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Optical Properties of PS-MgO Thin Films

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ABSTRACT

In this study, optical properties of thin films made of different volume ratios of polysulfone (PS) and magnesium oxide (MgO) thin film deposited on germania (GeO_2) were studied as a function of wavelength in the range 0.3 – 1.1 µm using Matlab. Refractive indices, extinction coefficients, and absorption coefficients were investigated. The transmittance spectra of the PS-MgO thin films of different thicknesses deposited on the GeO_2 substrate were also examined. The films were found to show an increase in transmittance with an increase in the MgO percentage the thin film. However, the absorbance of the film was found to be high in the ultraviolet. The results give good reason for the applications of MgO thin films in optoelectronic devices.

Keywords

Matlab, PS, MgO, Optical properties, Refractive indices, Substrate, Thin film.

Introduction

Polymer-metal oxide thin films are expected to receive considerable attention because of their many applications including in optoelectronics [1-3]. Polymers are multifunctional materials widely used in many fields [4]. The addition of low weight content of metal-oxide nanoparticles to the polymer enhances its physical, chemical, electronic, and optical properties and leads to more interesting and useful materials [5,6]. The change in the polymer properties being dependent on the dopant and the way in which it interacts with the polymer, theoretical studies might be the most cost and time effective way to predict various properties of composite nanomaterials.

In this study, thin films of polystyrene (PS) doped with magnesium oxide (MgO) of different weight fractions are used for the thin film. The films are produced by depositing a very thin layer of the composite material on the surface of a substrate, GeO_2. Polystyrene is low cost and has major characteristics including transparency, relatively high index of refraction, low water absorption, and good electrical insulation [7,8]. As for MgO, it has wide band gap, good chemical and thermal stability, high economical availability, and eco-friendly nature [9].

To predict the photoelectrical properties of the thin films, transmittance and reflectance of polystyrene-magnesium oxide thin films with different weight content and different thicknesses have been studied and analyzed on GeO_2 substrate to obtain the optimal configuration for the development of optoelectronic devices.

This paper is organized as follow: section II covers the theoretical calculations, section III shows the results and discussions, and section IV is the conclusion and future work.

Theoretical Calculations

Equations of reflectance and transmittance for thin films have been derived, then simulated using Matlab. Figure 1 [10] shows the model of an optical thin film of refractive index *n*, deposited on a transparent substrate with refractive index *s*.

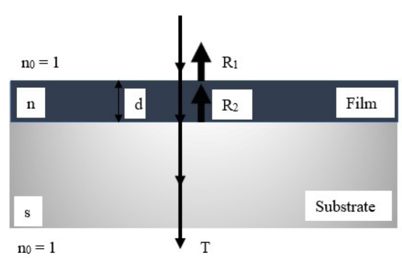

Figure 1: Model of optical thin film.

The thickness of the thin film d, is several orders of magnitude smaller than that of the substrate. The index of the surrounding air is n_0 = 1. As seen in Figure 1, for normal incidence, the incident light beam gives rise to a reflected beam and a transmitted beam, both perpendicular to the interface. The light reflected on the interface between air and film has intensity R_1, and the light reflected on the interface between the film and substrate has intensity R_2. Reflection at the interface between substrate and air is not considered. T represents the transmittance of light. In this work, PS-MgO is used as the thin film on GeO_2 substrate. Different concentrations of the thin films have been used as seen in Table 1.

Table 1: Concentrations of PS and MgO used**.**

	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
Volume fraction PS	1	0.985	0.975	0.96815	0.90
Volume fraction MgO	0	0.015	0.025	0.031850	0.10

The Cauchy-Urbach dispersion model is used to study the refractive index of the thin film as function of the wavelength [11]:

$$n = A + B/\lambda^2 + C/\lambda^4 \quad (1)$$

λ represents the wavelength of light in micrometers, and *A*, *B*, and *C* are fitting parameters.
Parameters utilized in reference [xiv] were used for PS and MgO and values are provided in Table 2.

Table 2: Fitting parameters for PS and MgO.

