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THE EFFECT OF NANOQUARTZ ON THE OPTICAL PROPERTIES OF IPP

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ABSTRACT

This study investigates the effect of nanoquartz (SiO_2) nanoparticles on the optical properties of isotactic polypropylene (iPP) composites. SiO_2 was added to iPP at various concentrations (1%, 3%, 5%, 7%, and 10%) to investigate changes in optical transmission, absorption spectra, and optical band gap. The results show a decrease in optical transmission as the SiO_2 concentration increases, with the material exhibiting stronger scattering and absorption effects. The absorption edge shifts toward longer wavelengths (redshift), indicating a narrowing of the optical band gap. This change was further confirmed by the Tauc method, which showed a decrease in band gap with increasing nanoparticle content. In addition, the Urbach energy, which reflects material disorder, was observed to increase with higher SiO_2 concentrations. This suggests that the incorporation of nanoparticles introduces localized defects and structural inhomogeneities into the polymer matrix. These results demonstrate that nanoquartz SiO_2 significantly modifies the optical behavior of iPP composites, enhancing their potential for use in optoelectronic devices where controlled optical properties such as light absorption and bandgap tuning are critical to performance.

1. Introduction

Polymers and polymer nanocomposites are widely used in all fields of science and technology. The use of solid nanoparticles as fillers opens up new possibilities for their application. With the addition of metal oxide nanoparticles in nanotechnology, new opportunities for their use arise [1,2,3]. Most of the scientific research in the field of polymer nanocomposites is dedicated to the application of metal oxides as fillers. Polymer-metal oxide nanocomposites, as composite materials, possess a number of unique properties [4,5,6]. Qualitatively new effects, properties and processes determined by quantum mechanics appear, improving certain properties: their electrophysical, strength, thermal stability and resistance to aggressive environments. They can be used as materials for photocatalysts, bioimaging, and also as sensors in optoelectronic materials. Polymer-metal oxide nanocomposites hold great promise in the fields of optics and optoelectronics, offering unique opportunities for the development of new devices and technologies [7,8]. Various studies have investigated the optical properties of polymer-metal oxide nanocomposites. However, the optical properties as a function of the percentage of nanofiller content, the changes in the optical properties depending on the size of the nanofiller, as well as the changes due to external influences for nanocomposites made of isotactic PP and nanocrystalline SiO2 are still insufficiently studied. These factors are among the most important issues in the selection of materials for research. Among polymeric materials, polypropylene (PP) is one of the polymers that has attracted significant interest due to its transparent and colorless properties. It has a long service life and excellent mechanical and chemical stability. The aim of this work is to investigate the optical properties of polymer nanocomposites. The choice of nanocrystalline silica as nanofiller for polymer nanocomposites is justified by their unique optical and mechanical properties, which allow the creation of materials with improved properties for various optical applications.

2. Experiments

For the composite matrix, isotactic PP granules with a size of 5 mm (Dema Import and Export Co. Ltd., China) with a density of 0.92 g/cm^3, a molecular weight of 300-700 thousand and a specific volume resistivity of 10^{14}-10^{15} Ω-m were used. The filler used in the study was nanocrystalline SiO_2 with particle sizes ranging from 25 to 35 nm and a density of 2.6 g/cm3 (Sigma-Aldrich, St. Louis, Missouri, USA). The preparation of PP+SiO_2 nanocomposites was carried out by introducing nanoparticles into a polymer solution [9]. The composites were obtained by hot pressing at the melting temperature of the polymer matrix under a pressure of 15 MPa for 10 min. Films with a thickness of 85 μm were prepared. The forbidden band energy was evaluated experimentally by measuring the variation of optical absorption intensity as a function of photon energy over a wide range from visible to vacuum ultraviolet wavelengths. Optical spectra in the UV and visible regions were measured using a Specord-250 spectrophotometer. The absorption spectra of the polymer-metal oxide nanoparticles were analyzed using the Tauc method to determine the band gap by approximating the curves [10]. By reconstructing the absorption spectrum and extrapolating the linear region of the spectrum to the abscissa axis, the width of the forbidden zone was obtained. The direct allowed band gap energy was calculated from the curves.

3. Results and discussion

Figure 1 shows the optical transmission spectra of the PP+SiO_2 nanocomposites at different filler volume fractions. At low filler content, the transmission coefficient decreases as the percentage of nanofiller increases. The transmission of the thin PP film is about 89%. The transmission edge for the polymer doped with metal oxide nanoparticles shifts to lower energies (red shift) compared to pure PP at room temperature. The strong interaction between the metal oxide nanoparticles and the polymer matrix leads to a change in crystallinity, which in turn changes the band structure and absorption percentage.

