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The Effect of Nickel Bromide Nanoparticles on Optical and Thermal Properties of Polystyrene Polymer

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The optical properties and thermal conductivity of conductive polymer composites made of polystyrene (PS) Nickel bromide Nanoparticles ($NiBr_2$) were studied under different measuring conditions: Nickel bromide filler concentrations (0, 2, 4, 8, and 12 wt. %), ultraviolet radiation wavelength, and temperature range (30-105 °C), The solid electrolyte thin films were prepared using the solution cast method, Absorption and reflectance spectra of UV-radiation were recorded in the wavelength range 300-800 nm using a spectrophotometer. The optical energy gap and the basic optical constants, refractive index, and dielectric constants of the prepared films have been investigated and showed a clear dependence on the $NiBr_2$ concentration. The analysis of the optical results showed that the electronic transitions are direct in the *k*-space. The thermal conductivity (*k*) of the prepared thin films was studied as a function of temperature, and $NiBr_2$ concentration. It was found that thermal conductivity is enhanced by the addition of the $NiBr_2$ content and temperature. During the heating process, the phonons are activated and electrons hopping to higher localized energy states, producing an enhancement in the thermal conductivity.

Keywords: Optical properties, Thermal conductivity, Polystyrene, Nickel bromide, PS/$NiBr_2$ thin films, Optical energy gap.

1. INTRODUCTION

In general, a composite can be defined as heterogeneous systems that consist of two or more components that differ in chemical composition and properties and are separated by distinct interfaces. Each composite material is characterized by two features. Firstly, the typical sizes of the separate structural elements are small in comparison with the whole composite sample. Secondly, the typical sizes of the structural elements are greater than the sizes of their individual atoms or molecules [1]. A composite material is formed by reinforcing a resin matrix with a proper material. The reinforcement can be fibers, particulates, or whiskers, and the matrix materials can be metals, plastics, or ceramics [2]. Both composites and nanocomposites have many promising mechanical, thermal, electrical, optical, and other interesting properties that make them a field of current active research interest both in academia and industry [3]. Thermoplastics consist of a series of long-chain polymerized linear or branched molecules, in which all the chains are separate and can slide over one another. The long chain molecules of thermoplastic polymer are held together by relatively weak Van Der Waals forces, but the chemical bonds along the chain are extremely strong [4, 5].

Polystyrene is a thermoplastic polymer that has been widely used for its specific properties. The ease of transportation and the special characteristics of polystyrene have made this polymer one of the most widely used polymers in various industries, such as the construction of car bodies and home appliances, building insulation, and packaging industries [6]. Styrene is an important feedstock in a variety of polymer production. Of the total amount of styrene produced, almost 50 % is used to make polystyrene. In solid form, polystyrene is a colorless and rigid plastic; however, this material may also be returned to a liquid state by heating and used again for molding or extrusion [7].

Nickel bromide is a bromide of nickel. Nickel is a chemical compound with the atomic number 28. It is found abundantly in nature in laterite ore minerals, such as limonite, garnierite, and pentlandite. Nickel has a biological role and is found in certain enzymes, including urease, hydrogenase, methyl-coenzyme *M* reductase, and carbon monoxide dehydrogenase [8]. Bromine is a halogen element with the symbol Br and atomic number 35. Diatomic bromine does not occur naturally, but bromine salts can be found in crustal rock. Nickel bromide ($NiBr_2$) is a kind of brown powder. It is a weak reducing agent. It is rhombohedral, hygroscopic, and is soluble in water and in ethanol. It dissolves in water to make a blue-green solution typical of soluble nickel (II) compounds [9]. It can

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be used as a source of bromide ion and used in the pharmaceutical industry. It reacts with bases to make nickel (II) hydroxide.

In this work, Polystyrene/Nickel bromide nanocomposite (PS/NiBr$_2$) was prepared with different concentrations experimentally. Optical and thermal properties of the composite were studied in detail.