	A	*B* (μm²)	*C* (μm⁴)
Polystyrene (PS)	1.611	$2.574*10^{-8}$	$7.688*10^{-15}$
MgO	2.02	$8.38*10^{-8}$	$8.91*10^{-15}$

The index of refraction of the composite thin film with different volume fractions of MgO have also be computed according to the equation:

$$n = n_{ps} * volume\ fraction\ (PS) + n_{MgO} * volume\ fraction\ (MgO) \quad (2)$$

Refractive indices of substrates are given by the Sellmeir dispersion model [12]:

$$s^2 = 1 + (A1*\lambda^2)/(\lambda^2-\lambda_1^2) + (A_2*\lambda^2)/(\lambda^2-\lambda_2^2) + (A_3*\lambda^2)/(\lambda^2-\lambda_3^2) \quad (3)$$

λ is the wavelength in micrometers, and A_1, A_2, A_3, λ_{ii} are Sellmeir coefficients. Table 3 includes Sellmeir coefficients for GeO_2.

Table 3: Fitting parameters for GeO_2.

	A_1	A_2	A_3	λ_1	λ_2	λ_3
GeO_2	0.80686642	0.71815848	0.85416831	0.068972606	0.15396605	11.84

From these fitting parameters, the indices of refraction of PS, MgO, PS-MgO composite, as well as GeO_2 as function of wavelength have been plotted as function of the wavelength using Matlab. Extinction and absorption coefficients, k and α respectively, of PS, MgO, and composite as a function of the wavelength have also been calculated and plotted according to the equations below:

$$k_{PS} = (5.45064*10^4)/4\pi * \lambda^{-0.498} \quad (4)$$

$$k_{MgO} = 1.84 \exp[1.23(1.242375/\lambda - 3.83)] \quad (5)$$

$$k = k_{PS} * volume\ fraction\ (PS) + k_{MgO} * volume\ fraction\ (MgO) \quad (6)$$

$$\alpha = (4\pi k)/\lambda \quad (7)$$

The values of R1 and R2 have been calculated by:

$$R_1 = [(n-1)^2 + k^2]/[(n+1)^2 + k^2 \quad (8)$$

$$R_2 = (s-n)^2/(s+n)^2 \quad (9)$$

The transmittance T of MgO thin film on different substrates is given by:

$$T = T_0 - 2*(R_1R_2)^{0.5}*\cos(\delta) \quad (10)$$

$$\delta = (4\pi nd)/\lambda + \pi \quad (11)$$

In (10), T0 is the transmittance without interference effect. It is found from:

$$\alpha = (1/d) * \ln[B_2/(B_3*T_0)] \quad (12)$$

where $B_2 = 16*n^2*s$ and $B_3 = (1+n)^3 * (n+s^2)$

The transmittance with interference effect is given by:

$$T_{interference} = T - T_0 \quad (13)$$

Results and Discussions

Optical properties were investigated in the region between 0.3 and 1.1 μm. The refractive indices for PS, MgO, and composite thin films, as well as the GeO_2 substrates are shown in Figures 2, 3, 4, and 5 respectively.

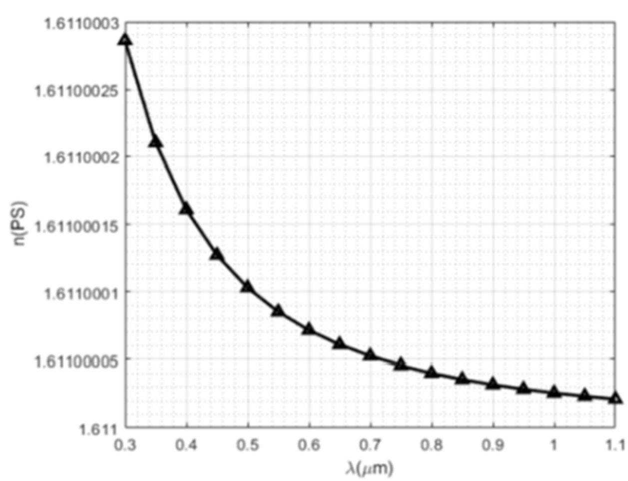

Figure 2: n(PS) as function of wavelength.

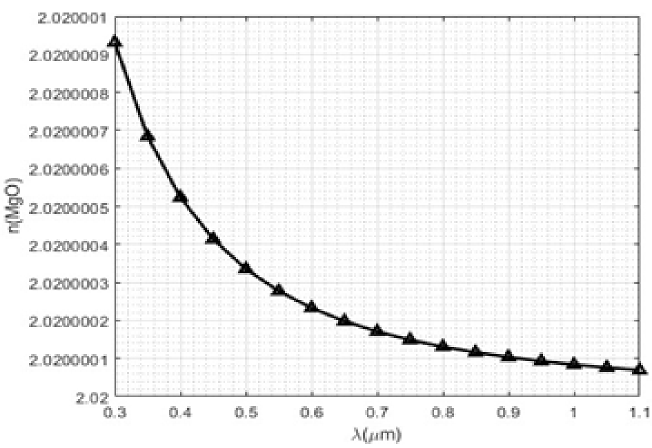

Figure 3: n(MgO) as function of wavelength.

