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MODELING OF SYSTEM THAT BASED ON NEMATIC LIQUID CRYSTALS, DOUBLE WALL CARBON NANOTUBE AND FULLERENE MOLECULES C60

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The paper presents the results of computer simulation of the behavior of nematic liquid crystals in the presence of fullerene molecules and a double wall carbon nanotube. 10 cases of arrangement of system components relative to each other were investigated. Arylpropargyl esters of phenols were used as nematic liquid crystals. It is shown that polarity complicates the processes taking place in the system. It was found that the temperature dependences of the information entropy of the liquid crystals correlate with a change in the orderliness of these compounds. It was found that the arrangement of fullerene molecules at the ends of carbon nanotubes leads to a decrease in the orderliness of the liquid crystals.

Keywords: liquid crystals, fullerenes, carbon nanotubes, modeling

Introduction

The discovery of numerous types of nanostructures, for example, carbon nanotubes (CNTs), fullerene molecules [1-2], led to the development of various methods for their production and their production on an industrial scale. The improvement in the physicochemical properties of nanocomposite materials determines the efficiency of the operation of optoelectronic devices based on them. Dispersing small amounts of nanostructures, such as carbon nanotubes, fullerenes [3-5] in the medium of liquid crystals, can significantly improve important characteristics-response times, threshold electric field voltages, and others. It is known [6-7] that carbon nanotubes often form aggregates of different configurations among themselves. Investigation of the behavior of liquid crystals [8-9] in the presence of parallel carbon nanotubes made it possible to detect the movement of LC molecules with one carbon nanotube to another. No less interesting is the fact that the crystal structure is formed by fullerene molecules [1-2].

In this respect, the question of the effect of aggregations of carbon nanotubes and fullerene molecules of various morphologies on the behavior of nematic liquid crystals is interesting in this sense. Therefore, the aim of this work was to study the effect of complexes of different structures containing carbon nanotubes and fullerene C60 molecules on the behavior of liquid crystal molecules by molecular dynamics methods.

1. The methodology of the analysis

Three-component clusters containing the polar molecule of the phenylpropargyl ether p-fluorophenol (PEF) [10], the nonpolar - phenylpropargyl ether p-cresol (PEK) [11], a double wall carbon nanotube and fullerene C60 molecules were created.

The type of the structure of a double wall carbon nanotube corresponded to a zigzag structure with a length of 29.919 nm, an internal (8.0) radius of 0.31 nm, an outer radius (17.0) of 0.66 nm. Clusters were 3 layers of LC molecules around a carbon nanotube. The distance between the planes (OZ) was 0.4 nm PEF and 0.5 nm PEK, by OY 1.6 nm for all molecules (this direction coincides with the direction of the director and the axis of the carbon nanotube) displacement along this axis between neighboring molecules 0, 7 nm.Neighboring LC molecules were located antiparallel to each other. The distance along the arc (OX) is 0.7 nm. The fullerene C60 molecules were arranged in two layers around the carbon nanotube: the nearest molecules in the layer were shifted in OY by 0.7 nm, the arc distance (OX) was 1 nm, from the surface of the carbon nanotube to the center of the nearest molecule - 1 nm and between the centers of neighboring nanotubes molecules of different series - 1 nm. In the inner layer contains 10, in the outer layer - 16 molecules of fullerenes. The distance between the fullerene molecule and the nearest LC molecule was 2 nm. The C-C distance in the carbon nanotube was 1.421 Å. The carbon nanotube was "frozen", and the fullerene molecules were not "frozen", that is, they were simulated, as well as the LC molecules.

