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# Polystyrene and silicon based nanocomposites: preparation and structure

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**Abstract**

The influence of the silicon nanoparticles on the structure and optic properties of the polystyrene-based nanocomposites was investigated. PS+Si nanocomposites were prepared by combinations of the solution blending and hot pressing methods. The EDS spectrum of Silicon characterizes the high purity of nanoparticles. The XRD study of the nanocomposite samples shows that silicon nanoparticles play not only the role of filler but also have a structure-formatted function in the nanocomposite. PL properties of the polymer nanocomposite also prove that silicon nanoparticles, play the role of the center of the structure to format a more ordered arrangement in the polymer matrix. It was clear that the PL emission of the nanocomposite enhanced with the introduction of the silicon nanoparticles at the $450 - 550\ nm$ region. This increase results in the expansion of the emission region of the pure polystyrene by the addition of a few amounts of silicon nanoparticles. This PS+Si nanocomposite could be an effective material for biomedical applications as a fluorescent marker for drug delivery systems.

**Key words:** *Silicon nanoparticles, polystyrene, nanocomposite, fluorescent markers for biomedical application*
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## 1. Introduction

Nanocomposites are a new class of materials with enhanced properties like optical, magnetic, and electrical, which is due to the unique nature of nano-sized additions [1-16]. Nanocomposites obtained on the base of the polymer matrix are one of the promising structures of modern material science. Especially thermoplastic

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polymer-based nanocomposites possess a wide range of application areas. Polystyrene (Ps) is a synthetic polymer made from monomers of aromatic hydrocarbon styrene and is considered one of the major industrial polymers [4]. Since Ps is a thermoplastic polymer, it softens and melts when heated and can be reused, which is very important for industrial applications.

Furthermore, polystyrene is widely used for drug delivery applications in biomedicine. The main advantage of polystyrene is its biocompatibility, which allows it to be used broadly for biomedical devices and the study of bio-nano interactions. Furthermore, their ability to not degrade in cellular environments proves an asset in biomedical applications [7, 11]. A unique property of polystyrene, like some other polymers, is its ability to fuse with proteins [14].

At the moment, the majority of research efforts are focused on creating nanocomposite materials with many qualities simultaneously, using those properties, and assessing how well they can be used. In the current study, thermoplastic called polystyrene is used to create a smooth, readily moulded, and repeatable polymer-based nanocomposite. Depending on the size, amount, distribution, and technique of acquiring the nano-sized additive included in the polymer, different materials may be created. Many of the issues that arise in the domains where traditional materials are used can be solved by derived materials. Because of their many industrially applicable features, Si-based polymer nanocomposites have a wide range of applications. Their domains of use are expanded by the peculiarity of nano Si structure and particularly surface characteristics. Lithium batteries, membrane technology, display screens, and packaging are a few of these application areas that have attracted attention [1].

In this study, the nanocomposite based on polystyrene and silicon nanoparticles was produced, and structural futures were investigated.

## 2. Materials

All chemicals were used without additional purification. High impact Polystyrene (HIPS 7240) with $1.04\ g/cm^3$ density was provided by the Petrochemical Company of Iran. Toluene (PLC) with high purity ($99.9\%$) was used as a solvent. The size of the silicon nanoparticles is about $50\ nm$.

Solution blending and hot pressing methods were used for polymer nanocomposite preparation [17]. PS+Si nanocomposites were prepared via the following technique: At first, PS powder was solved in toluene under $100℃$ for $20-30$ minutes. In addition, Si nanoparticles were dispersed in $10\ ml$ toluene by ultrasonic cavitation. Further, dispersed Si nanoparticles were added into the PS/toluene system and were mixed for two hours. To remove the solvent from the system obtained nanocomposite solution was evaporated in the open Petri dishes for $24$ hours. Af-

ter solvent evaporation, the white crack texture of the nanocomposite was obtained. The cracks texture of the nanocomposite is compressed under $100\ kPa$ pressure at $160℃$ up to a thin film is obtained. The thin films of polymer nanocomposite were produced for various mass concentrations of the filler, namely $1\ wt\%$, $1.5\ wt\%$, $3\ wt\%$.

## 3. Methods

Energy-dispersive spectrum (EDS) analysis of nanocomposite samples was taken on a Scanning Electron Microscope JEOL JSM-7600F. X-ray diffraction (XRD) analysis of the prepared samples was carried out on a Rigaku Mini Flex 600 XRD diffractometer at room temperature. In all the cases, CuK(a) radiation from a Cu X-ray tube (run at $15\ mA$ and $30\ kV$) was used. Diffraction patterns were obtained in the range of Bragg's angle $2\theta = 10° - 80°$. Photoluminescent properties of nanocomposite films were examined using a spectrofluorometer Varian Cary Eclipse at a wavelength range of $200 - 900\ nm$.

## 4. Results and discussion

The energy dispersion spectrum of silicon nanoparticles is given in figure 1. The peak at the EDS spectrum of Silicon is narrow, which characterizes the high purity of silicon nanoparticles.