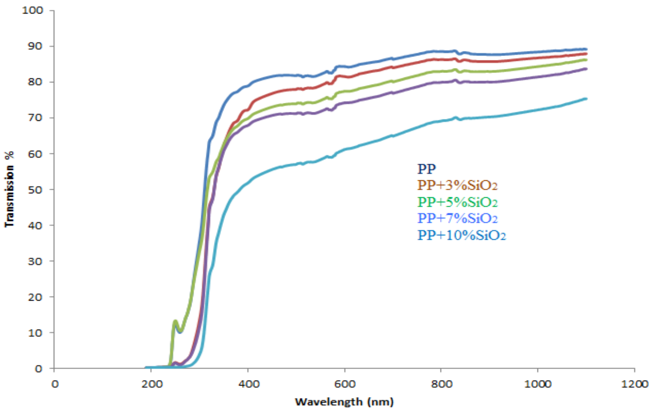

Fig. 1 Optical transmission spectra of PP+SiO_2 nanocomposites at different filler volume fractions.

These changes are associated with physicochemical processes occurring at the nanoscale, which depend on the type of nanoparticles, their concentration, and the nature of the polymer matrix. The addition of nanoparticles can cause changes in the microstructure of the polymer composite, which in turn affects the optical properties of the material. Nanoparticles can also interact with the polymer matrix, altering its energy state. This interaction may reduce the energy band gap, leading to a shift in the transmission edge towards longer wavelengths. As the percentage of SiO_2 increases, these nanoparticles may experience stronger inter-particle interactions, which could result in agglomeration, increased light scattering, and reduced transmission. Absorption increases with the nanoparticle content, as the free electrons in the nanoparticles can absorb the incoming radiation.

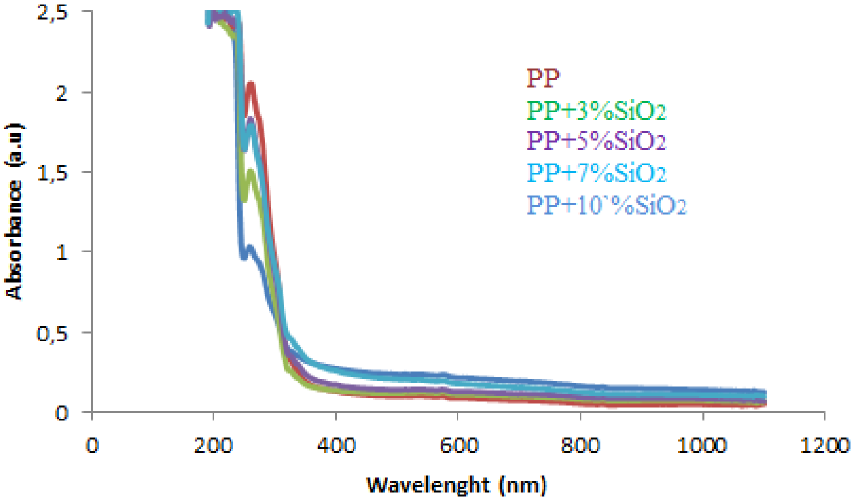

Fig. 2 Absorption spectra for the PP+SiO_2 nanocomposites.

From figure 2, a peak in the short wavelength region can be observed, which can be related to the presence of unsaturated (ethylene and carbonyl) groups in the structure of the blend [11]. This peak shifts towards longer wavelengths as the nanoparticle content increases, indicating a reduction in the band gap, an increase in the amorphous structure of the films and an improvement in the semiconducting behavior of the resulting films.

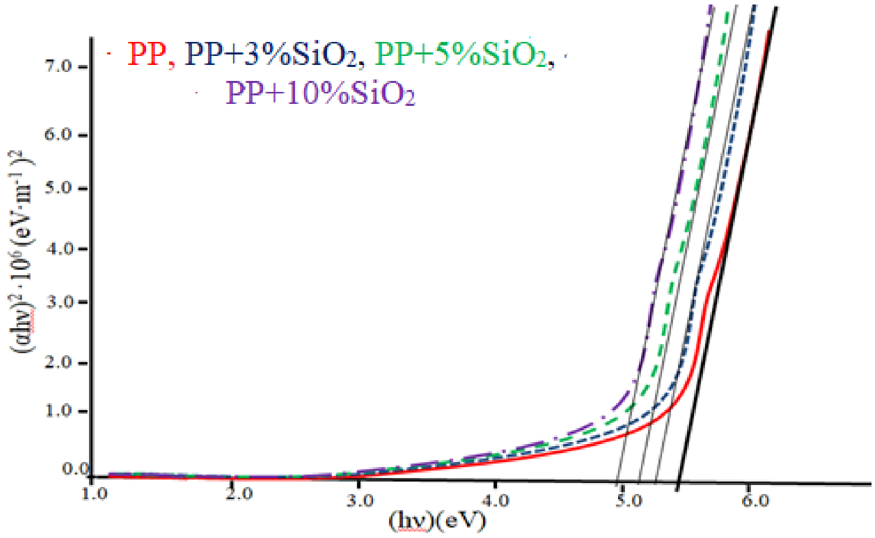

Fig. 3 Width of band gap of nanocomposites.