To simulate the behavior of these compounds, the molecular dynamics method based on the GROMACS program [12], version 3.3.1, was used in the approximation of the liquid aggregate state [13-15]. At modeling the NPT ensemble is used. The cutoff radii of the dispersion and Coulomb interactions were 2 nm. Sequential annealing in the heating mode was carried out. Computer simulation was carried out for the case of a planar orientation of LC molecules with respect to a carbon nanotube in the presence of an electric field. The annealing time at one temperature was 10 ps, but the cluster was located in the same cell as the liquid aggregate state of the system was realized, and the electric field strength was $1x10^7$ V / m and directed both along the axis of the carbon nanotube (Ey) and perpendicularly her (Ex). An input file was created to form a cluster in which the distance between molecules, rows and cluster layers in the XYZ directions was taken into account 10 cases of arrangement of system components relative to each other were investigated (Table 1).

Table 1 - Structure and number of components of the system "CNT-C60-LC"

№	Location C: 60 relative to CNTs	A molecule of LC	Number of LC	Number of C:60	Number of rows in layers			Number of LCD in a row
					1	2	3	
П1	centre	PEK	612	26	12	17	22	12
П2	centre	PEF	429	26	8	11	24	13
П3	end	PEK	612	26	12	17	22	12
П4	end	PEF	429	26	8	11	24	13
П5	centre - end	PEK	561	52	12	17	22	11
П6	centre - end	PEF	396	52	8	11	24	12
П7	end - centre - end	PEK	510	78	12	17	22	10
П8	end - centre - end	PEF	363	78	8	11	24	11
П9	end - end	PEK	561	52	12	17	22	11
П10	end - end	PEF	396	52	8	11	24	12

The technique for preparing and conducting experiments on computer modeling is described [12-15].

2 **Results and discussion**

The results of the studies are presented in Figures 1-6.

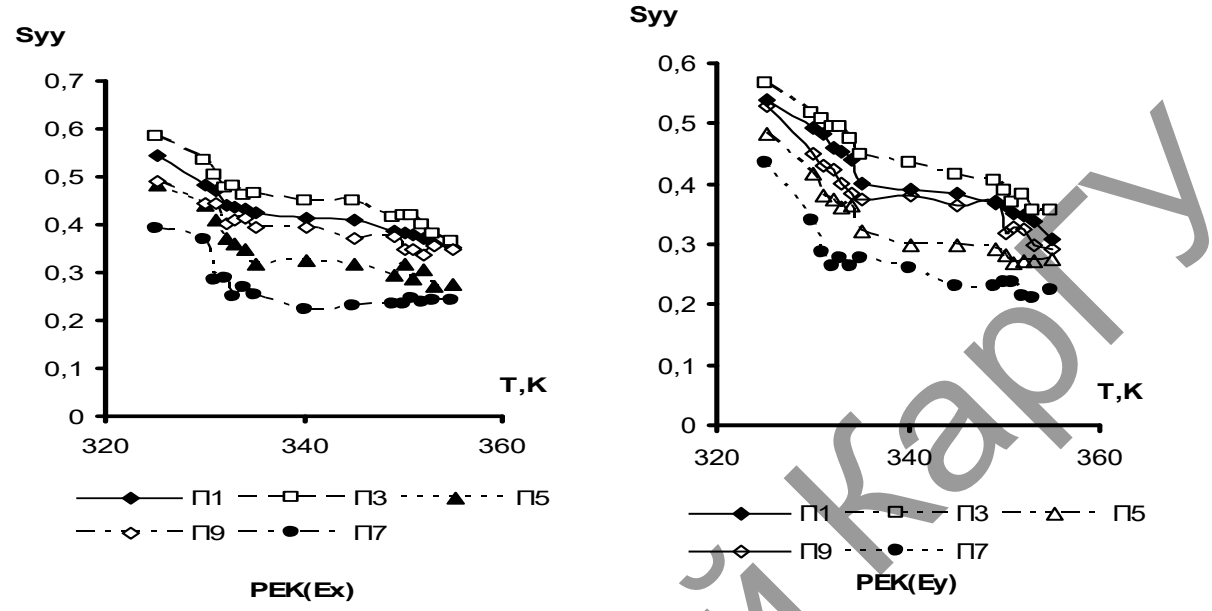

Fig. 1. Temperature dependence of the order degree of PEK for various directions of the electric field.

