

Fourier-IR Spectroscopic Study of the Structure of High-density Polyethylene Composites with Semiconductor Fillers GaAs and GaAs <Te>

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Abstract The method of Fourier IR spectroscopy was applied in the study of the structure of high-density polyethylene composites with semiconductor fillers GaAs and GaAs <Te> at room temperature. It was revealed that in case of 2-3 mass % content of GaAs and 5-8 mass % of GaAs <Te> in PE films the maximum degree of crystallinity is obtained. It is shown that GaAs and GaAs <Te> fillers with 50 micron dispersion in polyethylene compositions play a role of structure formers in the increase of the degree of crystallinity and a change in the supramolecular polymer structure.

Keywords High-density polyethylene, Semiconductor fillers GaAs and GaAs<Te>, Polymer composites, Degree of crystallinity, Fourier-Infrared (IR) spectroscopy, Absorption band, Supramolecular structure

1. Introduction

Obtainment of polymeric compositions with interesting electro-physical, strain-sensitive, electret, sensory, spectral-luminescent, optical and other properties largely depends on the nature of the filler, the shape, size and distribution of particles, as well as the degree of interaction between components[1-6]. Usually, new fillers lead to the enhancement of the practical application of the composite material as the nature of the aggregation of the filler particles, conditions of crystallization and a number of other factors change the morphology of the polymeric matrix, and as a result, composite materials obtained on their basis acquire unique properties[1-2]. In this respect, of particular interest are composites based on high density polyethylene (HDPE) with compound semiconductors GaAs and GaAs <Te>. The reason of the fact is that these semiconductors have peculiar crystal and band structures, and are promising materials in micro-and optoelectronics[5-8]. Choice of HDPE (C_{2n}H_{2n+2}) as a binding agent caused a good knowledge of the material[9-10]. It should be noted that actually there exists no literature data on the optical and spectral properties of the composites and HDPE-GaAs and HDPE-GaAs <Te>.

Therefore, in this paper we present the results of Fourier-IR spectroscopic studies of composite HDPE films with GaAs and GaAs <T> fillers (the content of which is 1-10

mass %) at room temperature. IR spectroscopy allows us to follow the structural changes caused by the introduction of micro-particles to the polymer matrix, and identify patterns associated with these changes[9, 11].

2. Experimental

Of HDPE and GaAs and GaAs <Te> semiconductors powders (with particle size ~50 micron) there was prepared homogeneous mixture prepared through mechanical mixing. Then homogeneous mixture was within 15 minutes exposed to hot pressing at T = 140°C temperature and cooled to room temperature within 30 min. This method allows obtainment of HDPE film with uniform distribution of microparticles in the volume of the polymer, which is a necessary factor for optical studies. The uniform distribution of the microparticles in HDPE films was controlled against Fourier-IR absorption spectra. The thickness of the original and composite films was equal to d = 50-100 microns. The content of GaAs and GaAs <Te> microparticles varied from 1 to 10 mass %. (1,2,3,4,5,6,7,8,9,10 mass %).

Fourier-IR absorption spectra of virgin samples of the initial HDPE and its composites were recorded on Varian 640 FT-IR spectrometer at room temperature in the 4000-400 cm⁻¹ frequency range. Structural changes in PE films connected with the introduction of particulate fillers was traced in the frequency range $\nu = 750-700$ cm⁻¹ corresponding to pendular oscillations of CH₂ group PE, as well as in the deformation ($\nu = 1500-1400$ cm⁻¹) and valence ($\nu = 3000-2800$ cm⁻¹) areas symmetric and asymmetric vibrations of CH₂ groups[11].

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The crystallinity degree of the samples was calculated based on the optical densities by the following formula[7].

$$K = \frac{1,4 \cdot (D_{730}/D_{720})}{1 + 0,4 \cdot (D_{730}/D_{720})} \quad (1)$$

Where D_{730} and D_{720} are optical density of 730 and 720 cm^{-1} bands in the IR spectra of HDPE + GaAs and HDPE + GaAs <Te> films.

