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## **X-ray diffractometric study of HDPE/GaAs and HDPE/GaAs<Te> composites**

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High-density polyethylene sheets (HDPE), HDPE/GaAs and HDPE/ GaAs<Te> composites with GaAs and GaAs<Te> semiconductor fillers were studied by X-ray diffractometry at room temperature. The degree of crystallization of these samples was calculated and it was determined that the inclusion of fillers in the polymer matrix (x=1-10% composite) leads to an increase in the degree of crystallization by 1.3-1.4 times. The obtained results are explained by the change of the upper molecular structure of the polymer.

**Keywords:** high density polyethylene, GaAs, GaAs<Te>, composites, X-ray diffractometry method.

*Received 16 November 2022; Accepted 27 January 2023.*

### **Introduction**

It is known that the introduction of new fillers leads to the expansion of the possibility of using composite materials. From this point of view, polymer-semiconductor filler polymer composite materials are of special interest [1-3]. The introduction of semiconductor fillers into the polymer matrix leads to changes in its structure and properties. From this aspect, composites based on high-density polyethylene HDPE/GaAs and HDPE/GaAs<Te> semiconductor fillers are important [4,5]. Using these materials as modifying additives for polymers can lead to the production of new composites with different properties. X-ray diffraction (XRD) analysis is the most reliable experimental method for obtaining information about the structure and dynamics of the crystal lattice of solid bodies. It gives a three-dimensional image of macromolecules, which is necessary for understanding the features of structure formation in polymer composites. An important technological application of XRD analysis is the measurement of the degree of crystallinity in polymer composites. This method is considered an ideal analytical method for studying any type of sample. The reviewed article presents the results of X-ray diffractometric analysis of

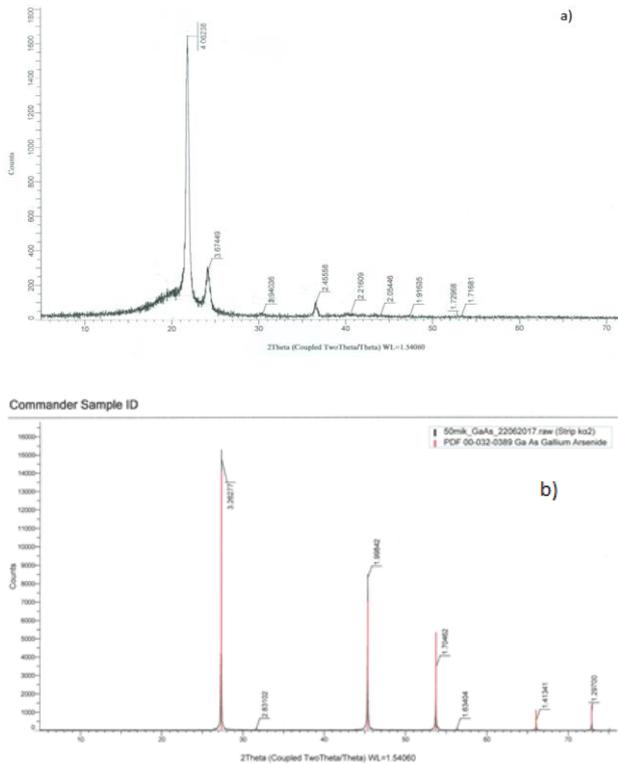
HDPE/GaAs and HDPE/GaAs<Te> composites.

### **I. Experimental part**

The diffractograms of the primary HDPE, HDPE/xwt.%GaAs and YSPE/x wt.%GaAS<Te> (x=1-10% composite) layers were obtained on a D2 Phaser (Bruker company, Germany) x-ray diffractometer. CuK $\alpha$  source and Ni filters were used during the experiment. The values of the degree of crystallization in the studied samples were calculated by the program. This method allows to monitor structural changes caused by the introduction of microparticles into the composition of the polymer matrix [6].

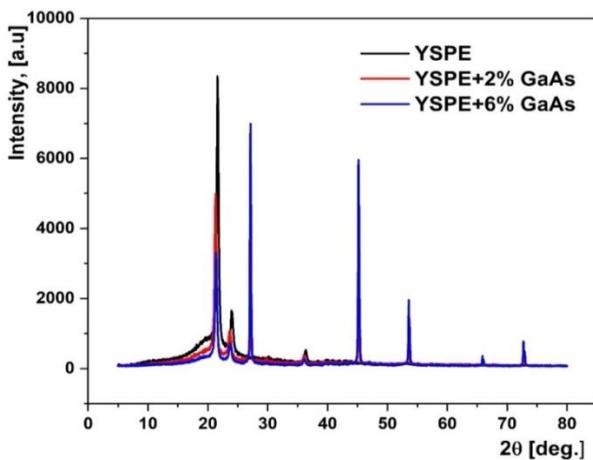
### **II. Discussion of results**

The diffractogram of the initial HDPE (1) layer is given in figure 1 (a). As can be seen from Figure 1(a), the initial HDPE layers are characterized by a set of reflections:  $2\theta=220$  and  $240$ . The given lines are characteristic lines for HDPE polymer.