2. EXPERIMENTAL WORK

2.1 Composite Materials and Preparation

The studied composite films are made of polystyrene (PS) filled with different Nickel bromide NiBr$_2$ concentrations by using the casting method. Polystyrene and acetone were mixed and stirred continuously by using a magnetic stirrer for 24 hours at 70 °C until the polymer completely dissolved. Then NiBr$_2$ is added to the solution and shaken manually for a few minutes until the mixture reaches a homogeneous viscous molten appearance. The mixture was immediately cast to thin films on a glass plate ,and the acetone was allowed to evaporate completely at room temperature and under atmospheric pressure for a few days. The composite films were dried in an oven at 40 ºC for 2 days. The films obtained have thicknesses of about 70 mm and Nickel bromide concentrations of 0 %, 2 %, 4 %, 8 %, and 12 % by weight.

2.2 Optical Measurements

The most direct and perhaps the simplest method for probing the band structure of materials is to measure their absorption spectrum. The optical absorbance (*A*) and reflectance (*R*) spectra of the sample sheets were taken in the wavelength (*λ*) range (300-800 nm) using the UV-spectrophotometer.

2.3 Thermal Conductivity Measurements

The measurements of thermal conductivity were done using the heat-pulsed method, which is based on sending an electrical pulse to transmit across double test specimens separated by a current coil placed in a sample holder connected to thermocouples for temperature measurements. The cell assembly, which is surrounded by an insulating jacket to minimize the heat loss, is placed in an oven. Temperature readings were taken every half hour until the steady state of thermal equilibrium was reached. Measurements were taken within the temperature range: 30-105 ºC.

3. RESULTS AND DISCUSSION

3.1 Optical Results

When solids absorb an amount of light of intensity I$_o$, optical transitions appear if the energy of photons absorbed is greater than or similar to the energy gap. If the required energy is almost equal to the difference between the lowest level of the conduction band and the highest level of the valence band, electrons will immigrate from the valence band to the conduction band.

The absorption coefficient $\alpha(\omega)$ was then calculated from the absorbance $A(\omega)$ spectra using the relation [10]:

$$I = I_0 \cdot \exp \cdot [-\alpha x] \tag{1}$$

Hence,

$$\alpha(\omega) = \frac{2.303}{x} \log\left(\frac{I_0}{I}\right) = \frac{2.303}{x} A(\omega), \tag{2}$$

where I and I_0 are the incident and transmitted intensities UV-radiation, respectively, and x is the sample thickness about ($x = 0.7$ mm). The absorption coefficient $\alpha(\omega)$ was then calculated from the absorbance (*A*). After correction for reflection, $\alpha(\omega)$ was calculated using the equations (2).

Figure 1 shows the absorption spectrum for neat PS, 2, 4, 8, 12 wt. % thin films samples. One can clearly notice that absorption decreases rapidly with increasing the UV-wavelength.
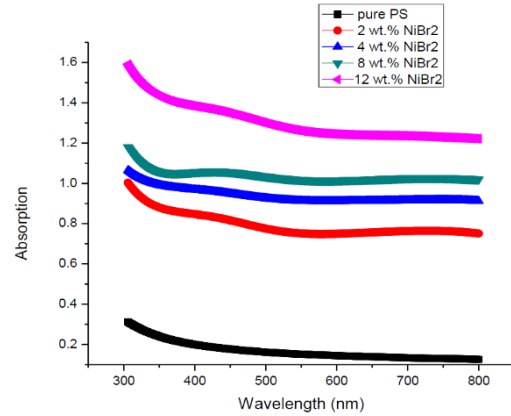

Fig. 1 – Absorption spectra for PS/NiBr$_2$ thin films

The absorption coefficient $\alpha(\omega)$ for a non-crystalline material can be related to the energy of incident photon energy ($\hbar\omega$) according to the formula [11]:

$$\alpha(\omega)\hbar\omega = \beta\left(\hbar\omega - E_{opt}\right)^r \tag{3}$$

where β is a constant, E_{opt} is the optical energy gap, and the exponent r is an index determined by the type of electron transition causing an optical absorption event and can take values of 1/2, 3/2 for direct and 2, 3 for indirect transitions, respectively.

