UDC:544.252.22:541.1:539.21:535.37

RESEARCH OF THE ELECTRIC FIELD INFLUENCE ON THE PROPERTIES OF NANOCOMPOSITES WITH NEMATIC LIQUID CRYSTALS AND SINGLE-WALLED NANOTUBES

Agelmenev M.E., Muldakhmetov Z.M., Bratukhin S.M., Polikarpov V.V. , Irgasheva O.B., Ibrayeva A.D.

Institute of Organic Synthesis and Coal Chemistry, Alikhanov street, 1,
Karaganda, 100008, Kazakhstan, e-mail: amaxut@mail.ru

The paper presents the results of the computer modeling of the behavior of nematic liquid crystals in the presence of single-walled nanotubes. It was found that the behavior of non-polar liquid crystals molecules corresponds to Fredericks transitions. It is shown that carbon nanotubes enhances the liquid crystals ordering. The inversion of influence of electric field on this process is possible by decreasing the electronegativity. The appearance of biaxial states was found.

Keywords: liquid crystals, nematic liquid, modeling, electric field, nanotube

Introduction

Different types of nanomaterials: metal nanoparticles, carbon nanotubes (CNTs), doped in liquid crystals (LC) exhibit interesting phenomena, such as the expansion of LC electro-optical properties, nonvolatile memory effect, enhanced photoluminescence, electrical conductivity, induction of LC ordering, reducing the working voltage consumption and the device response speed, etc. [1-9]. CNTs arouse the greatest interest because of its electrical and mechanical properties [10]. Researchers around the world doped LC with single-walled and multi-walled CNTs to improve dielectric, magnetic, electro-optical properties, dynamic performance and other physical parameters of the last one [11-16].

Theoretical part

In [17] there was established the existence of "guest - host" effect in LC- CNT cell, where CNT molecules are oriented in accord with LC molecules in the presence of electric fields. As to the interaction between LC molecules and single-walled CNTs, in [18] there were determined that the energy of the electrostatic interaction between LC molecules and CNT walls is on the order of 2 eV. It is much more than the Van der Waals forces and adsorption energy.

Because of anisotropy of diamagnetic and dielectric susceptibility, the free energy of the NLC molecules ensemble in external electric or magnetic field has the minimum at the definite orientation of the molecular axis (the director) relative to the field. At positive values of the dielectric anisotropy, the director tends to establish along the field, and at negative values - perpendicular to it. If in the initial state directions of the field and the NLC director do not match the minimum of free energy at the sufficiently strong field, can overcome the NLC elastic force, director will reoriented and new steady-state distribution will be established [19]. This effect was discovered and studied in detail by Fredericks and coworkers [20-21].

Interest to the interaction between LC and electric field is still relevant. It is largely due to the advent of biaxial states in phase transitions [22]. Authors reviewed the one-dimensional symmetric π-cell with thickness of 1 mm, which were 5CB nematic LC with unlimited energy of adhesion with 2 substrates. The electric field strength was varied within $1.8\text{-}9*10^7$ V/m. It was shown that the increase of field leads to the more rapid establishment of biaxial state.

The influence of electric field is revealed in interaction of its intensity vector with available in the LC molecules own vector of the dipole moment and the moment determined by the LC polarizability. This interaction often leads to molecules reorientation relative to the vector of the

external field. Studies that we have been carried out earlier show [23] that polar LC with increasing electric field intensity and temperature influence increase their ordering. The appearance of long CNTs in the system, apparently, can affect physical and chemical properties, which explains the early considered effects.

Therefore, to determine characteristics of LC behavior based on APEF in the presence of the CNT with the variation of value and direction of the electric field there were carried out experiments of computer simulations of molecular dynamics in the liquid state approximation [24-26].

Experimental technique

For conduction of the study one-component clusters containing phenylpropargyl ether of p-chlorophenol (PEC), phenylpropargyl ether of p-fluorophenol (PEF), phenylpropargyl ether of p-cresolphenol (PEK) [27-28], located on the surface of single-walled CNT were developed.

For modelling of the behavior of these compounds molecular dynamics method based on the program GROMACS [29] version 3.3.1 in liquid state approximation [24-26] was used. The NPT ensemble was used for modelling. The cutoff radius of dispersion and Coulomb interaction were 2 nm. The successive annealing in the heating mode were held. Computer modeling was carried out for the case of planar molecular orientation relative to the lateral CNT surface in the presence of electric field. The direction of the electric field was chosen as parallel to the CNT axis, so as perpendicular to it. Direction of the director coincides with the CNT axis. The annealing time at a given temperature was 10 ps, but the cluster was located in one cell, whereby system liquid aggregate state was achieved and the electric field strength was varied from $1{,}0x10^7$V / m to $65x10^7$ V / m.