According to the Tauc theory

$$\alpha h\nu = B(h\nu - E_g)^P \qquad (1)$$

where: α-alpha is the absorption coefficient, hν is the photon energy, Eg is the optical band gap, B is a constant that depends on the material and the type of optical transition (direct or indirect), the index P refers to the distribution of the density of states. This index can take values of 1/2,3/2, 2, or 3 depending on the nature of the electronic transition. In this case, P=2

Figure 3 shows the dependence of the absorption coefficient on the photon energy for the nanocomposites. As shown in the figure, the band gap of the pure polymer is larger than that of the nanocomposites for all types of nanofillers. Doping with metal oxide nanoparticles affects the transmission band of the polymer structure. As the nanofiller concentration increases, the optical band gap decreases. Thus, effective control of the transmission band can be achieved by introducing a specific concentration of nanofillers into the polymer matrix.This effect can be explained by the interaction between the nanoparticles and the polymer matrix, which changes the local distribution of electronic states. Such interactions can modify the energy of electronic transitions within the composite, thereby influencing the bandgap width. In addition, as the concentration of nanoparticles in the polymer matrix increases, the electronic structure of the material changes due to changes in interparticle interactions and the state of surface atoms. The addition of nanoparticles alters the density of states at the polymer-nanoparticle interface, leading to changes in the electronic structure and consequently the bandgap [12]. The introduction of nanofillers can modify the dynamics of electronic transitions in the material by interacting with phonons (lattice vibrations). Depending on the nature of these interactions, the band gap width can either increase or decrease.

Thus, the variation in bandgap width with increasing nanofiller concentration in polymer composites is attributed to the quantum size effect, interphase interactions, and changes in the electronic structure of the material. According to Urbach's theory [13], an increase in disorder within a material leads to a broadening of the band edges and a reduction in the band gap width. When nanoparticles are introduced into the polymer matrix, they can create local perturbations in the polymer structure. These perturbations can include structural defects, inhomogeneities, and interfacial interactions between the polymer and the filler. Such perturbations increase the disorder in the system, which, according to Urbach's theory, can result in a reduction of the band gap width and a shift of the absorption edge toward the long wavelength region of the spectrum. Therefore, as the percentage of nanofillers in the polymer matrix increases, the structural disorder intensifies, leading to a decrease in the band gap width and the appearance of a more pronounced "Urbach tail". This also leads to changes in the optical properties of the nanocomposites, which can be observed in the absorption and transmission spectra. The energy associated with this tail is known as the Urbach energy (Eν), which can be determined using the following relationship [14]:

$$\alpha(\nu) = \alpha_0(\nu) exp \frac{h\nu}{E_\nu} \qquad (2)$$

The Urbach energy in polymer composites characterizes the distribution of energy levels within the band gap and indicates how rapidly light absorption decreases as photon energy increases. [15,16]

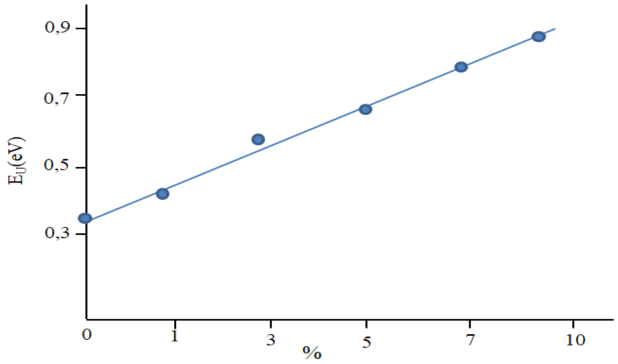

Fig. 4 Dependence of Urbach energy on the nanofiller concentration for the PP+SiO_2 composite

Figure 4 shows the dependence of the Urbach energy on the concentration of composites. As can be seen, the Urbach energy increases with increasing nanofiller concentration.This increase is likely due to the creation of additional surface defects and disordered regions within the polymer that affect the energy levels and density of states at the valence and conduction band edges. This structural disorder contributes to the increase in the Urbach energy, which characterizes the degree of disorder in the material.

4. Conclusion

The incorporation of nanoquartz SiO_2 into isotactic polypropylene significantly alters its optical properties by reducing transmittance, shifting the absorption edge, narrowing the band gap, and increasing the Urbach energy. These changes are attributed to nanoparticle-induced changes in electronic structure, interfacial interactions, and quantum confinement effects. The results highlight the potential of iPP + SiO_2 nanocomposites in optical and optoelectronic applications where controlled light absorption and tailored bandgap properties are required.