Figure 2 shows the product of absorption coefficient (α) and photon energy ($\alpha\hbar\omega$)$^{1/r}$ versus photon energy ($\hbar\omega$) at room temperature for neat PS, 2, 4, 8, and 12 wt. % thin film samples. A good straight line is obtained with $r = 1/2$. This indicates that the transition energy for electrons is direct in k-space.
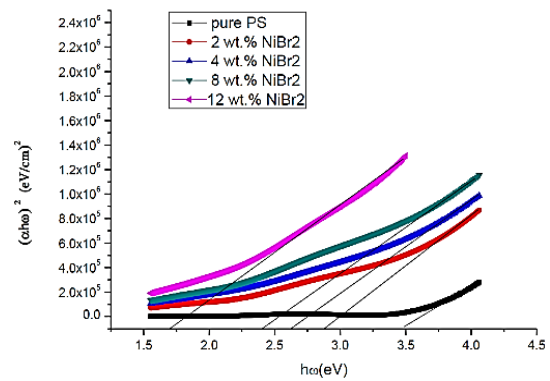

Fig. 2 – $(\alpha\hbar\omega)^2$ versus the incident light photon energy for PS/NiBr$_2$ thin films

Extrapolation of the linear portion of these curves gives the optical energy band gap (E_{opt}). Table 1 includes the measured values of (E_{opt}) which decrease with increasing the NiBr$_2$ concentration.

The decrease in the optical gap by doping may be explained on the basis of the fact that incorporation of a small amount of dopants forms charge transfer complexes in the host matrix as the dopants concentration is increased, the dopants charges start bridging the gap separation between the two localized states and lowering the potential barrier between them, thereby facilitating the transfer of charge carriers between the two localized state [12, 13]. The variation of the optical energy gap with the filler concentration is shown in Fig. 3.

Table 1 – Optical results

Thin films	E_{opt} (eV)	ΔE (eV)
Pure	3.52 ± 0.1086	0.72 ± 0.0072
2 %	3.01 ± 0.0903	0.73 ± 0.0073
4 %	2.77 ± 0.0831	0.77 ± 0.0076
8 %	2.55 ± 0.0765	0.79 ± 0.0078
12 %	1.72 ± 0.0546	0.82 ± 0.0081

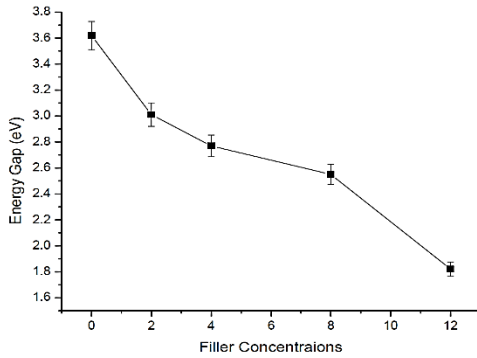**Fig. 3** – Energy gap with filler concentration

At a high absorption level ($\alpha > 10^4$) cm^{-1}, in the range of (1 to 10^4) cm^{-1}, which is associated with interband transition, the absorption coefficient $\alpha(\omega)$ is described by the Urbach formula [14]:

$$\alpha(\omega) = \alpha_o \exp\left[\frac{\hbar\omega}{\Delta E}\right], \qquad (4)$$

where α_0 is a constant and ΔE is the energy gap tail (or energy which is interpreted as the width of the tail of localized states in the band gap) [15].

Figure 4 presents the Urbach plot for the samples. The values of ΔE were obtained and listed in Table (1). The exponential dependence of $\alpha(\omega)$ on $\hbar\omega$ for these samples indicates that they obey the Urbach's rule. These tails become higher as the concentration of the NiBr$_2$ increases, which is consistent with E_{opt} variation. The variation of the Urbach energy tails with NiBr$_2$ concentration is shown in Figure 5. Since ΔE generally represents the energy difference between the localized states in the valence band and extended states in the conduction band or vice versa.

The increase of the tail width with the NiBr$_2$ concentration can be explained by the fact that the increase in NiBr$_2$ concentration could lead to the creation of disorder and imperfections in the structure of the thin films,

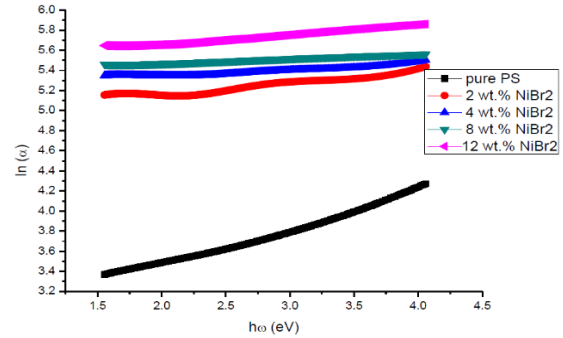a case that may increase the localized states within the forbidden gap.