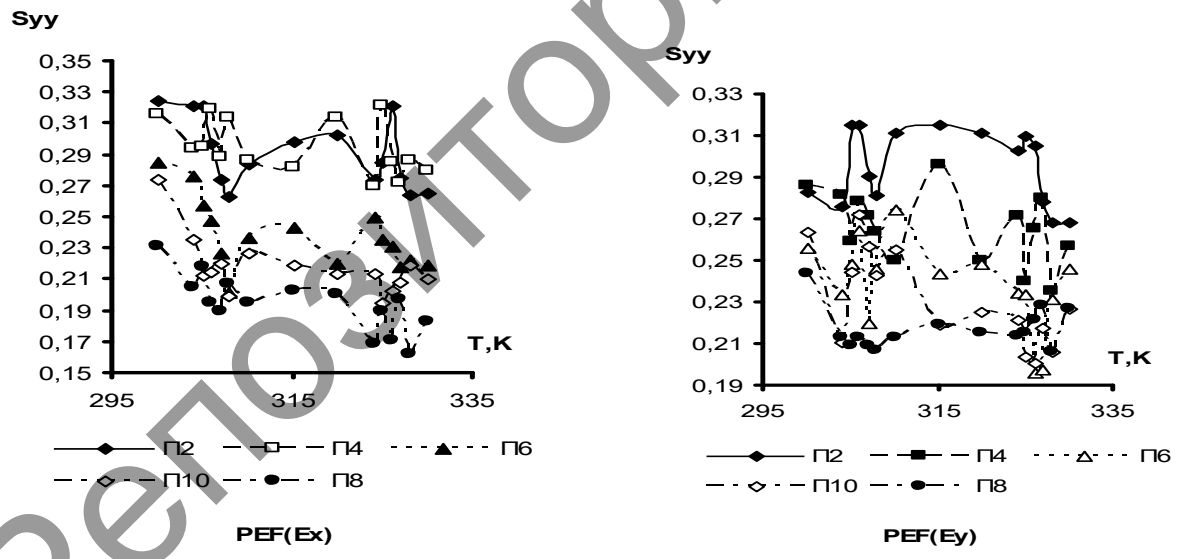

Fig. 2. Temperature dependence of the order degree of PEF for various directions of the electric field.

As can be seen in Fig. 1, the order degree of PEK decreases with increasing temperature, and, especially, in cases of spatial limitation of fullerene molecules by LC molecules (П5, П7, П10). The direction of the electric field does not change this pattern. In the case of the polar molecule PEF (Figure 2), the situation is complicated by the decay of dimers in the mesophase region [16]. This leads to a loss of a monotonic decrease in the curves with increasing temperature. But here again the spatial limitation of LC by fullerene molecules leads to a decrease in order

