Using the relation in equation (31) the electrical conductivity, \( \sigma_1 \) was computed for all the samples and the results are presented as shown in figure 8. It is observed from the figure 8 that the electrical conductivity increases exponentially with increasing dopant concentration. This observation illustrates that doping improves the conductivity properties of the material to a significant degree.

From figures 4(b) and 8 it is clearly observed that there is a close relationship between the optical conductivity, \( \sigma_1 \) and the imaginary part of the dielectric constant, \( \varepsilon_2 \).

![Figure 8. Electrical conductivity spectra](image)

**4. Conclusion**

In this work, fluorine-doped tin oxide films were modeled successfully using a dielectric constant of a combined the Drude and Lorentz model. From the analysis, it was shown that the films had high visible transmittance of > 60% for all the samples and high infrared reflectance of 81.8% for the highly doped sample. The results imply the possibility of the films to be employed as spectrally selective coating materials. From the analysis, it can be concluded that an increase in the doping concentration improves the optical and electrical properties of tin oxide to a greater extent. From the study it can also be concluded that the film thickness also affects the transmittance and reflectance properties of the films. An increase in film thickness leads to an increase in reflectance and a decrease in transmittance. From the study of the optical constants it can also be concluded that, in practice, it is only \( \varepsilon_f \) that be negative.

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**References**

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