Type of nanotube structure corresponds to the zigzag structure (12, 0), the CNT length was 29.919 nm, and radius was 0.47 nm. The number of LC molecules was equal to the 406 (PEC, PEF) and 585 (PEK). Clusters were 3 layers around CNT, while in the first layer there were 6 (PEC, PEF) and 10 (PEK) series, in the second one - 10 (PEC, PEF) i15 (PEK), in the third one - 13 (PEC, PEF) and 20 (PEK) rows, respectively. In each row, there were 14 (PEC, PEF) and 13 (PEK) molecules. The distance between the planes (OZ) was 0.4 nm (PEC, PEF), 0.5 nm (PEK); by OY – 1.6 nm for all molecules (this direction coincides with the direction of the Director and the CNT axis). C-C distance in the nanotube was 1,421 Å. 2 cases were reviewed - when the electric field vector was parallel to the CNT axis and the director (OY), and when it was perpendicular to it.

Methods of preparing and carrying out experiments of computer modeling were described in [24-26].

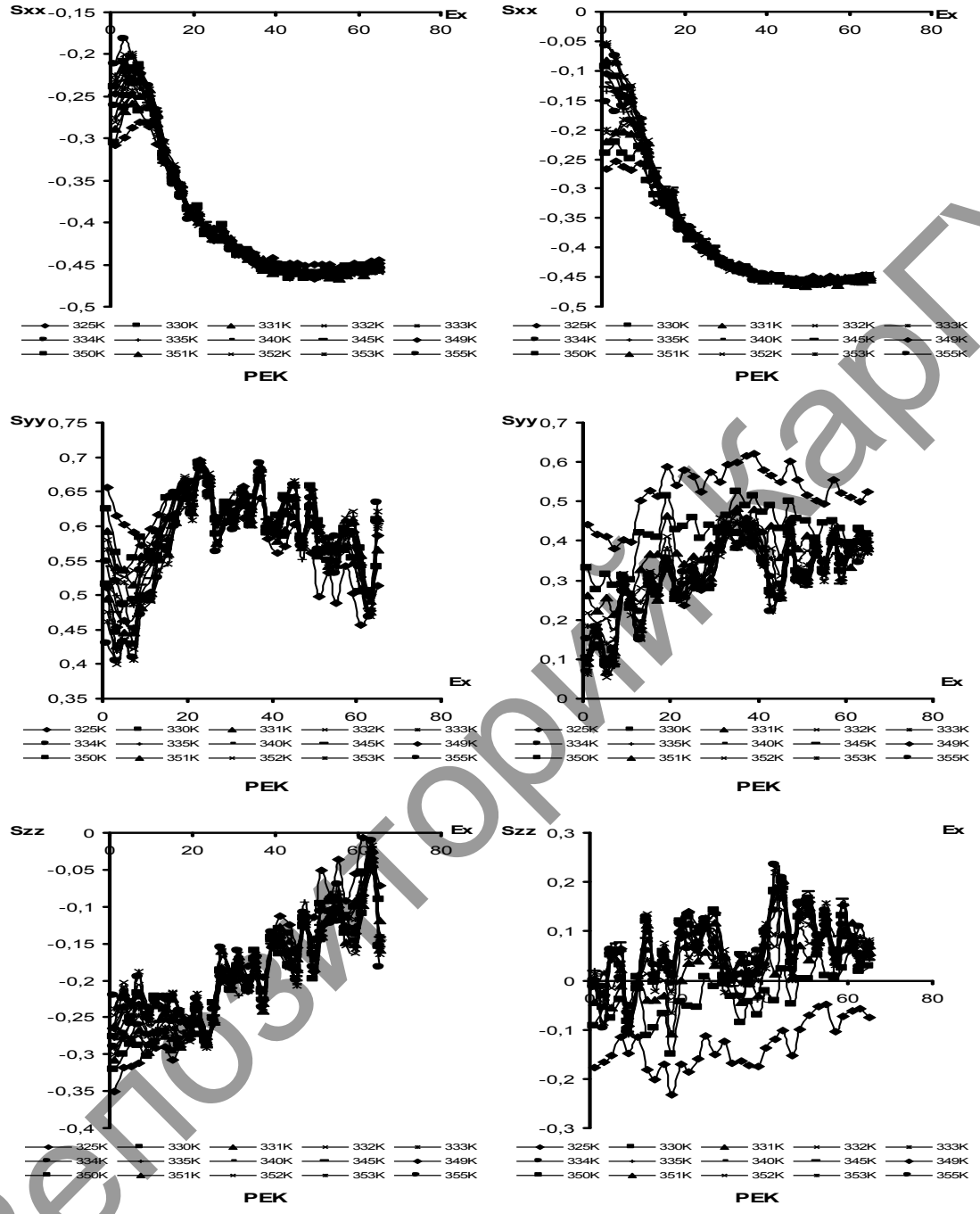
Results and discussion

The results of these studies are presented in Figures 1-20.

a) phenylpropargyl ether of p - cresolphenol (PEK)

Figures 1-2 show dependence curves of the coordinate components of S PEK molecules ordering degree on the electric field E intensity. The cases with and without CNT were presented. In the last case, the cluster was 4 layers of 13x13 PEK molecules, the bottom of which in the XOY plane was frozen and represented a substrate. In order to comply with the CNT case by the molecules number 5th layer of 6x13 molecules was added. The distance between molecules corresponds to the case with CNT.

As seen in Figure 1, when E||OX there is enhanced of ordering in both cases. Which is not surprising. The observing molecules have a negative dielectric constant [27-28], so the director tends to locate perpendicular to the field [19-21]. However, as it can be seen from the dependence Sy (E) in the case with CNT ordering is higher, where the maximum is observed at $23x10^7$V / m and without CNT - 19 $*10^7$ V / m. There is less influence of temperature on the curves nature in the presence of CNT.



with CNT without CNT

Fig.1. Dependence of the PEK ordering degree on the intensity at different temperatures. Intensity vector is E||OX. [E] = $1{,}0 \times 10^7$ V/m.

