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## Short Communication

# Small Angle X-ray Scattering in Nanocomposite: Nanoparticles $BaTiO_3$ with Modified Surface in Polystyrene

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By small angle X-ray scattering (SAXS) investigated the structure of polystyrene matrix composites filled by barium titanate nanoparticles with different volume fraction. Found that the percolation threshold for these systems is about 15 % of the content of the nanoparticles. Estimate the average distance between nanoparticles composites with different volume fraction.

**Keywords:** Small angle X-ray scattering, Barium titanate, Nanoparticles, Composites.

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## 1. INTRODUCTION

Composites of ferroelectric nanoparticles in the polymer matrix has a high dielectric and optical nonlinearity properties and are considered as promising materials in nanoelectronics and photonics. For example, based on composites of nanoparticles of barium titanate in different polymeric matrices have been created capacitors with high energy storage density [1], memory elements [2], photonic crystals [3], absorbing microwave coating [4]. However, agglomeration of nanoparticles in the polymer during the synthesis of these composites is the high heterogeneity in their properties and prevents their widespread practical use. A possible solution to this problem is the modification of the surface of nanoparticles with different chemical compounds. Modifying layer preventing agglomeration and may be cause changes interfacial adhesion [5], the dipole-dipole interaction between the particles and forming an electret state at the interface [6]. Thus, structural changes can lead to changes in the mechanical and dielectric properties of the composites.

## 2. EXPERIMENTAL SECTION

The method of producing composites with 5-35 % volume fraction of nanoparticles $BaTiO_3$ with modified surface described in [7].

Studies with SAXS were conducted with the help of facility SAXSessmc[2] (Anton Paar) in the linear collimation mode. To this end a typical X-ray tube was used with copper anticathode and a monochromator with X-ray radiation of 0.154 nm $K_\alpha$ line.

## 3. RESULTS AND DISCUSSION

According to the obtained data, structure of pure polystyrene matrix and composites with 5 and 10 % volume fraction of $BaTiO_3$ nanoparticles characterized by two Bragg peaks $d$:

$$d = 2\pi / q_{peak}, \qquad (1)$$

where $q_{peak}$ – backscattering vector.

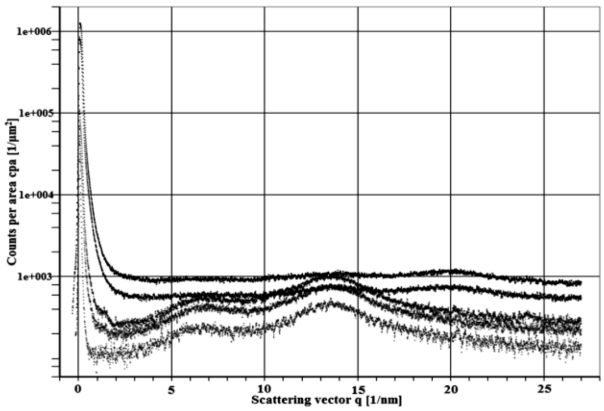


**Fig. 1** – SAXS curves from polystyrene and composites with 5 %, 10 %, 15 % and 30 % volume content of $BaTiO_3$ nanoparticles with modified surface from below upward

This peaks characterized objects with radii of 0.47 and 1 nm, respectively, describing the structure of the matrix of polystyrene. This fact confirmed detection of such structural elements in polystyrene films by scanning near-field optical microscopy in [8]. Further increase in the concentration of nanoparticles $BaTiO_3$, as seen in (Fig. 1), accompanied by the disappearance of these peaks, due to the change in the structure of the composite with passing through the percolation threshold [9] and the formation of infinite cluster of $BaTiO_3$ nanoparticles in a matrix.

Since composites was prepared from polydisperse nanoparticles powder $BaTiO_3$, for analyze of the degree of their agglomeration was obtaining the size distribution (Fig. 2), based on polydisperse hard-sphere model with using Percus-Yevick solution:

$$I_6(q, r) = P_4(q) \cdot S_3(q), \qquad (2)$$

where $P_4(q) = \Delta\rho^2 \sum_i D_i \left(4r_i^3\pi/3\right) P_1(q, r_i)$ – the form-factor of the particles, $P_1(q)$ – form-factor homogeneous monodisperse particles, $S_3(q)$ – structure factor [10, 11]. The size distribution of $BaTiO_3$ nanoparticles in composites calculated by generalized indirect Fourier trans-

  