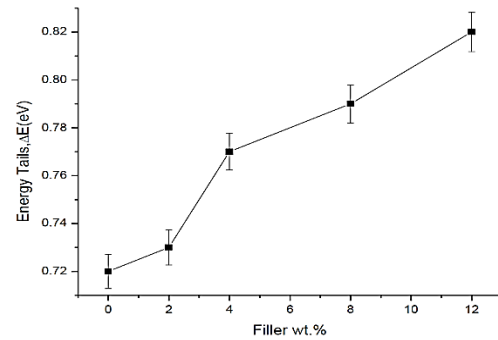**Fig. 4** – Natural logarithm of (α) versus the incident light photon energy

Fig. 5 – Variation of the urbach energy tails vs NiBr$_2$ concentration

The refractive index (n) values of the samples were obtained from the following
Equation [16]:

$$n = \left\{\left[\frac{4R}{(R-1)^2} - k^2\right]^{1/2} - \frac{R+1}{R-1}\right\} \qquad (5)$$

where R is the reflectance, k is the extinction coefficient that is related to the absorption coefficient and wavelength by:

$$k = \frac{\alpha\lambda}{4\pi} \qquad (6)$$

Figure 6 shows the variation of the extinction coefficient for the neat PS, 2, 4, 8, and 12wt. % thin film samples. The figure shows that the extinction coefficient (k) increases with increasing the wavelength, because (k) is directly proportional to the absorption coefficient as seen in equation (6). The value of extinction coefficient increases with increasing NiBr$_2$ concentration because it is directly proportional to the absorption coefficient. Extinction coefficient values exhibit changes with increasing of the NiBr$_2$ content.

Figure 7 shows the variation of the refractive index (n) obtained from equation (5), which shows that the refractive index decreases with increasing the applied wavelength, i.e., dispersion behavior. The variations of refractive index with the wavelength show that some interactions take place between incident photons and localized electrons.
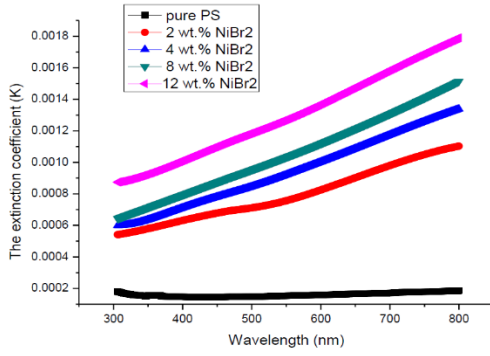
Fig. 6 – The variation of extinction coefficient for doped films with the photon wavelength
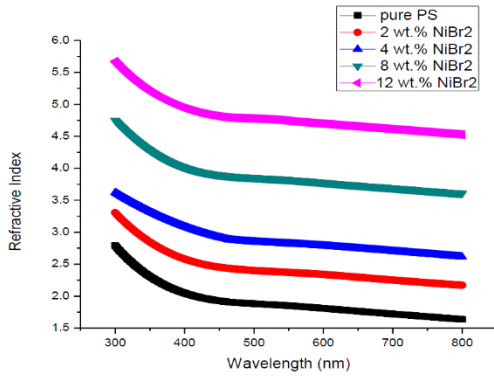

Fig. 7 – Refractive index vs Photon wavelength

Figure 8 shows the variation of the refractive index at ($\lambda = 600$ nm) for different NiBr$_2$ thin films doped. This shows the refractive index increases with increasing the concentration of the NiBr$_2$ in the PS matrix.
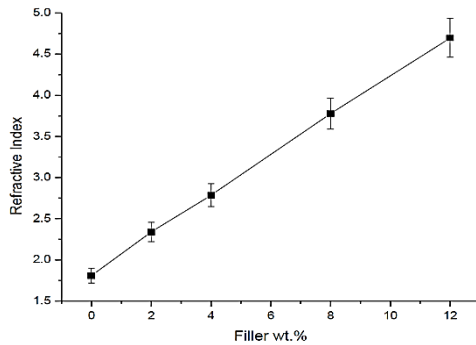

