Linear and Nonlinear optical study of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ /PVP nanocomposites for Photonic applications

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Abstract For use in flexible optical devices, new Polyvinylpyrrolidone (PVP) nanocomposite films doped with $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass have been created using the solution casting technique. Films optical constants were computed based on the spectral information measured in the wavelength range using a UV-visible spectrophotometer 400–800 nm is the range. It was discovered that the permitted indirect optical transition in these films has an energy gap that drops from 2.38 eV for pure $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ to 1.95 eV for the Se82Te15Bi1.0Sn2.0/PVP nanocomposites.

Keywords: Chalcogenide glasses, nanocomposite film, optical band gap, refractive index.

1. Introduction:

Composite materials are typically created to create a novel material that combines the advantageous or distinctive qualities of specific components. These days, the creation of clever, multifunctional materials depends heavily on nanocomposites [1, 2]. Organic electronics applications have been widely commercialized, primarily in the display (such as smartphones' displays), photovoltaic, and transistor technologies. A wide range of organic materials are being used for flexible optical and electronic applications, including solar cells, batteries, organic light emitting diodes, thin-film transistors, sensors, lasers, and organic semiconducting devices like organic field effect transistors, which previously used inorganic materials for their layered structures. Polymers in these organic materials are becoming more and more common due to its adaptable qualities, which include simplicity of processing, simple fabrication techniques, a reasonably strong electric breakdown field, mechanical flexibility, etc.[3] Furthermore, by adding inorganic components, their qualities may be changed [4-6]. Numerous polymers have been investigated for their properties for this purpose, including polyvinyl pyrrolidone (PVP), polymethyl methacrylate (PMMA), poly(diallyl dimethyl ammonium chloride (PDADMAC), polyvinylidene fluoride (PVDF), polyvinyl chloride (PVC), polyvinyl alcohol (PVA), and polymer blends like polyethylene glycol-polyvinyl alcohol (PEG-PVA) [7-10]. Inorganic materials, like amorphous chalcogenides, which are created when specific chalcogens (S, Te, and Se) are combined with elements like As, Sb, Bi, Sn etc., are part of the significant class of photonic materials because of their low phonon energy (375 cm-1), extended transmission window from visible to infrared, and ease of fabrication in the form of bulk and thin films [11-14]. A novel class of materials with promising and adjustable physical and optical properties is shown by the combination of polymer and chalcogenide glass to create nanocomposite[15-17] . A certain amount of work has been published on polymer chalcogenide composites' optical, electrical, thermoelectric, and dielectric characteristics [18-20].The present work reports the study of optical properties of new $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites.

2. Experimental

The standard melt quenching method has been used to create a bulk sample of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass [21].Using the solution casting method, films of pure PVA and its nanocomposites containing varying weight percentages of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass were created. Colloidal $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass solution was mixed with PVP solution in varied volumes to create $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP

nanocomposite films with variable concentrations of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass. To guarantee a uniform composition, the combined solutions were agitated for a further twenty-four hours. Ultimately, the solutions were placed into glass Petri plates and allowed to dry for 24 hours at 60-degree Celsius in a hot air oven. The $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposite thin films were separated from the petri dishes to form free-standing films with an average thickness of 100 µm. A Cary 5000 UV-VIS-NIR computer-controlled spectrophotometer from Agilent was used to examine the samples normal incidence absorption, transmission, and reflection spectra at room temperature (300 K) in the transmission range of 400-800 nm. From these spectra, the optical characteristics of the nanocomposites have been examined.

3. Result and discussions

The absorption spectra of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass and $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites are shown in Figure1. By utilizing the intersection of the abruptly declining region of the spectra with the baseline, one may directly estimate the wavelength corresponding to the absorption edge from the absorption graph.

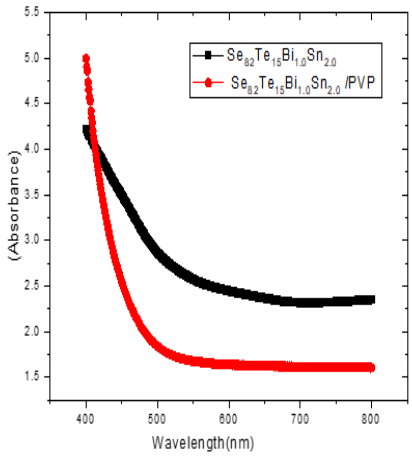

Fig.1. Absorption spectra of nanocomposites $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass and $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites.

The band gap of the material can be ascertained via fundamental absorption, which is the transmission from the valence band to the conduction band. The relation between absorption coefficient (α) and the incident photon energy (hν) is given by

$$\alpha h\nu = B(h\nu - Eg)^2 \quad (1)$$

where E_g is the material's optical band gap, B is a constant that determines the electron transition probability.

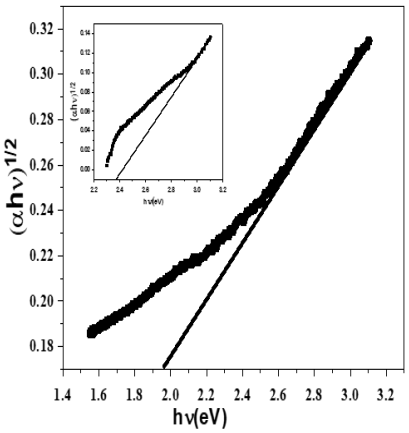

Fig. 2. $(\alpha h\nu)^{1/2}$ vs. hν for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites and the inset show $(\alpha h\nu)^{1/2}$ vs. hν for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ chalcogenide glass.