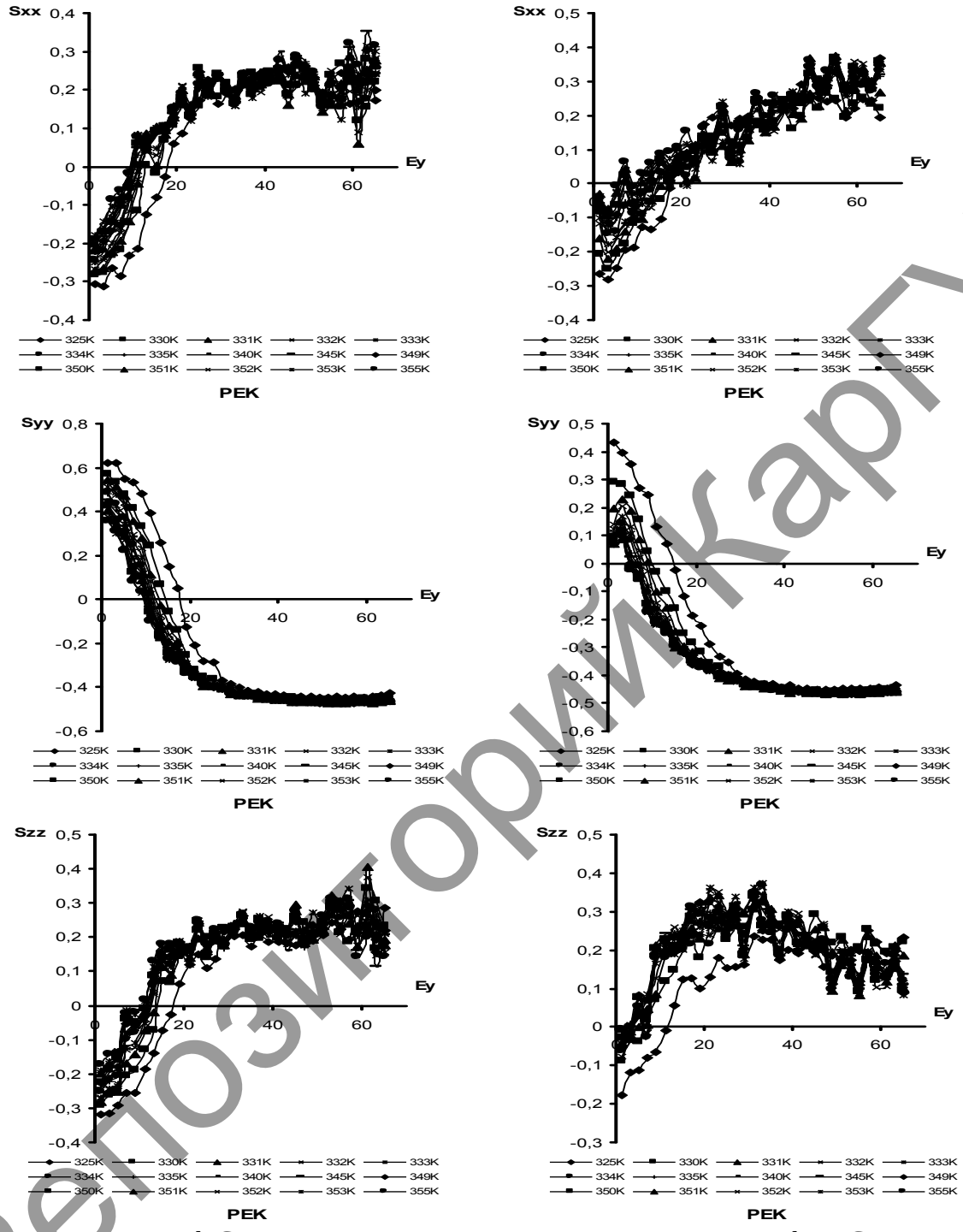
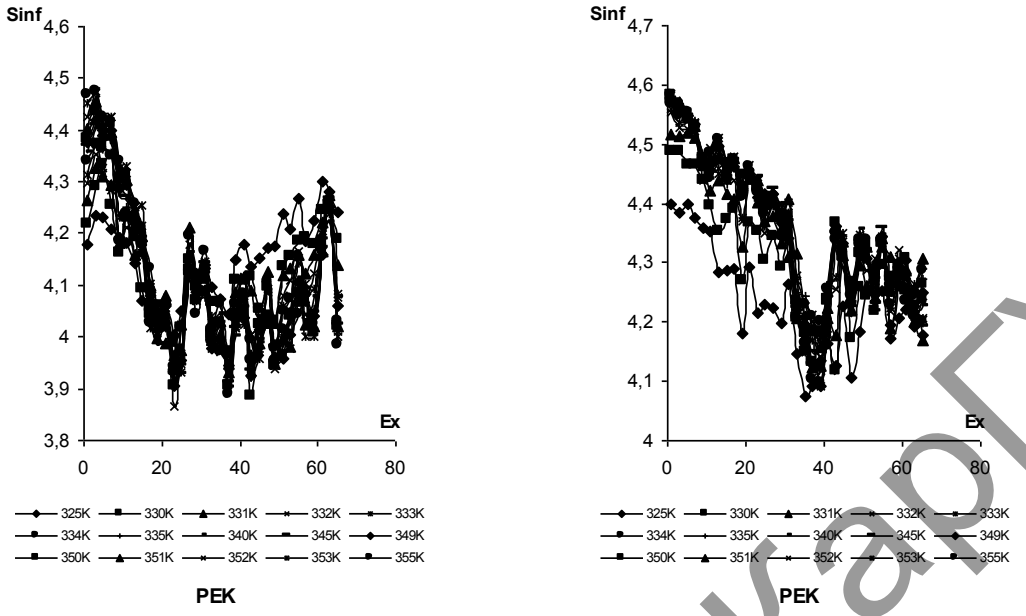


Fig.2. Dependence of the PEK ordering degree on the intensity at different temperatures. Intensity vector is E || OY. [E] = 1,0x10^7 V/m.

CNT also does not much affect on the character of Sx (E) dependencies curves. However, for Sz (E) curves the lack of CNT leads to the appearance of biaxial state, ordering and in the OZ direction at small values of the electric field intensity at the high temperatures.

Sinf (E) information ordering dependence curves (Figure 3), marked features in Figure 1. The observed difference between Sy (E) and Sinf (E) in the case of CNT absence when the ordering maximum Sinf (E) falls on the values 39x10^7 V/m, and for Sy (E) - 19x10^7 V/m. It is due, presumably, to the presence of biaxial state [66], which leads to such shift.