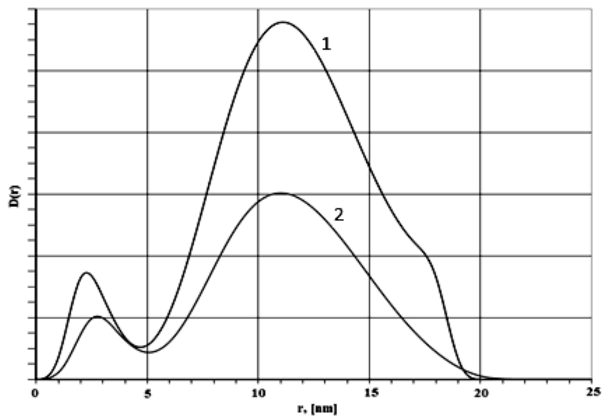


**Fig. 2** – Size distribution of the $BaTiO_3$ nanoparticles in composites with 10 % (1) and 5 % (2) volume content

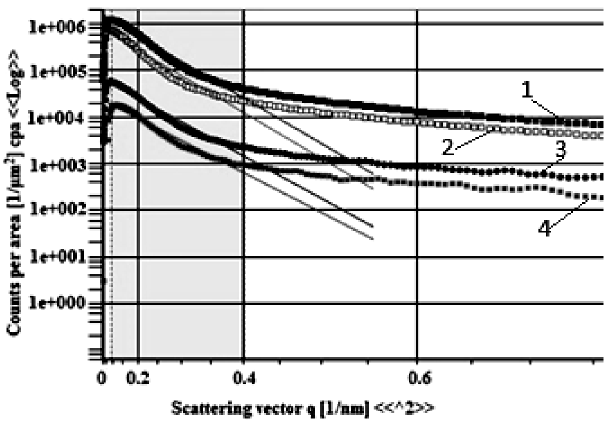


**Fig. 3** – For the calculation of the radius Guinier for composite with % (1), 10 % (2), 15 % (3), 30 % (4) volume content

form (GIFT) in the software package PCG Software 4.05.12 (Fig. 2) [12, 13].

The existence peak, characterized objects with radii about 2 nm may be due to the presence of agglomerates of sodium oleate molecules unbounding with surface of $BaTiO_3$ nanoparticles, which can have a significant influence on the processes of charge transport in these structures. Passing through the percolation threshold prevents the possibility to obtain size distribution of nanoparticles in composites with a high concentration of filler. However, for these composites using a specified software package PCG 4.05 Software may be calculate the Guinier radius $R_g$ (Fig. 3) according to the formula:

$$R_g^2 = \frac{3}{5} R_h^2 , \qquad (3)$$

where $R_h$ – average radius of monodisperse particles (Table 1).

Thus (Fig. 1, 2) for composites with 5 and 10 % volume content of $BaTiO_3$ average size of the nanoparticles obtained under polydisperse hard-sphere model and the radius, estimated by mean Guinier radius $R_g$ are in good agreement and account for about 22 nm, which confirms the applicability of this model for investigated composites.

**Table 1** – The calculated values of the Guinier radii $R_g$ and average radii monodisperse particles $BaTiO_3$ for composites

| Vol. fraction, % | $R_g$, nm | $R_h$, nm |
|---|---|---|
| 5 | 8.16 ± 0.11 | 10.53 ± 0.11 |
| 10 | 8.41 ± 0.10 | 10.86 ± 0.13 |
| 15 | 8.74 ± 0.14 | 11.28 ± 0.18 |
| 30 | 8.71 ± 0.10 | 11.24 ± 0.13 |

The average distance between the particles $L$ can be expressing as [5]:

$$L = \left[ \left( \frac{4\pi}{3\eta} \right)^{1/3} - 2 \right] \cdot \frac{D}{2} , \qquad (4)$$

where $\eta$ – the concentration, $D$ – average diameter of nanoparticles. Thus, calculated average distance between particles in the composites with 5 and 10 % volume content of the nanoparticles are 25 and 15 nm, respectively.

## 4. CONCLUSIONS

It is known that nanoparticles of in these structures are stress concentrators and the thickness of the boundary layer, which decreases the magnitude of these stresses on the order in comparison with the value at the interface is ~ 1,7 $D$ [14]. Thus, sample composite with 5 and 10 % volume content of $BaTiO_3$ nanoparticles thickness of the layer is greater than the average distance between particles in the composite, which allows to conclude the distribution of deformations throughout the entire volume of the matrix in the composites.

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