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Effect of SiO_2 Nanoparticle Concentration on the Mechanical Properties of PS-Based Nanocomposites

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Abstract

The impact of SiO_2 nanoparticle concentration on the structure and mechanical characteristics of polystyrene-based polymer nanocomposites was examined. PS+SiO2 nanocomposites were made using the solution mixing techniques. The crystalline structure of the polymer was not substantially changed by the addition of SiO_2 according to XRD patterns. According to tensile test the addition of the 1 wt% SiO_2 nanoparticles into the polymer leads to raise the tensile strength from $14.05\ MPa$ to $15.48\ MPa$. Conversely, as the amount of SiO_2 nanoparticles increased, the elongation at break decreased. The observed mechanical behavior was attributed to interfacial interactions and the dispersion state of SiO_2 nanoparticles, where well-dispersed particles enhance load transfer, while agglomeration at higher concentrations reduces deformability.

Keywords: polystrene, silica,nanoomposite, mechanical properties
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Introduction

Polymer materials are used and processed across a wide application area. Especially, because of their high mechanical and barrier performance, heat impedance, and wide availability at comparatively low cost, petrochemical-based plastics like polyethylene terephthalate (PET), polyvinyl chloride (PVC), polyethylene (PE), poly-

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propylene (PP), and polystyrene (PS) are primarily utilized in different fields of industry [1-5]. With the advancement of nanotechnology, organic/inorganic polymer nanocomposites are in the focus of attention of both scientific researchers and industrial enterprises due to their high mechanical, magnetic, optical, electrical, and chemical resistance. Composite materials in which polymers are used as a matrix are quite diverse. The main advantage of using polymers as a matrix is that they are economically inexpensive [6-8].

It is known that new materials formed as a result of the combination of organic polymer and inorganic filler that differ from each other in both their physical and chemical structure and properties exhibit their own completely new properties, which creates the basis for them to act as a new material different from the original material. Thus, the composite, while maintaining a number of functional and operational properties of its original components, at the same time demonstrates new or more advanced properties compared to the previous ones due to the effects that occur at the phase boundary and a number of physical interactions. In the formation of the properties of any composite, in addition to the individual properties of both components, the ratio in which they are taken, the dimensions of the distributed phase, the degree of aggregation and the nature of their interaction with the polymer also play a significant role. Several instances showing the notable benefits of nanocomposites over matrix materials have recently been reported. These days, nanostructured composites are widely used in many engineering applications [9, 10].

At the same time, several studies address the difficulties in creating thermoplastic-based composites with various nanoparticle kinds and achieving the required qualities. As is well known, the composite characteristics can be severely harmed by the propensity of nanoparticles to agglomerate. Methods for stabilizing nanoparticles and introducing them into polymer matrices to achieve the necessary mechanical properties of the final material are the subject of numerous papers. Considering the above challenges, the development of methods that can ensure the uniform distribution of nanoparticles in a polymer matrix using a simple and effective method is quite relevant. In this study, polymer nanocomposites based on PS polymer and SiO_2 nanoparticles were obtained and the dependence of the mechanical performance of these nanocomposites on the amount and degree of dispersion of SiO_2 nanoparticles in the polymer was studied.

1. Experimental Section

The object of this study was the polystyrene (PS) polymer. The chemically pure high-impact polystyrene (HIPS 7240) used in the research was produced by an Iranian petrochemical company. The melt flow index of this material at a temperature of $200°\mathrm{C}$ under a $5\ kg$ load is $4.5g/10min$. Polymer nanocomposites were prepared by combining mechanical mixing of solutions using a magnetic stirrer (until a homogeneous solution was obtained through intensive stirring) and hot pressing. PS powder was dissolved at $120℃$ in the organic solvent toluene for approximately 30 minutes with the aid of a magnetic stirrer. Than SiO_2 nanoparticles was added into the polymer solution and was stirred for $2\ h$. The resulting polymer mixture was left in a Petri dish for 24 hours to ensure complete solvent evaporation, yielding polymer ingots. From these ingots, samples were produced by hot pressing (under a pressure of $10\ MPa$ at a temperature of $160℃$ for 5 minutes) followed by cooling in water at room temperature (cooling rate of $200℃/min$). To minimize the influence of stress concentrations arising from the loading of specimen grips, the samples were cut into dumbbell-shaped specimens with a total length of $110\ mm$ using a knife in accordance with the standard recommended for uniaxial tensile testing (ASTM D638-03). The specimens were marked $32\ mm$ from each end, and the remaining gauge section was divided into four equal parts for measurement. The average of these measurements was taken as the mean thickness of the specimen. The samples were fractured in a tensile testing machine under a load of several kilograms-force, and the elongation was recorded in millimeters to determine the relative strain. Using these data, the tensile strength at break (in MPa) was calculated. Consequently, the mechanical strength of the material was determined as a function of the filler content.