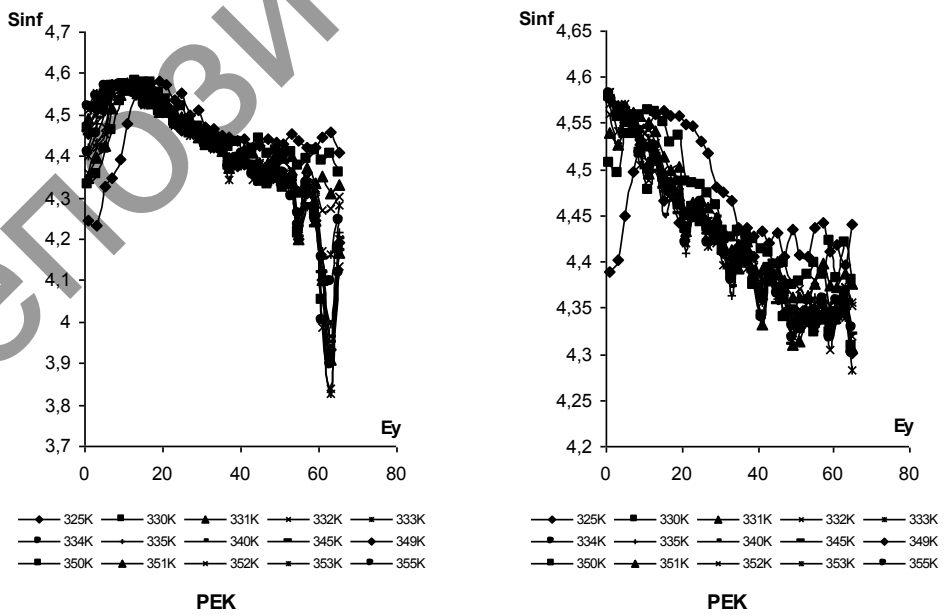


with CNT without CNT

Fig.3. Dependence of the PEK informational entropy on the intensity at different temperatures. Intensity vector is E || OX. [E] = 1,0x10^7 V/m

The behavior of PEK molecules in the case of E || OY (Figures 2 and.4), is consistent with the results [23]. Molecules unfold perpendicular to the E electric field direction. On the Sy (E) curves without CNT (Figure 2) ordering disappears when electrical field values goes from 15 to 5 x10^7 V/m with temperature increase. The CNT introduction leads to the interval from 17 to 11 x10^7 V/m with increasing temperature, when there is the disappearance of order in the OY direction, in the assigned original cluster. In both cases, there is appearance of the biaxial state, ordering in the OX and OY directions. This is clearly can be seen in the Sx (E), Sz (E) curves on Figure 2.

The dependence of information entropy Sinf (E) (Figure 4) shows that the CNT presence leads to ordering increase and less influence of temperature on the curves nature.



with CNT without CNT

Fig.4 .Dependence of the PEK informational entropy on the intensity at different temperatures. Intensity vector is E||OY. [E] = 1,0x10^7 V/m.

Evaluation of the interaction energy of LC molecules and the substrate, constructed by taking into account the geometry of the original cluster (length along the OY is 23 nm) and certain ranges of field values in which ordering by OY disappears (see above). For the case without CNT the energy is changing in 3.7 - 1.1 eV interval with temperature increase, and with CNT - in 3.9 - 2.5 eV interval with temperature increase. It is easy to see that the energy increases in the CNT presences. It accord well to previously obtained dependence of the degree of order and information entropy. The energy values are close to the values obtained in [18]. The greatest amount of energy corresponds to the crystalline phase of PEK molecules.

Analysis of the dependence of the total molecular dipole moment from the field shows that the curves represent monotonically increasing smooth curves while increasing the field. It applies to both orientations of the electric field relevant to the CNT axis.

In Fig. 5 it is shown that the increasing E value of field leads to changing the form of lines of D distribution of molecular pairs function [24-26]. The asymmetry between the left and right sides increases, the shape of curve narrows, the number of molecular pairs with small angles between each other increases. Staring from E = $17x10^7$ V/m the maximum value of function in crystalline state becomes less in comparison with the other phase states. Dynamics of changes of D function is consistent with the order change.

