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XRD study was utilized to understand the effect of Al₂O₃ nanoparticle concentration on the amorphous structure of polystyrene.

The XRD pattern of Al₂O₃ nanoparticles is presented in Fig. 1(a). A pattern of the sample is characterized by diffraction peaks at diffraction angles 20.6, 22.3, 39.7 and 41.3°, respectively. Transmission electron microscope (TEM) analysis was carried out to study the morphology of Al₂O₃ and determine the actual size of the Al₂O₃ nanoparticles.

TEM micrograph of Al₂O₃ nanoparticles is shown in Fig. 1(b). The particles were found to be nearly spherical in shape. The average particle size was estimated to be 31 nm. The XRD patterns of the pure PS and PS loaded with different concentrations of Al₂O₃ nanoparticles are shown in Fig. 1 (c). The XRD patterns of pure PS are characterized by one peak at 19.06°.

After the addition of Al₂O₃ nanoparticles with different concentrations, three sharp peaks appear in nanocomposites. These numbers of sharp peaks reflect the polycrystalline structure of PS after the addition of Al₂O₃ nanoparticles with different concentrations. These figures show a broad noncrystalline peak from 10° to 30° of polystyrene and sharp diffraction peaks for Al₂O₃ nanoparticles. The amalgamation of Al₂O₃ nanoparticles results in neither a new peak nor a shift with respect to PS, showing that Al₂O₃ nanoparticles consist of polymer and nanoparticle phases. The effect of Al₂O₃ nanoparticle additives on the crystallinity of PS is also investigated by XRD measurements. The percentage of crystallinity CC of the films is calculated by the following equation 18:

(1) Where A is the total area of the peaks and A_0 is the total area under the diffraction pattern.

Fig. 2(a). Shows that the percentage of crystallinity increases with an increasing in Al₂O₃ nanoparticles concentrations, which may be attributed to an increase in the density of nanoparticles. This also associated with the observed decrease in peak intensity and FWHM.

It means that the amorphicity of the samples decreases with increasing of Al₂O₃ nanoparticles concentrations, which reflects the formation of an ordered system after the addition of Al₂O₃. The increase in ordering in PS samples can be due to the strong intermolecular interaction of PS chains and intermolecular hydrogen bonding. Further, the addition of Al₂O₃ nanoparticles to PS causes repulsion between the additive molecules, resulting in an increase in ordering character of the chains, which raises the crystallinity of PS.

Average crystallite size L was calculated using Scherrer formula given by 19:

(2) Where k is a constant of proportionality (called the Scherrer constant), Δ is the full width at half maximum (FWHM) of the peak (in radian), λ is the wavelength of a copper target of X-ray ($\lambda = 1.5418 \text{ \AA}$) and θ is the diffraction angle. Fig. 2(b). Shows that the crystallite size of PS increases after introducing Al₂O₃ to different ingredients, due to the observed decrease in the FWHM. Increase in crystallite size is generally associated with an increase in the crystallinity of the PS/ Al₂O₃ nanocomposites, as the crystallite size is influenced by the width of a diffraction peak. The change in

interplanar spacing d and interchain separation R , along with Al₂O₃ nanoparticles concentrations, is calculated by the following relation 20, 21,

$$\text{Interplanar spacing (D)} \quad (3)$$

$$\text{Interchain separation (R)} \quad (4)$$

As seen in Fig. 2(c).

Both d and R decrease after the incorporation of Al₂O₃ into PS polymer chains, which may be due to the presence of specific interactions between PS and nanoparticle interplanar spacing (d) phases. The penetration of polymer molecules into nanoparticles leads to a decrease in the interlayer distance of nanoparticles, thereby decreasing D and R ; this may also be due to the increase in crystallinity. UV-visible studies The ultra-violet visible (UV-vis) absorption of pure polystyrene (PS) and polystyrene filled with different concentrations of Al₂O₃ nanoparticles was recorded. The absorption is shown in Fig. 3(a). It is clear that the fundamental absorption edge shifted toward higher wavelength side with increasing Al₂O₃ nanoparticles concentration. The absorption increased as the loading concentrations of Al₂O₃ increased.

This was due to excitations of donor-level electrons and conduction bands at these energies. A significant decrease in film transmittance was observed when Al₂O₃ nanoparticle additives increased, shown in Fig. 3(b). This was due to an increase in surface roughness.

A Rayleigh scattering of all nanoparticles lowered the transmittance.

Moreover, a layer of covalent bonds formed between the polymer chains and additives decreased incident-light transmission. Moreover the electrons in

the outer orbits travelled to higher energy-level locations and occupied vacant energy-band positions. Thus, part of the incident light did not penetrate the layer of covalent bonds. This reduced the transmittance.

Optical band gap and activation energy
The most direct method of probing the band structure of a polymer film is to measure its absorption spectra.

The absorption coefficient was calculated for the region using the following expression 22:

(5) Where A is the absorbance and t is the thickness of the samples.

The optical band gap of the pure PS and the PS filled with various Al₂O₃ nanoparticle concentrations was obtained by considering the linear portion of the UV-vis spectra at the edge of the absorption. The optical band gap was calculated using Davis and Mott's model 23,

(6) Where $a(n)$ is the absorption coefficient, a_0 is a constant and n is an index which characterizes the transition process. Shown in Fig 4 (a). The best fit for the absorption spectra, found using Equation (6), was $n = 2$. Therefore, the electrons transition is allowed indirect in the k -space. As shown in Fig. 4(a). The optical band gap of the PS decreased as the Al₂O₃ nanoparticle concentrations increased.

This was due to the incorporation of small amounts of conducting fillers that formed charge-transfer paths in the host matrix. It may have also been due to modifications in the electronic structure of the PS matrix. The modifications were caused by the appearance of various polaron and defect levels.

The polaron and defect levels contributed to the conditions of the band edges, lowered the Fermi level and affected the energy gap.