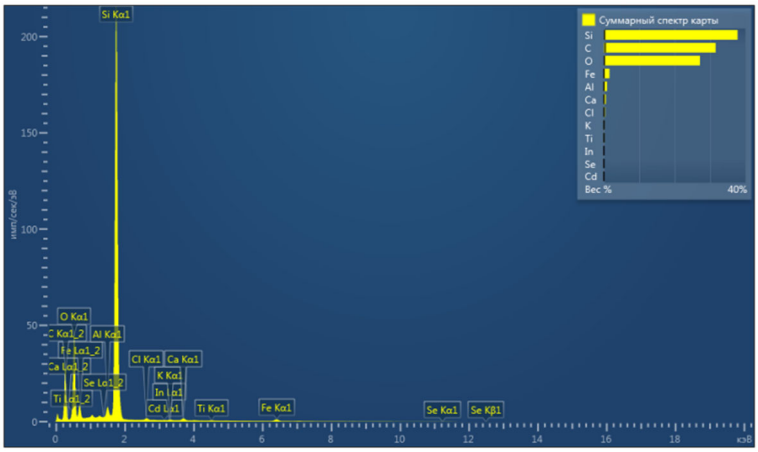


**Figure 1.** Energy dispersion spectrum of silicon nanoparticles

The X-ray diffraction pattern of pure PS, Si-nanoparticles and PS+Si nanocomposites is given in Figure 2. The broad peaks at $9.74°$ and $19.7°$ of $2 - 2\ theta$ angle correspond to polystyrene. The peaks at $2\theta = 9.74$ indicate the presence of amor-

phous material in the PS polymer, while the peaks at 19.8 indicate the presence of a crystalline phase [18]. The peaks positions at 28.46 [111], 47.36 [220], 56.21 [311] indexed with silicon phase (Si-NPs) [19-20]. The diffraction patterns of PS+1%Si and PS+3%Si nanocomposites possess diffraction lines of both PS and Si. With the increase of the Si nanoparticles, the intensity of the characteristic X-ray line corresponding to these particles is observed.

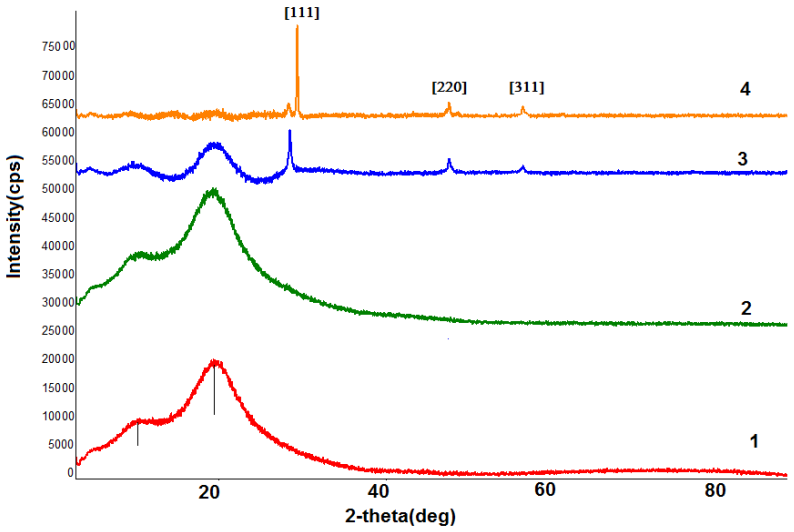


**Figure 2.** X-ray difraction patterin of polystyrene and sılıcon based nanocomposıtes:
1) Polystrene, 2) PS+1%Si, 3) PS+3%Si, 4) Si

Furthermore, the characteristic lines of the polymer were decreased. The result suggests that Si nanoparticles act as structural centers in the polystyrene medium. The Debye-Scherrer equation is used to estimate the size of crystallites in materials from X-ray diffraction (XRD) data. For polystyrene, which is amorphous but can have crystalline regions, the equation helps determine the size of these crystalline domains by analyzing the broadening of XRD peaks:

$$D = \frac{k\lambda}{\beta \cos\theta}, \tag{2}$$

where $\lambda$ is the wavelength of X-rays (1.54 Å), $\theta$ is the diffraction angle. For pure Ps sample $2\theta = 19.7\ deg$. $\beta$ is the full width at half maximum ($FWHM = 8.68\ deg$), and D is the crystallite size was found to be $0.97\ nm$. By the addition of the silicon nanoparticles into the polymer matrix, the diffraction peak of the Ps polymer corresponding to the crystalline phase shifted to $2\theta = 18.73\ deg$ and the calculated

crystalline size increased up to $2.9\ nm$. This change in the crystalline size of the polymer crystalline phase indicated that the macromolecule chain wrapped around the nanoparticles. In other words, X-ray diffraction pattern of the nanocomposites based on the silicon and polystyrene, and calculated value of the crystallites demonstrated that silicon nanoparticles play the role of the structure formation center in the polymer matrix. In other words, polystyrene polymer and silicon nanoparticles show good intercalation with each other.