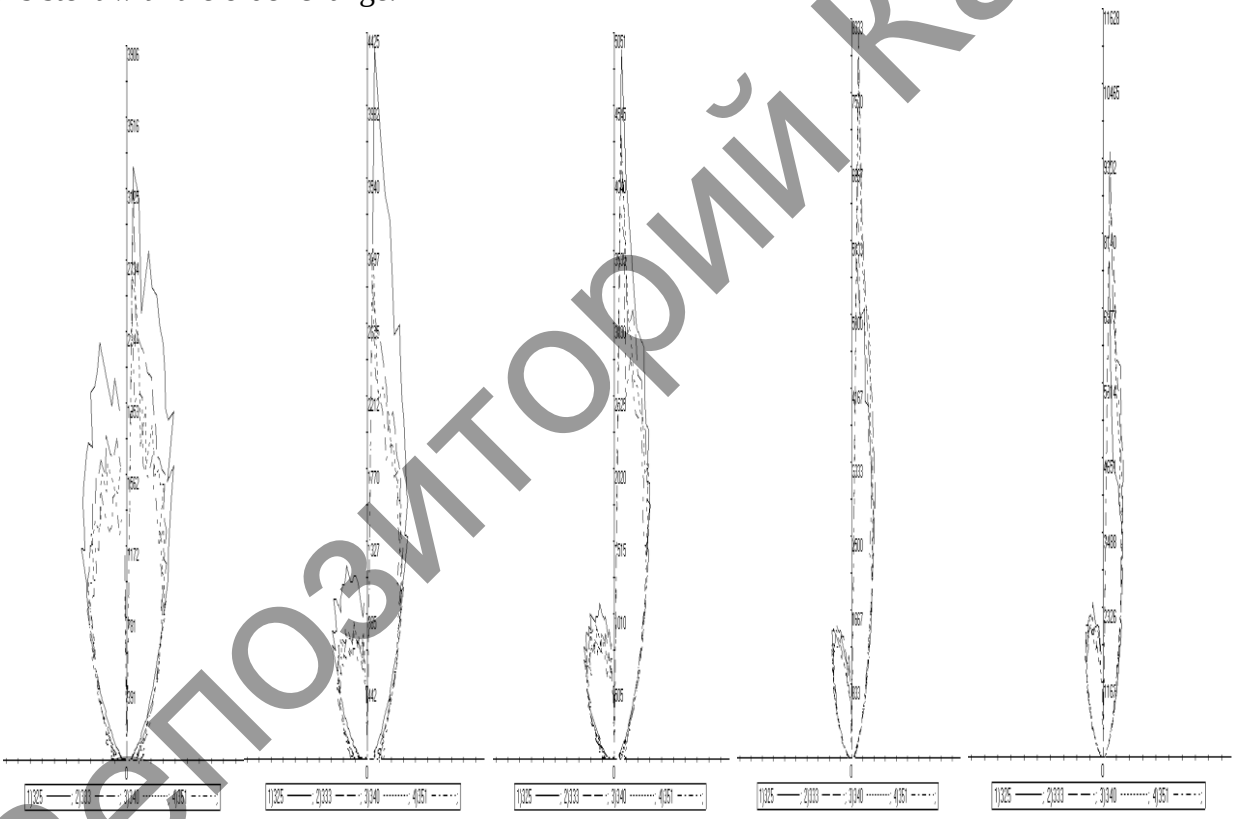