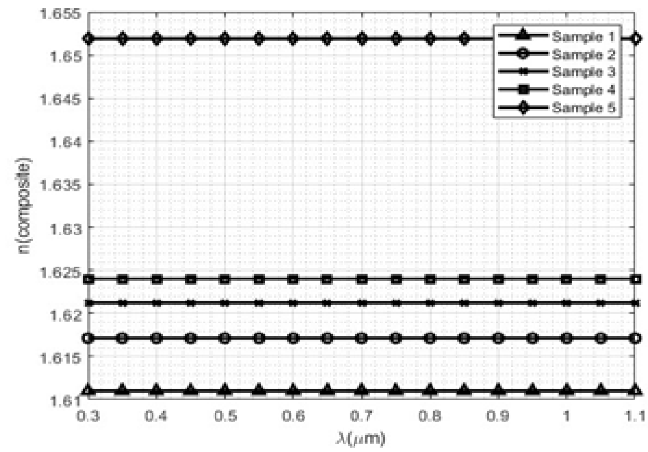

Figure 4: n(thin film) vs wavelength for different volume fractions.

It is observed that between 0.3 and 0.8 µm, the refractive indices decrease exponentially with the wavelength. After 0.8 µm, the evolution of the refractive index is linear. It is also noted that for the composite material, the index of refraction increases as the volume fraction of MgO increases.

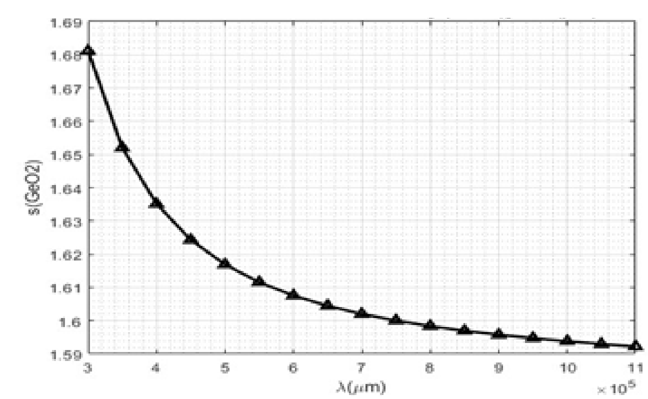

Figure 5: Refractive index of GeO_2 vs wavelength in µm.

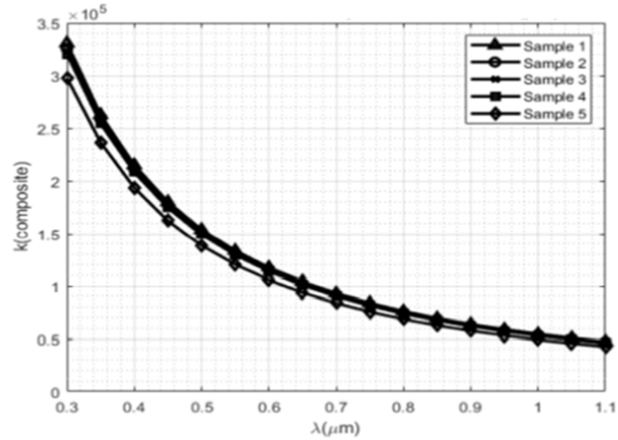

Figure 6: Extinction coefficient of composite thin film vs wavelength in µm with different volume fractions, k = k(composite).

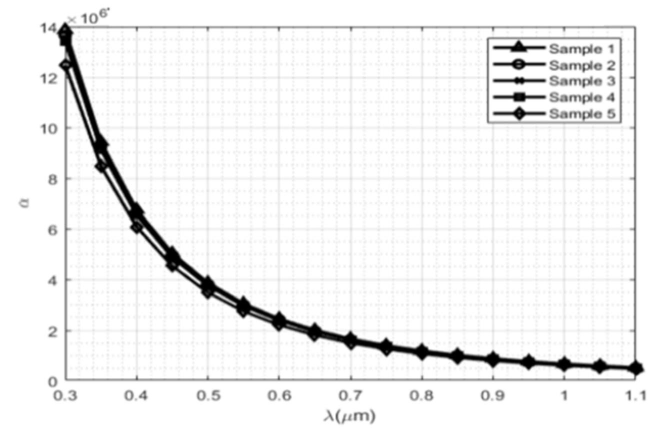

Figure 7: Absorption coefficient of composite thin film vs wavelength in µm with different volume fractions.