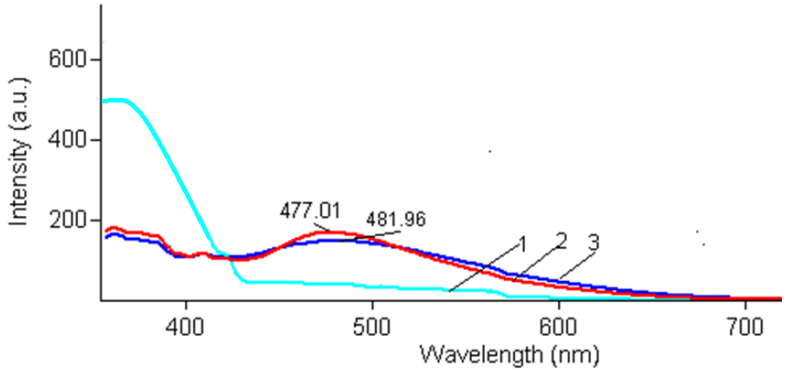


**Figure 3.** PL spectrum of the pure polystrol and PS+Si nanocomposite:
1) Pure polystrene; 2) PS+1%Si; 3) PS+3%Si

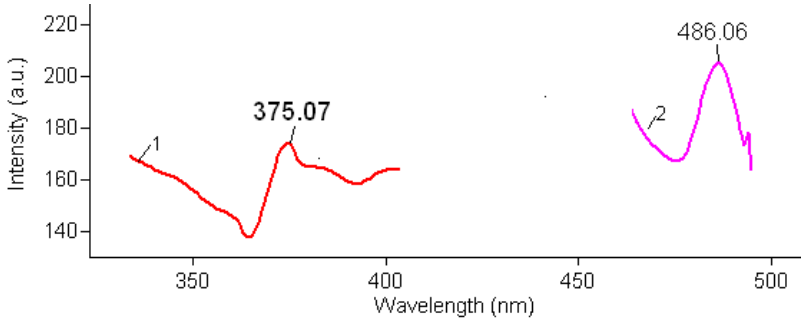


**Figure 4.** Emission and excitation spectrum of the peak at 481.96 nm:
1) Excitation spectrum; 2) Emission spectrum

Figure 3 shows the PL spectrum of the pure polystyrene and PS+Si nanocomposite. The excitation wavelength was 250 nm. The emission spectrum was investigated in the range of $350 - 700\ nm$. According to the PL spectrum of the samples it was clear that the intensity of the emission spectrum of the polystyrene polymer increased with the introduction of the silica nanoparticles. Polystyrene is known as

a luminescent polymer. The emission band typically occurs around $300$ to $400$ nanometers. This emission is often due to various structural defects and exciton interactions within the polymer. The exact position can vary based on factors like molecular weight and any additives or modifications in the polystyrene. It is also known that Silicon nanoparticles (Si NPs) exhibit strong visible photoluminescence (PL) [21]. However, the interaction of the two photoluminescent components namely polystyrene and silicon does not investigate very well. Since polystyrene is a synthetic hydrocarbon polymer that is widely adaptive and can be used for a variety of purposes in drug delivery and silicon possesses a range of properties that make it ideal for a variety of biomedical use, to study the combination of these two components is effective for the production of the new materials for biomedical applications. The PL spectrums of the PS+Si nanocomposite were obtained at the $350 - 700\ nm$ region. It is clear that the incorporation of the Si nanoparticles leads to increasing the intensity of the luminescence spectrum of polystyrene at the $450 - 550\ nm$ region. The addition of a few amounts of silicon nanoparticles leads to expansion of the emission region of the pure polystyrene [22-24]. The addition of the silicon nanoparticles leads to the observation new peak at the $450 - 550\ region\ nm$, which is related to the surface defect of silicon. Figure 4 demonstrates the emission and excitation spectra of the polystyrene and 1% silicon nanoparticle-based nanocomposite. The interaction of the polymer and silica nanoparticles in the interface region leads to an increase in the luminescence intensity.

## 5. Conclusions

The preparation process, structural analysis, and optical properties of silicon nanoparticles and polystyrene polymer-based nanocomposites were presented in the current work. Solution mixing and hot pressing techniques were used to create polystyrene and silicon-based nanocomposites with different concentrations of Si. XRD and Pl-emission spectroscopy methods were used to examine the impact of silicon nanoparticles on the structural and optical characteristics of polystyrene-based nanocomposites, respectively. It can be estimated that silicon nanoparticles play the role of the structure formation centre in the polymer matrix. The inclusion of silicon nanoparticles causes the polymer matrix's crystalline size to rise. Moreover, the $350 - 700\ nm$ range was where the PS+Si nanocomposite's PL spectra were obtained. It is evident that the addition of Si nanoparticles increases the luminescence spectra of polystyrene in the $450 - 550\ nm$ wavelength range. The emission spectra of pure polystyrene expand when a small amount of

silicon nanoparticles is added.

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