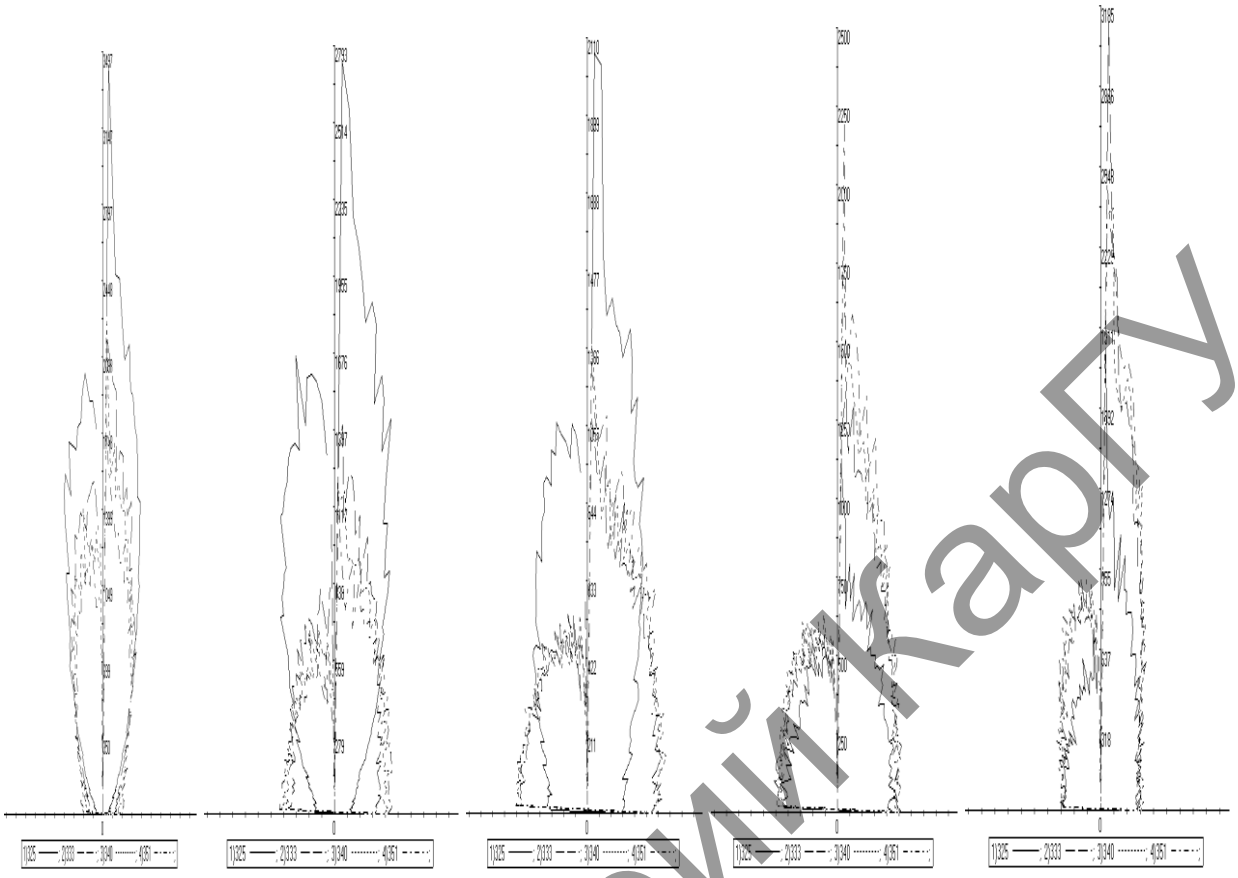