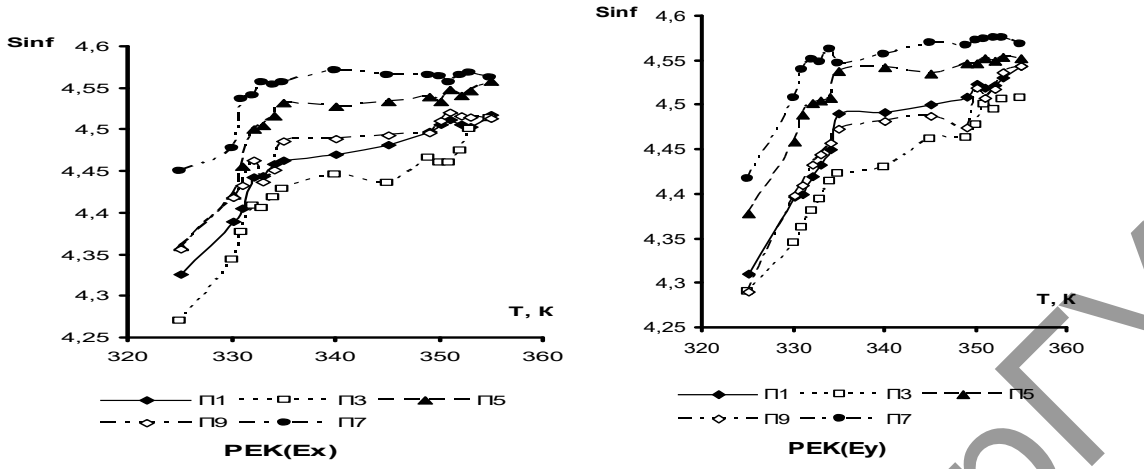

Fig.3. Temperature dependence of the information entropy PEK for various directions of the electric field.

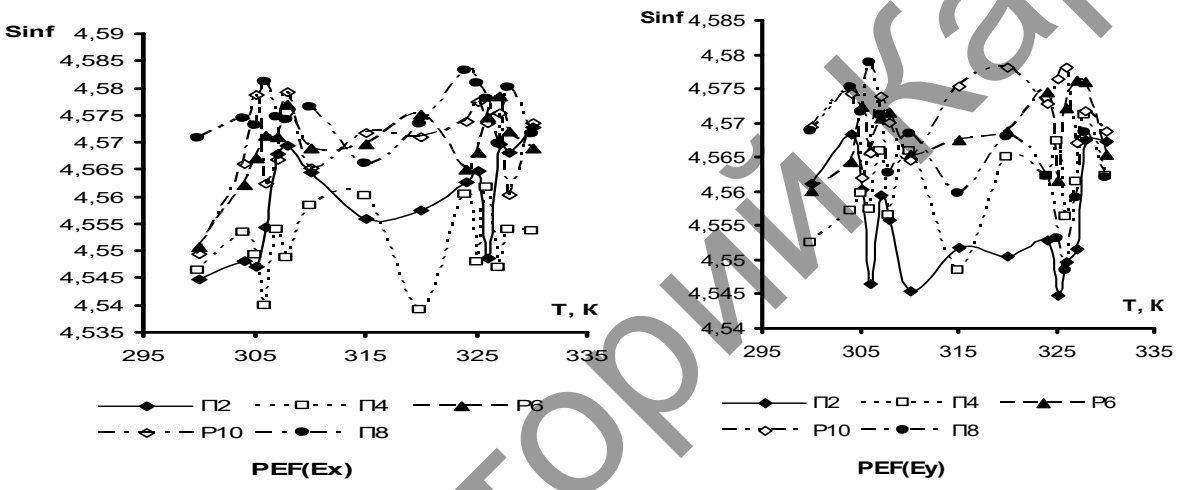

Fig.4. Temperature dependence of the information entropy PEF for various directions of the electric field.

The temperature dependences of the information entropy of PEK and PEF (Figures 3 and 4) are consistent with a change in the orderliness of these compounds.