Figure 6 describes how the extinction coefficient varies as function of wavelength. It is observed that it decreases exponentially between 0.3 and 0.7 µm, and after that, it is almost constant with a value very close to zero. Figure 7 describes how the absorption coefficient varies as a function of wavelength. It also decreases exponentially between 0.3 and 0.7 µm, and then becomes almost zero at higher wavelengths. This small value is explained by the very absorption in this region. For film thicknesses of d = 0.2 µm, 0.6 µm, and 1 µm deposited on GeO_2 substrate, the transmittance have been determined by Matlab.

Figure 8, Figure 9, and Figure 10 show the transmittance of thin films of different thicknesses deposited on GeO_2. It is observed that there are interference peaks with maxima and minima. The interference fringes are produced due to multiple reflection of light between the top surface of the film on contact with air and the bottom surface of the film in contact with the substrate. It can also be seen that the number of peaks increase with the increase in thickness and it is maximum with sample 5 of 10% MgO. Thus, it can be said that the effect of interference increases with the increase in thickness.

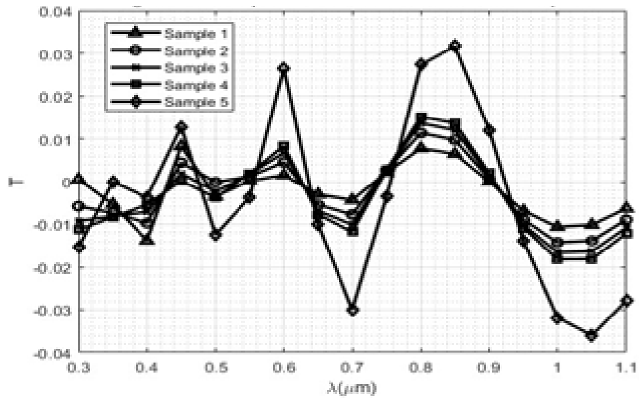

Figure 8: Transmission spectra of MgO/PS film deposited on GeO_2 for 0.2 micrometers.

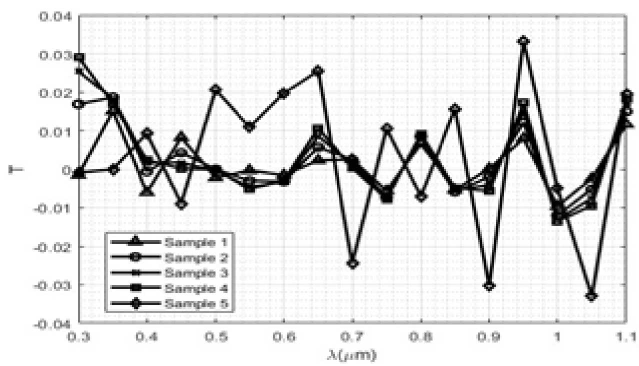

Figure 9: Transmission spectra of MgO/PS film deposited on GeO_2 for 0.6 micrometers thickness.

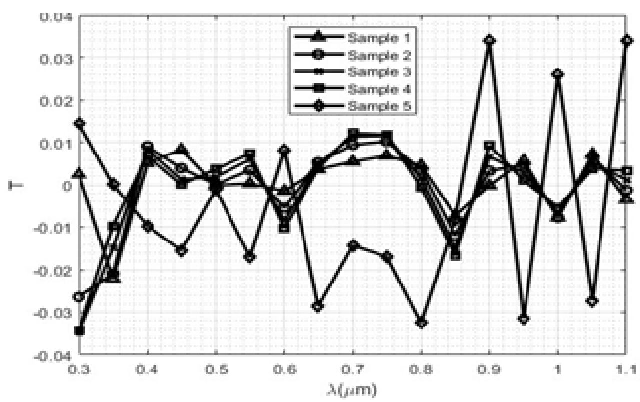

Figure 10: Transmission spectra of MgO/PS deposited on GeO_2 for 1 micrometers thickness.

Conclusion

The optical properties of PS-MgO thin films of different thicknesses deposited on GeO_2 were investigated to obtain an optimal thin film-substrate configuration. A thin film with 10% MgO exhibited the highest transmittance when the wavelength range was between 0.8 and 1.1 µm. Future work will focus on studying optical properties of different polymer-metal oxide thin films for various uses in optoelectronic devices.

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