Fig.5. Distribution functions of D pairs of molecules in crystalline phase at the temperature of melting, mesophase and enlightenment in the CNT presence. Intensity vector is E || OX. [E] = $1,0x10^7$ V/m

When electric field is directed along the CNT axis, with the increase of its value leads to broadening of D function curve shape, and temperature increase leads to the reduction of the asymmetry and the number of molecular pairs, which have small angles between them (Figure 6). However, starting from E = $13x10^7$ V/m with temperature increase, there is the reverse process of changing the shape of the distribution function. This is due to the establishment of the biaxial state in PEC.



E = 1 7 11 17 23

Fig.6. Distribution functions of D pairs of molecules in crystalline phase at the temperature of melting, mesophase and enlightenment in the CNT presence. Intensity vector is E||OY. [E] = 1,0x10^7 V/m

The analysis of PEK molecules images E||OX shows that even for small values of the field molecules clearly aligned along the CNT axis. As an example, there is given the state of the cluster in the mesophase at E = 17x10^7 V/m (Figure 7).

At E||OY with increasing of intensity, molecules are perpendicular to the CNT axis, as it is shown in Figure 8. Starting with the value of E = 29x10^7 V/m separate clusters fly out from the surface of cluster, and at E = 43x10^7 V/m, this process significantly increases. Displaced molecules under the field influence line up at define angles (Figure 9), creating with other molecules biaxial state of LC cluster.

The analysis of the results of computer modelling of the CNT-PEK shows that the CNT presence increases the ordering degree of the LC molecules. It was found that at E||OX with increasing electric field intensity molecules are aligned along the CNT axis, while there are noted the slight effect of temperature and lack of biaxial states. The S maximum is observed in the region of 23x10^7 V/m, and without CNT - 19x10^7 V/m.

It is shown that in case of E||OY the ordering disappears at field values from 17 to 11x10^7 V/m with temperature increase, and the appearance of biaxial state is observed. The evaluation of the interaction energy between LC molecule and CNT gives values in the range 3.9 - 2.5 eV for different temperatures. It was found that the energy increases in the CNT presence. The dynamics of changing the shape of the curves of the distribution function of molecular pairs is shown and influence of orientation of the electric field on it is established.