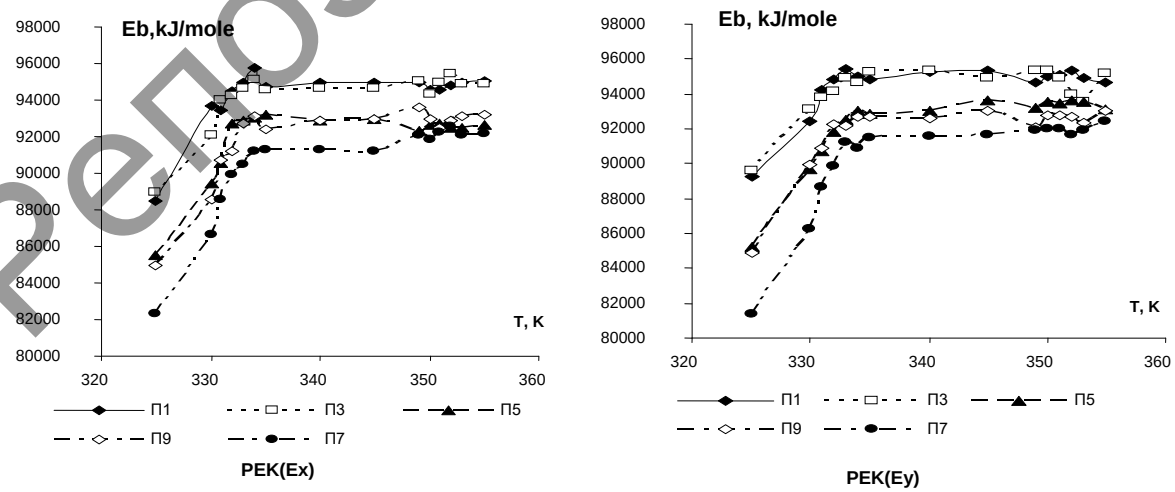

Fig.5. Temperature dependence of the information entropy PEK for various directions of the electric field.

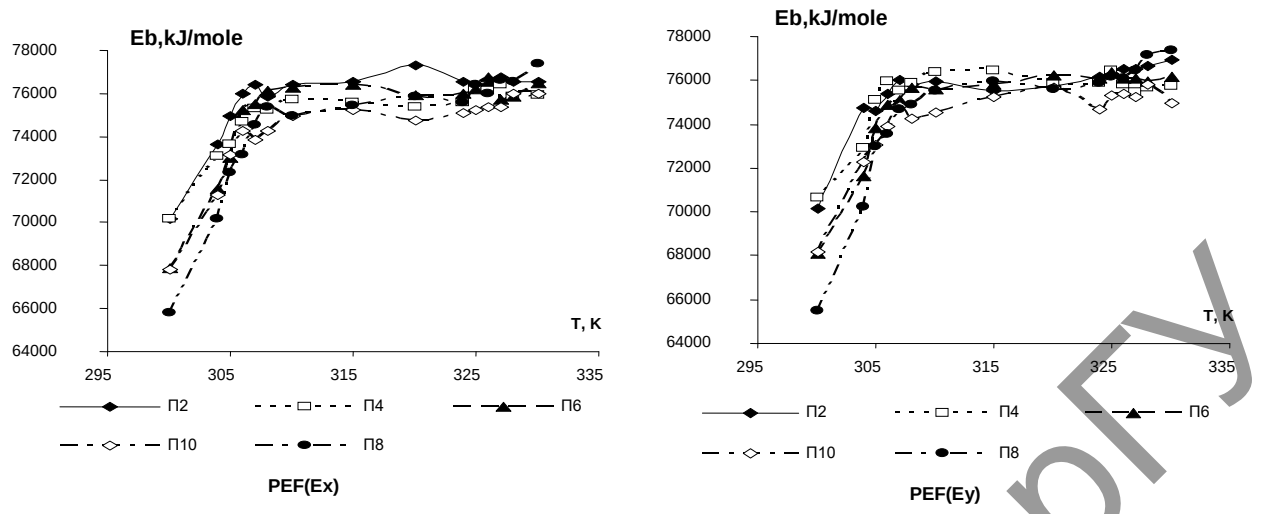

Fig.6. Temperature dependence of the information entropy PEF for various directions of the electric field.

A change of the configuration of the system under study shows that the restriction of LC to fullerene molecules leads to a decrease in the ordering of the LC. This leads to a decrease in the binding energy between the LC molecules (Figures 5 and 6). The analysis of the images of the system under study shows that the components are stable in their initial positions under temperature influence.

Conclusion

As is known, the results of many technological processes lead to a simultaneous combination of different carbon nanostructures. We have various 10 combinations of fullerene molecules and a carbon two-walled nanotube in the presence of nematic liquid crystals. Earlier, we showed that the morphology of the combination of nanotubes strongly affects the behavior of liquid crystals. Arylpropargyl esters of phenols were used as nematic liquid crystals. It was found that the temperature dependences of the information entropy of the LC correlate with a change in the orderliness of these compounds. It was found that the arrangement of fullerene molecules at the ends of CNTs leads to a decrease in the orderliness of the LC.

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