Fig. 8 – The dependence of the refractive index on NiBr$_2$ concentration at (600 nm)

The dielectric constant (ε') and the dielectric loss (ε'') are calculated from the relations [17]:

$$\varepsilon' = n^2 - k^2, \qquad \varepsilon'' = 2nk \qquad (7)$$

The variations of the dielectric constant and dielectric loss of the thin film samples with the incident wavelength are shown in Figures 9 and 10, respectively. The curves follow the same dispersive pattern in the UV-wavelength as shown in the refractive index behavior. The dielectric constant value of neat PS, 2, 4, 8, and 12wt. % thin film samples is greater for high NiBr$_2$ concentration and is attributed to space charge polariza-

tion, a phenomenon that appears in heterogeneous media consisting of phases with different electronic conductivity.
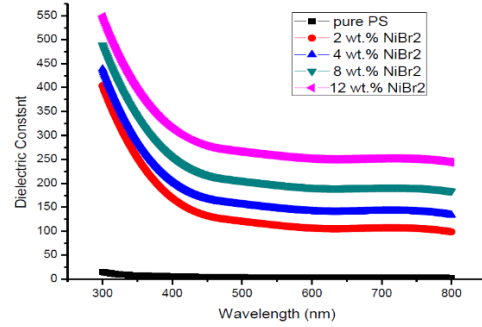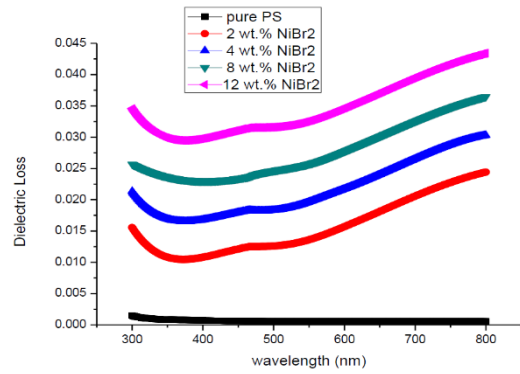

Fig. 9 – Dielectric constant vs Wavelength

Fig. 10 – Dielectric loss vs Wavelength

3.2 Thermal Conductivity Results

The thermal conductivity k for the five thin films samples, with different NiBr$_2$ concentration was measured in temperature range from 30 ºC to 105 ºC and calculated using equation [18]:

$$k = q_s \left(\frac{l}{\Delta T_s} \right) = \frac{IVl}{2A\Delta T_s} \quad \text{(W/m·ºC)} \qquad (8)$$

where q_s are the heat flux, I – the electrical current, V – the electrical voltage, and A – the area of the heating foil. Factor 2 is due to the symmetrical distribution of heat flux on both sides of the apparatus [19]. This is because we used two circular disks of identical thickness l.
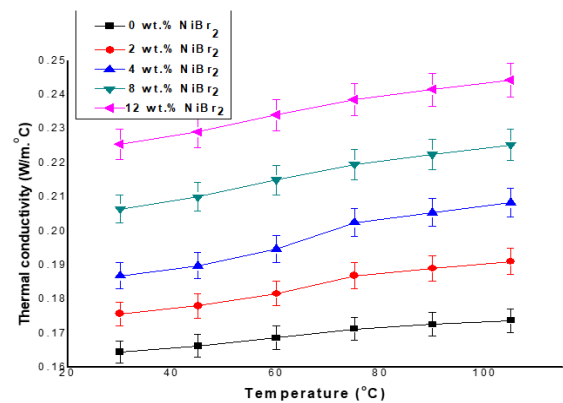

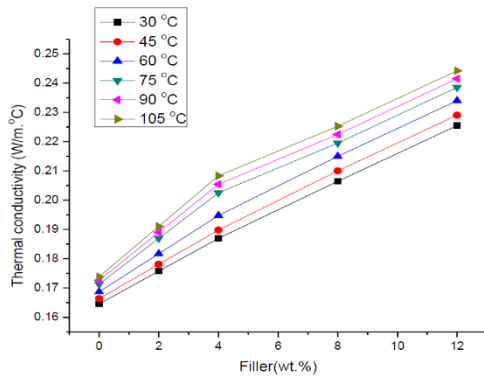**Fig. 11** – Thermal conductivity with temperature