3. Results and Discussion

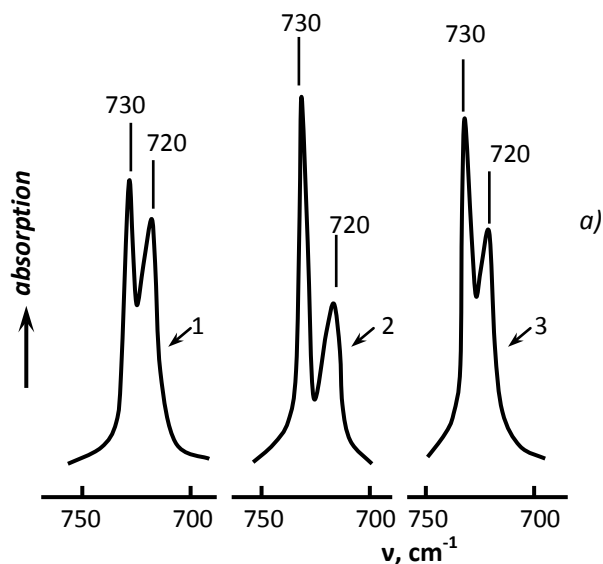


Figure 1a. Fourier IR-absorption spectra of the initial (1) and composite HDPE films containing 2 (2), and 6 mass% of GaAs microparticles (3)

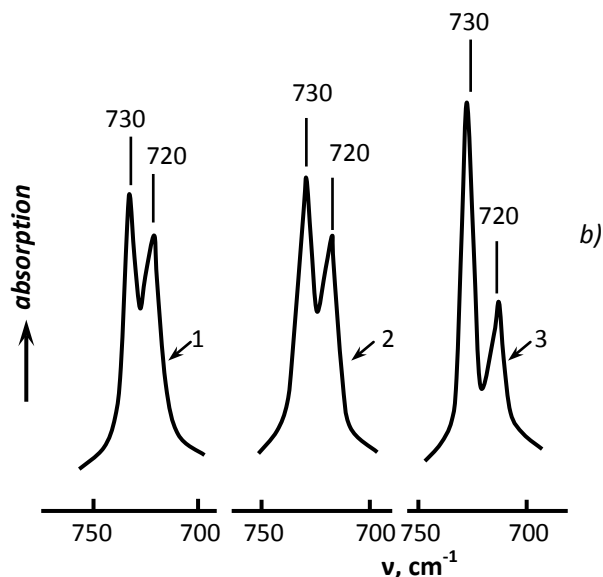


Figure 1b. Fourier IR- absorption spectra of the initial (1) and composite HDPE films containing 2 (2), and 6 mass% of the GaAs <Te> microparticles (3)

Fig. 1a and 1b show examples of Fourier IR absorption spectra of the starting PE films without microparticles (curve 1) and containing 2,4 and 6 mass% of gallium arsenide (GaAs) and gallium arsenide doped with tellurium

(GaAs <Te>) microparticles (curves 2 4) in the band area 722cm^{-1} , corresponding to pendular oscillations of the CH_2 group in crystalline PE cell. The doublet observed in the IR spectrum emerges due to the splitting of the 722 cm^{-1} band. The 730cm^{-1} band characterizes the crystalline area of PE, and the 720cm^{-1} band - the crystalline region with amorphous layers[11]. It obvious from the spectrum that in the result of introduction of GaAs and GaAs <Te> microparticles redistribution of the doublet band intensities takes place. By formula (1) there calculated the degree of crystallinity of the starting sample constituting 65%, and PE specimens with GaAs and GaAs <Te> fillers in an amount from 1 to 10 mass % varies from 70 to 92 mass%.

Fig. 2 shows the variation of the relative degree of crystallinity (C/C_0) of PE + GaAs and PE + GaAs <Te> films depending on the weight content of the GaAs and GaAs <Te> microparticles. Areas of highest degree of crystallinity are observed. For the PE+GaAs composite, this area is formed at 2-3 mass% concentrations of GaAs. Characteristic area of the maximum degree of crystallinity for the composite films PE+GaAs <Te> is obtained at GaAs <Te> 5-8 mass % concentration. Comparing areas of maximum degrees of crystallinity for composite materials with fillers GaAs and GaAs <Te> shows that for the first filling it is narrow and the second is quite broad.

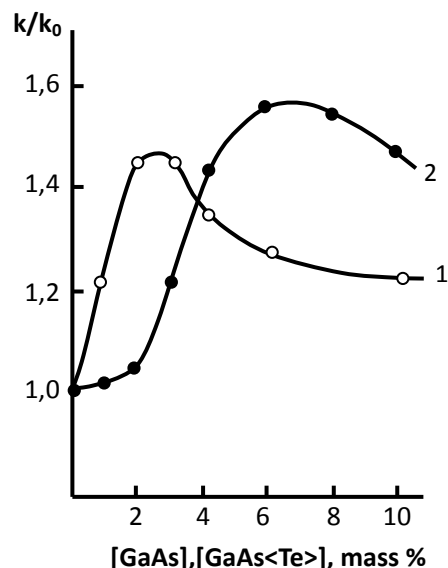


Figure 2. Dependencies of the relative degree of crystallinity of HDPE + GaAs (1) and HDPE + GaAs <Te> (2) samples on the mass content of the microparticles of GaAs and GaAs <Te> filler in HDPE films