The relation [22] was utilized to determine the absorption coefficient (α).

$$\alpha = \frac{2.303 \times abs}{d} \quad (2)$$

where 'abs' is the absorbance and d is the thickness of the film.

Tauc's relation was utilized to calculate the energy band gap based on the absorption coefficient [23]. Plotting the values of $(\alpha h\nu)^{1/2}$ as a function of (hν) for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass and $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites and Fig. 2 shows the optical band gap energy value obtained by extrapolating the linear component to α=0.

Figure 3 displays the transmission spectrum of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass and $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites that were taken from a spectrometer.

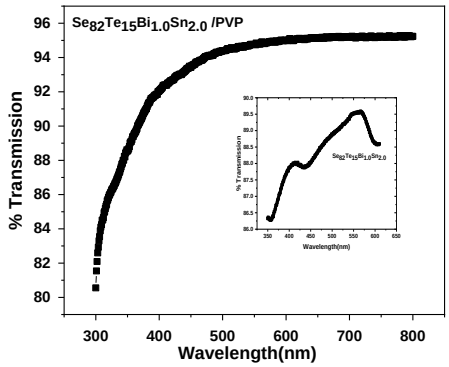

Fig.3. Transmission spectra for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites and the inset show transmission spectra for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ chalcogenide glass.

The absorption coefficient has a significant influence on the extremely complex functions of optical transmission (T) and reflection (R). Swanepoel's simple approach is used to calculate a number of optical properties for the thin film that has been prepared [24]. Important characteristics of photonic materials are the refractive index (n) and extinction coefficient (k). Values of *n* and *k* can be calculated from transmission and reflection spectra using the relation:

$$K = \alpha\lambda/4\pi \qquad (3)$$

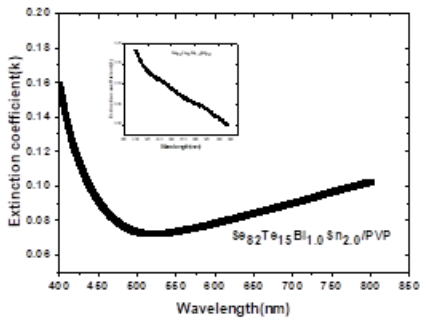

Fig.4. Behavior of K with wavelength for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites and the inset show behavior of K with wavelength for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ chalcogenide glass.

The extinction coefficient decreases as wavelength increases, indicating that more light is lost as a result of scattering.

The refractive index (n) has been calculated using the relation [25]

$$R = \frac{(n-1)^2+K^2}{(n-1)^2+K^2} \qquad (4)$$

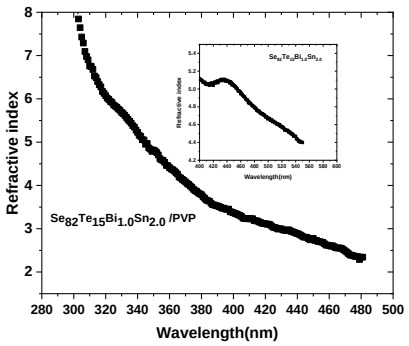

Fig.5. Behavior of refractive index(n) with wavelength for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites and the inset show behavior of refractive index(n) with wavelength for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ chalcogenide glass.

Values of K and n are tabulated in Table 1. These materials high refractive index values improve optical intensities for nonlinear interactions and are beneficial for strong optical confinement.

3.1 Nonlinear Refractive index(n_2)

The nonlinear refractive index (n_2) and susceptibility χ^{3} can be estimated using a straightforward empirical relation based on generalised Miller's rule. By combining Miller's generalised rule [26] with the low-frequency linear refractive index(n_0) one may calculate the non-linear refractive index (n_2) and susceptibility (χ^{3}).

$$\chi^{(3)} = \frac{A(n_0^2-1)^4}{(4\pi)^4} \qquad (5)$$

Here n_0 is static refractive index and estimated A value is $1.7*10^{-10}$ (for χ^{3}) in (esu) [26]. The nonlinear refractive index (n_2) can be estimated by the relation:

$$n_2 = \frac{12\pi\chi^{(3)}}{n_0} \qquad (6)$$

The obtained values of nonlinear refractive index (n_2) and susceptibility (χ^3) are incorporated in Table 1. It is discovered that the nonlinear refractive index of the studied films varies as well, based on the band gap. These materials high refractive index values are beneficial for nonlinear interactions and strong optical confinement [27].

Table 1. Values of E_g, k(at 450 nm), n(at 450 nm), n_0 , $\chi^{(3)}$ and n_2 for $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ and $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites

Sample	E_g	k	n	n_0	(χ^3)	n_2
$Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$	2.38 (eV)	0.101	5.01	4.3	$6.39x10^{-10}$esu	$5.60x10^{-9}$esu
$Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP	1.95(eV)	0.091	2.74	2.60	$7.52x10^{-12}$ esu	$1.08x10^{-10}$esu

4. Conclusion

The transmission spectra of $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$ glass and $Se_{82}Te_{15}Bi_{1.0}Sn_{2.0}$/PVP nanocomposites thin films in the 300–800 nm spectral range were used to study the thin films optical characteristics. The Tauc method was used to estimate the optical energy gap and it was discovered that the interband transitions were of the indirect kind. For the composite films, calculations have been made for the non-linear susceptibility $\chi^{(3)}$, and non-linear refractive index (n_2).

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