2. Discussion of Results

Figure 1 shows the X-ray diffractogram of PS+SiO_2-based polymer nanocomposites at different filler concentrations compared to pure PS. For PS+SiO_2-based polymer nanocomposite samples, the maximum of the spectrum is obtained when the 2θ angle is $21.8°$, i.e. a strong diffraction peak is formed. Since both polystyrene and SiO_2 nanoparticles are amorphous, the addition of filler particles does not cause significant changes in the polymer X-ray diffraction.

Table 1 provides a summary of the samples' mechanical property results. Pure PS was found to have a tensile strength of about $14.05\ MPa$. The tensile strength rose to $15.48\ MPa$ with the addition of 1 weight percent SiO_2 nanoparticles, which represents an improvement of almost 10% over the pure polymer. Strong interfacial interactions between the PS matrix and the SiO_2 nanoparticles, which promote effective load transfer across the polymer–filler interface, are primarily responsible for this improvement [11, 12].

Nevertheless, the tensile strength increased somewhat to $16.77\ MPa$ when the SiO_2 concentration was raised to 3 weight percent, suggesting a modest improvement. The reinforcement effect tends to plateau at increasing filler contents, although a moderate rise is seen. The reason for this is that at high concentrations, nanoparticles have a tendency to aggregate, which decreases the effective surface area available for stress transfer and may serve as local stress concentrators instead of reinforcing sites.

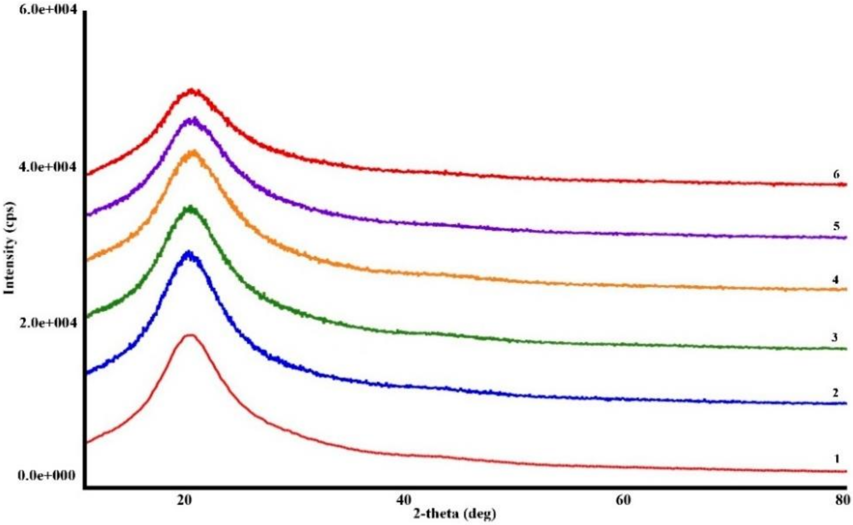

Figure 1. X-ray diffraction pattern of PS+SiO_2 based polymer nanocomposite materials: 1) Pure PS, 2) PS+1%SiO_2, 3) PS+3%SiO_2, 4) PS+5%SiO_2, 5) PS+7%SiO_2, 6) PS+10%SiO_2

Table 1. Tensile test results of PS and PS+SiO_2 nanocomposites

No	Sample	Specimen No.	Average Thickness (mm)	Tensile Force (kg)	Tensile Strength (MPa)	Elongation (mm)	Relative elongation (%)
1	PS	1	1.22	11.2	14.12	20	80
		2	1.24	11.2	13.89	20	80
		3	1.21	11.5	14.62	24	96
		4	1.21	11.7	13.60	18	72
	Average		1.22	11.15	14.05	20.5	82
2	PS+1% SiO_2	1	1.13	11.3	15.38	6	24
		2	1.09	10.7	15.10	5	20
		3	1.07	10.9	15.67	5	20
		4	1.11	11.4	15.80	5	20
	Average		1.10	11.07	15.48	5.25	21
3	PS+3% SiO_2	1	1.22	13.1	16.51	3	12
		2	1.17	13.0	17.09	3	12
		3	1.18	12.7	16.55	3	12
		4	1.18	13.0	16.94	3	12
	Average		1.18	12.95	16.77	3	12

For pure PS, the elongation at break was roughly 82%. It is common for amorphous thermoplastics to have this high ductility. However, there was a noticeable decrease in elongation when SiO_2 nanoparticles were added (figure 2). The material becomes more brittle when stiff inorganic particles are present because they limit the movement of polymer chains. The total deformability of the composite is decreased by this restriction in chain mobility, particularly in the interfacial region surrounding the nanoparticles. The dispersion of nanoparticles and the strength of the interfacial interaction with the matrix have a significant impact on the mechanical behavior of polymer nanocomposites [13].