REFERENCE LIST

The Journal follows APA Style Referencing:

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- Tamayo, L., Palza, H., & Bejarano, J. (2019). Polymer composites with functionalized nanoparticles. In Zapata, P. A. (Ed.), Polymer-based nanocomposites for energy and environmental applications (pp. 249–286). Elsevier. https://doi.org/10.1016/B978-0-12-814064-2.00008-1.
- Tauc, J. (1974). Optical properties of amorphous semiconductors. In Tauc, J. (Ed.), Amorphous and Liquid Semiconductors (pp. 159–200). Plenum Publishing Co. https://doi.org/10.1007/978-1-4615-8705-7

JOURNAL ARTICLES:

12. Bhol, P., Mohanty, M., & Mohanty, P. S. (2021). Polymer-matrix stabilized metal nanoparticles: Synthesis, characterizations and insight into molecular interactions between metal ions, atoms and polymer moieties. Journal of Molecular Liquids, 325, 115135. https://doi.org/10.1016/j.molliq.2020.115135
13. Dikshit, P. K., Kumar, J., & Das, A. K. (2021). Green synthesis of metallic nanoparticles: Applications and limitations. Catalysts, 11(8), 902. https://doi.org/10.3390/catal11080902
14. Ghazzy, A., Naik, R. R., & Shakya, A. K. (2023). Metal–polymer nanocomposites: A promising approach to antibacterial materials. Polymers, 15(9), 2167. https://doi.org/10.3390/polym15092167
15. Zadehnazari, A. (2022). Metal oxide/polymer nanocomposites: A review on recent advances in fabrication and applications. Polymer-Plastics Technology and Materials, 62(5), 655–700. https://doi.org/10.1080/25740881.2022.2129387

16. Hilmi, A. R., & Purnamasari, N. D. (2022). Thermomechanical and optical characteristics of nanoquartz- and nanozircon-filled poly(methyl methacrylate) composites. Journal of Applied Polymer Science, 139, 52923. https://doi.org/10.1002/app.52923
17. Nguyen, T. P. (2011). Polymer-based nanocomposites for organic optoelectronic devices: A review. Surface and Coatings Technology, 206(4), 742–752. https://doi.org/10.1016/j.surfcoat.2011.07.010
18. Nakata, K., & Fujishima, A. (2012). TiO_2 photocatalysis: Design and applications. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 13, 169–189. https://doi.org/10.1016/j.jphotochemrev.2012.06.001
19. Ibrahimova, H. S., Rzayev, R. M., & Mustafayeva, E. M. (2024). Thermophysical properties of PP/ZrO_2 nanocomposites before and after electrothermal polarization. Journal of Inorganic and Organometallic Polymers and Materials, 4655–4660. https://doi.org/10.1007/s10904-024-03062-y
20. Al-Muntaser, A. A., Abdelghany, A. M., & Abdelrazek, E. M. (2020). Enhancement of optical and electrical properties of PVC/PMMA blend films doped with $Li_4Ti_5O_{12}$ nanoparticles. Journal of Materials Research and Technology, 9(1), 789–797. https://doi.org/10.1016/j.jmrt.2019.11.019
21. Sharifov, D., Niyazbekova, R., Mirzo, A., Shansharova, L., Serekpayeva, M., Aldabergenova, S., Ibzhanova, A., Machnik, R., & Bembenek, M. (2024). The study of composite materials properties based on polymers and nano-additives from industrial wastes from Kazakhstan. Materials, 17(12), 2959. https://doi.org/10.3390/ma17122959
22. Studenyak, I., Kranjec, M., & Kurik, M. (2014). Urbach rule in solid state physics. International Journal of Optics and Applications, 4(3), 76–83. https://doi.org/10.5923/j.optics.20140403.02
23. Urbach, F. (1953). The long-wavelength edge of photographic sensitivity and of the electronic absorption of solids. Physical Review, 92, 1324. https://doi.org/10.1103/PhysRev.92.1324
24. Ota, M., Ando, S., Endo, H., Ogura, Y., Miyazaki, M., & Hosoya, Y. (2011). Influence of refractive index on optical parameters of experimental resin composites. Acta Odontologica Scandinavica, 70(5), 362–367. https://doi.org/10.3109/00016357.2011.600724
25. Darwesh, A. H. A., Aziz, S. B., & Hussen, S. A. (2022). Insights into optical band gap identification in polymer composite films based on PVA with enhanced optical properties: Structural and optical characteristics. Optical Materials, 113007. https://doi.org/10.1016/j.optmat.2022.113007