Increasing the degree of crystallinity may occur through the formation of the third transition phase, as proposed in[11] three-phase model of the supramolecular structure (SMS) of amorphous-crystalline polymer consisting apparently, mostly of the rectified chains (RC). According to X-ray data, RC may have a three-dimensional structure with $\lambda = 50\text{-}60\text{ nm}$ [1, 12]. RC constitute an integral part of the highly oriented PE. The value of λ for PE fibers corresponds to the lengths of trans sequences in crystalline lamel regions. Apparently, at concentrations of GaAs 2-3 and GaAs <Te>

5-8 mass % microparticles in the PE, their introduction into the transition layer leads to the increase in the number of RC and increase the proportion of the crystalline phase of PE. This may be due to the fact that at these concentrations GaAs and GaAs <Te> microparticles are centers of further crystallization. When the concentration of particulate fillers in the PE increases more than 3 mass % for GaAs and 8 mass % for GaAs <Te> cluster sizes begin to strongly exceed the value of the frequency of RC, which is shown in the reduction of the relative degree of crystallinity. Apparently, the increase in the sizes of microparticles prevents rectification of the chains and the crystallization process. Increasing of the concentration of fillers leads to the formation of clusters, reduction of surface energy and stabilization of the crystallization processes of the polymer.

Structural changes in the composite films of HDPE+GaAs and HDPE+GaAs <Te> were traced as in areas of stretching ($2800-2900\text{ cm}^{-1}$) and deformation ($1450-1480\text{ cm}^{-1}$) oscillations of CH_2 -groups. Since the increase of the concentration of fillers from 1 to 10 mass% leads to redistribution of the intensities of both symmetrical 1472 and 2850 cm^{-1} and asymmetrical 1462 and 2857 cm^{-1} oscillations [12,13]. The ratio of the intensities and I_{1472}/I_{1462} and I_{2857}/I_{2850} with the increase in the concentration of GaAs and GaAs <Te> microparticles increases 2 and 1.5 times. Increase of intensity ratios of the of the bands absorption of symmetric and asymmetric deformation and valence oscillations of the CH_2 -groups indicates a change in the length of trans- sequences in the crystalline regions of lamels and rectified chains (RC). In this case, with the increase of concentration of fillers from 1 to 10 mass%, intensity of the absorption band of 1368 cm^{-1} of the amorphous phase (CH_2 -torsional oscillation) gradually decreases[13]. This band actually disappears from the spectrum at 10wt% concentration of fillers. On the contrary the characteristic band of crystallinity at 1176 cm^{-1} of the polymer with increase of concentration begins to appear in the spectrum and has maximum intensity at 10 mass% values of fillers. It should be noted that in the 720 cm^{-1} and 1460 cm^{-1} area doublets emerge either through the interaction of two polyethylene chains forming one crystallographic cell or doublet structure in these regions is possibly the result of crystallinity. The latter is shown by the splitting of the absorption bands in the symmetric and asymmetric valence oscillations of CH_2 groups ($\nu = 2800-3000\text{ cm}^{-1}$). Reflectance spectra of composite films at concentrations of 1-10 mass% of fillers absorption bands are not observed in the area of lattice oscillations ($\nu=600-400\text{ cm}^{-1}$) of GaAs and GaAs <Te>, which shows 4TO indicates a uniform distribution of the microparticles throughout its whole volume.

4. Conclusions

The possibility of applying the Fourier IR spectroscopy method of study of structural changes connected with the introduction of microparticles in the matrix of the polymer.

In the area of concentration of fillers of GaAs up to 2-3 mass%, and GaAs <Te> up to 6-8 mass %, an area of maximum crystallinity of HDPE is observed which is conditioned by the change in the third transition phase of the supramolecular structure (SMS) of the amorphous crystalline polymer. Increase of the concentration of fillers above these values leads to the formation of clusters, decrease in surface energy and stabilization up to the crystallization processes of the polymer.

By varying the concentration of fillers and type of the polymer can change the degree of crystallinity and SMS of the polymer matrix. Fillers GaAs and GaAs <Te> with 50 microns dispersed in composites with HDPE play a role of a structure former in the growth of the degree of crystallinity and a change in SMS.

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