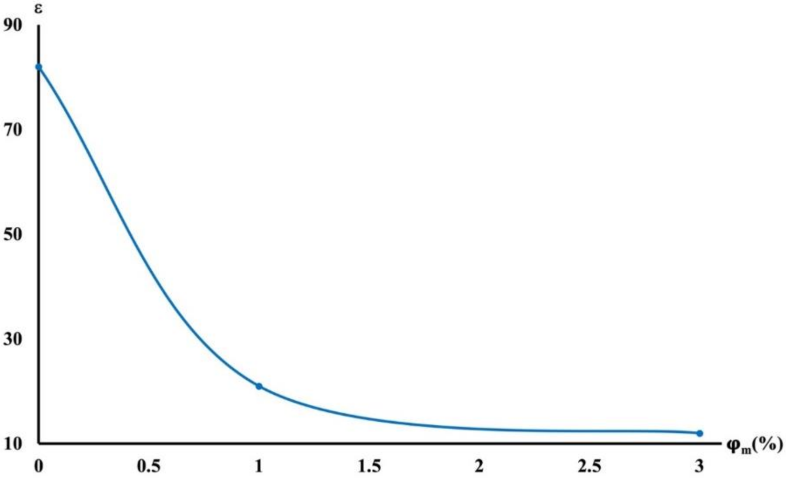

Figure 2. Dependence of the relative elongation of PS+SiO2-based polymer nanocomposite materials on the amount of filler

The nanoparticles are probably evenly distributed throughout the PS matrix at lower SiO_2 concentrations, allowing for effective stress transfer and increased mechanical strength (figure 3). On the other hand, particle agglomeration intensifies when the filler level rises to $3\,wt\%$. Under loading, these agglomerates produce microvoids and localized stress sites that negate the nanoparticles reinforcing function and cause a large loss in elongation.

3. Conclusion

The object of the study, the $PS+SiO_2$ nanocomposite, is obtained by purposefully modifying the structure of the polymer due to the SiO_2 filler. PS polymer is one of the most widely used thermoplastics. The chemical stability and large surface area of amorphous SiO_2, in turn, allow the introduction of amorphous silicon dioxide into materials of various compositions, including composite materials, to form

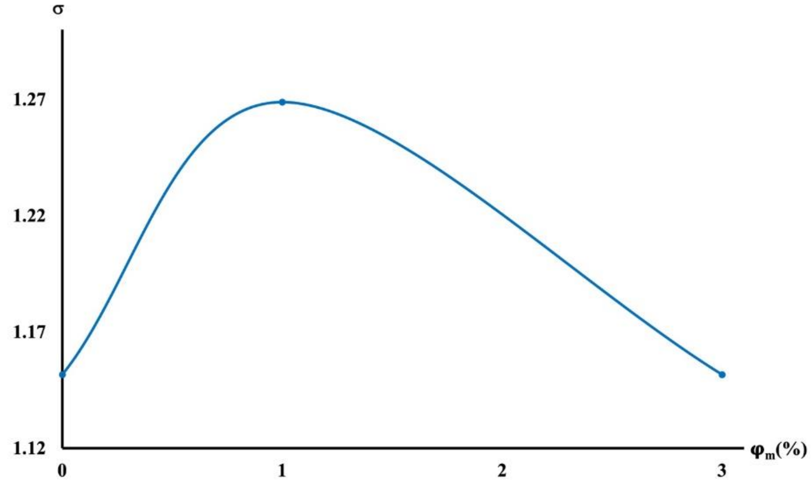

Figure 3. Dependence of tensile stress of PS+SiO2-based polymer nanocomposite materials on the amount of filler

new operational properties without changing their chemical structure. In the considered research work, layers with a thickness varying in the range of 95-100 μm were obtained. The structure and mechanical properties of the obtained layers were studied. Analysis of mechanical measurements shows that as the amount of SiO_2 nanoparticles in the polymer increases, the mechanical properties of the pure polymer change fundamentally. The nanocomposite with a 1% SiO_2 nanoparticle content demonstrates optimal strength and elasticity. This makes PS+1%SiO_2 nanocomposite samples potentially suitable for engineering applications where moderate reinforcement is required without loss of strength. At higher SiO_2 loadings ($3\ wt\%$), the system becomes stiffer but more brittle, which could be beneficial for structural components that require stiffness rather than deformation.

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