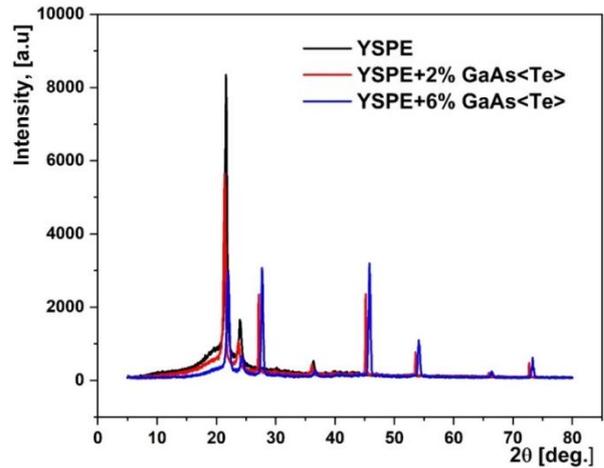


**Fig. 1.** Diffractograms of HDPE (a) and GaAs (b) samples.

Incorporating 2 wt.% GaAs microparticles into the matrix results in stronger 270 and 450 as well as weaker lines compared to the new 53.50 and 72.50. The observed new lines belong to GaAs (Fig. 1b). When GaAs alloyed with 2 wt.% tellurium is included in the matrix, the same diffraction lines (reflexes) are observed in the diffractogram, they are distributed as in HDPE/GaAs. When the concentration of microparticles included in the composition of the polymer matrix is increased from 2 wt.% to 6 wt.%, the diffraction lines shift (Fig. 2 and 3). The strongest lines are considered to be:  $2\theta=27$ ; 45 and 53.50.



**Fig. 2.** Comparative diffractograms of HDPE polymer matrix, HDPE/2wt%GaAs and HDPE/6wt%GaAs composites.



**Fig. 3.** Comparative diffractograms of HDPE polymer matrix, HDPE/2wt%GaAs<Te> and HDPE/6wt%GaAs<Te> composites.

At this time, a noticeable change in the intensities of the lines of the crystalline phase of HDPE is observed. Based on the data, the degrees of crystallization of the primary HDPE layer, HDPE/GaAs and HDPE/GaAs<Te> composite layers were calculated using a known program. At this time, it was determined that with increasing concentration, the degree of crystallization of HDPE/GaAs composite materials increased by 1.3 times (from 54 to 71.4%) compared to the initial sample, and in HDPE/GaAs<Te> composites by ~1.4 times (from 54 to 73.9%) increases (table).

**Table 1.**  
Crystallization degree values of HDPE, HDPE/wt.%GaAs and HDPE/wt.%GaAs<Te> composites

№	Sample	Crystallization degree,%
1	HDPE	54
2	HDPE/2wt.%GaAs	68,7
3	HDPE/6wt.%GaAs	71,4
4	HDPE/2wt.%GaAs<Te>	70,2
5	HDPE/6wt.%GaAs<Te>	73,9

The observed increase in the degree of crystallization is due to the possibility of a decrease in the size of the crystallites and an increase in their dispersion. The obtained experimental results are in good agreement with the results of Fourier-IR spectroscopic studies [7, 8].

Thus, on the basis of comparative X-ray diffractometric analysis, it was determined that the degree of crystallization of composite layers increases by x=12-16% compared to the degree of crystallization of primary layers. The observed effects are related to the change of the molecular structure and degree of crystallization (K) of the polymer, so that GaAs and GaAs<Te> fillers with a dispersion of 50 μm increase the degree of crystallization in polyethylene composites (these microparticles play a central role in crystallization) and the molecular structure of the polymer. it plays the role of creating a structure in its change. The increase in the degree of crystallization can occur due to the formation of the third transition phase [7].

According to X-ray results, AB (aligned bonds) have a three-dimensional structure with a periodicity of  $\lambda=50-60$  nm [4]. AB is an integral part of highly oriented PE. For HDPE fibers, the quantity  $\lambda$  corresponds to the length of the trans-sequences in the crystalline region of the lamellae. Apparently, the concentration of 2-6 wt.% of GaAs microparticles and 2-8 wt.% of GaAs<Te> microparticles in HDPE leads to an increase in the amount of AB in the transitional crystalline layer of HDPE. This is due to the fact that at these concentrations GaAs and GaAs<Te> microparticles act as centers of additional crystallization. When the concentration of microparticles of fillers in HDPE increases, the sizes of clusters become larger than the values of periodicity.

## Conclusion

Pure HDPE, GaAs, GaAs<Te>, HDPE/GaAs and HDPE/ GaAs<Te> composites with semiconductor filler were studied by diffractometry method. Crystallization degrees of these samples were calculated. It was determined that the inclusion of fillers in the polymer matrix leads to an increase in the degree of crystallization. This increase is related to the change of the upper molecular structure of the polymer.

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## Рентгенівське дифрактометричне дослідження композитів HDPE/GaAs та HDPE/GaAs<Te>

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Листи поліетилену високої щільності (HDPE), композити HDPE/GaAs і HDPE/ GaAs<Te> з напівпровідниковими наповнювачами GaAs і GaAs<Te> досліджували методом рентгенівської дифрактометрії при кімнатній температурі. Розраховано ступінь кристалізації цих зразків і встановлено, що включення до полімерної матриці наповнювачів (x=1-10% складу) призводить до збільшення ступеня кристалізації в 1,3-1,4 рази. Отримані результати пояснюються зміною високої молекулярної структури полімеру.

**Ключові слова:** поліетилен високої щільності, GaAs, GaAs<Te>, композити, метод рентгенівської дифрактометрії.