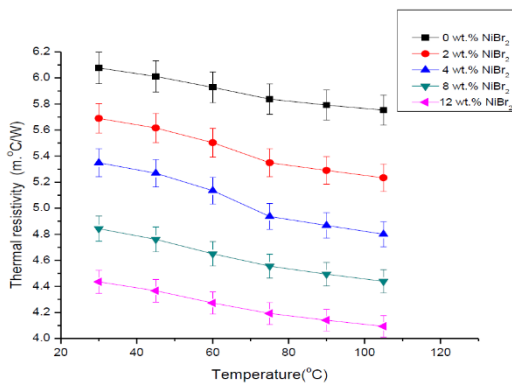**Fig. 12** –Thermal conductivity with NiBr$_2$ concentration

Fig. 13 – Variation of thermal resistivity ($r = 1/k$) with temperature

Figure 11 shows comparative graphs of thermal conductivity for four types of thin films and neat PS. It can be seen that the thermal conductivity increases with increasing the temperature.

Figure 12 shows an increase of thermal conductivity with NiBr$_2$ concentration. It can be seen that the thermal conductivity increases with increasing concentration of the filler content. This observed increase in k is raised from impurities, existing in the NiBr$_2$ deposit. Figure 13 displays the dependence of the thermal resistivity ($r = 1/k$) on temperature.

Table 2 shows the values of thermal conductivity and thermal resistivity for five samples at temperature 30 °C

Table 2 – Thermal conductivity results at ($T = 30$ ºC)

Thin films	Thermal conductivity (W/m·ºC)	Thermal resistivity (m·ºC/W)
0 wt. %	0.16 ± 0.0032	6.08 ± 0.12
2 wt. %	0.17 ± 0.0035	5.69 ± 0.11
4 wt. %	0.18 ± 0.0037	5.35 ± 0.10
8 wt. %	0.20 ± 0.0041	4.84 ± 0.09
12 wt. %	0.22 ± 0.0045	4.44 ± 0.08

4. CONCLUSIONS

The optical properties and thermal conductivity of solid polymer electrolyte PS/NiBr$_2$) were studied as a function of UV wavelength, NiBr$_2$ concentration, and temperature. By analyzing the results obtained. Some conclusions can be drawn from the results obtained: The optical energy gap value decreases, while the band energy tails increase with increasing concentration of NiBr$_2$. The extinction coefficient increases with increase in the UV wavelength. The observed dielectric constant and the refractive index increase with increase in NiBr$_2$ concentration.

The thermal conductivity is enhanced significantly with an increasing NiBr$_2$ weight fraction and increasing temperature. The highest thermal conductivity value reached 0.245 W/m·°C at 105 °C for 12 wt. % NiBr$_2$ compared with 0.172 W/m·°C for pure PS at the same temperature.

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Вплив наночастинок броміду нікелю на оптичні та теплові властивості полістиролу

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Оптичні властивості та теплопровідність електропровідних полімерних композитів із наночастинок полістиролу (PS) та наночастинок броміду нікелю ($NiBr_2$) були досліджені за різних умов вимірювання: концентрації наповнювача броміду нікелю (0, 2, 4, 8 та 12 мас. %), довжини хвилі ультрафіолетового випромінювання та діапазону температур (30–105 °C), тонких плівок твердого електроліту. Спектри поглинання та відбиття УФ-випромінювання реєструвались на спектрофотометрі в діапазоні довжин хвиль 300-800 нм. Оптична енергетична щілина та основні оптичні константи, показник заломлення та діелектрична проникність отриманих плівок були досліджені та показали чітку залежність від концентрації $NiBr_2$. Аналіз оптичних результатів показав, що електронні переходи є прямими в k-просторі. Теплопровідність (k) отриманих тонких плівок досліджували як функцію температури та концентрації $NiBr_2$. Було виявлено, що теплопровідність підвищується за рахунок додавання вмісту $NiBr_2$ і температури. Під час процесу нагрівання фонони активуються, а електрони стрибають до вищих локалізованих енергетичних станів, що призводить до підвищення теплопровідності.

Ключові слова: Оптичні властивості, Теплопровідність, Полістирол, Бромід нікелю, Тонкі плівки PS/$NiBr_2$, Оптична щілина.