The visualization of LC clusters states under electric field was made.

b) phenylpropargyl ether of p - fluorophenol (PEF)

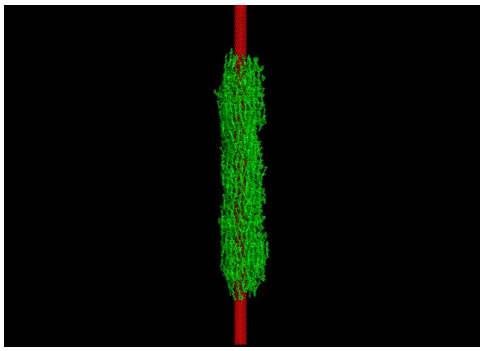


Fig.7. Image of PEK cluster in the XOY plane in the mesophase (345K).

Intensity vector is E||OX. E = 17x10^7 V/m

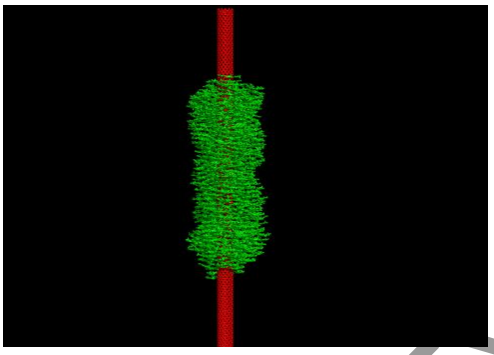


Fig.8.Image of PEK cluster in the XOY plane in the mesophase (345K). Intensity vector is E||OY.

E = 23x10^7 V/m

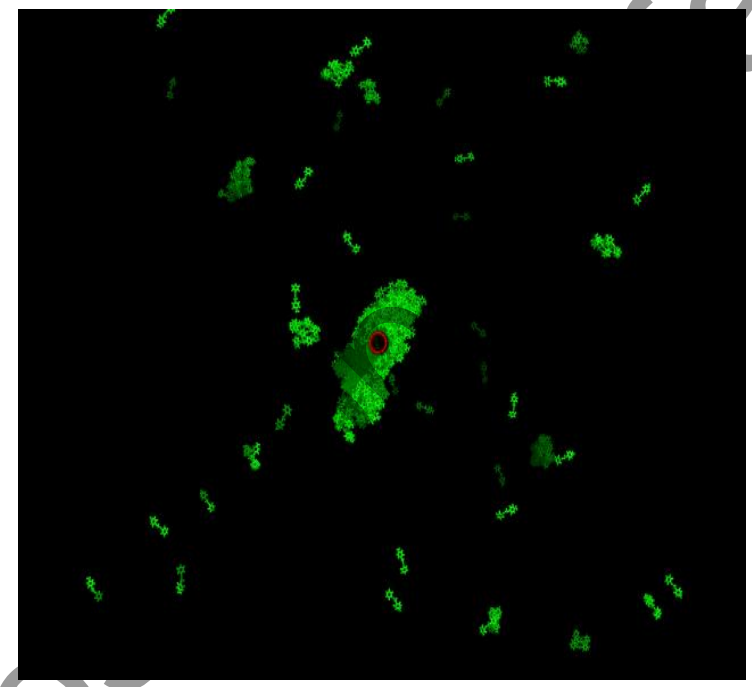


Fig. 9. Images of PEK cluster in the XOZ plane in the mesophase (345K).
Intensity vector is E||OY. E = 59x10^7 V/m

As can be seen from Figure 10, the polarity of the PEF molecule leads to differences in S (E) dependence in comparison with the PEK at E||OX (see Figure 1). The degree of order of Sy disappears in the range from 7-11x10^7 V/m at different temperatures and appears - in the range of 31-35x10^7 V/m. While the ordering in the OX direction is established.. It can be argued that the effect of the field leads to the complex reorientation of molecules due to the presence of electronegative fluorine atom in the *pair*-position. There are elements of the LC biaxial state.

In Figure 11 it can be seen that the temperature has little effect on the character of the Sinf (E) curves. It should be noted that entropy is decreasing at E = 7x10^7 V / m.

In the case of E||OY the transition in the biaxial state is observed. In the range of the electric field intensity from 39-43 x10^7 V/m depending on the temperature there is the disappearance of the Sy ordering degree and the appearance of positive values along the OX and OZ axes, as seen in Figure 12.

The evaluation of the interaction energy between PEF molecule and single-walled CNT was 9,0-9,9 eV, depending on the cluster temperature. It exceeds energy values for the non-polar molecule of PEK.

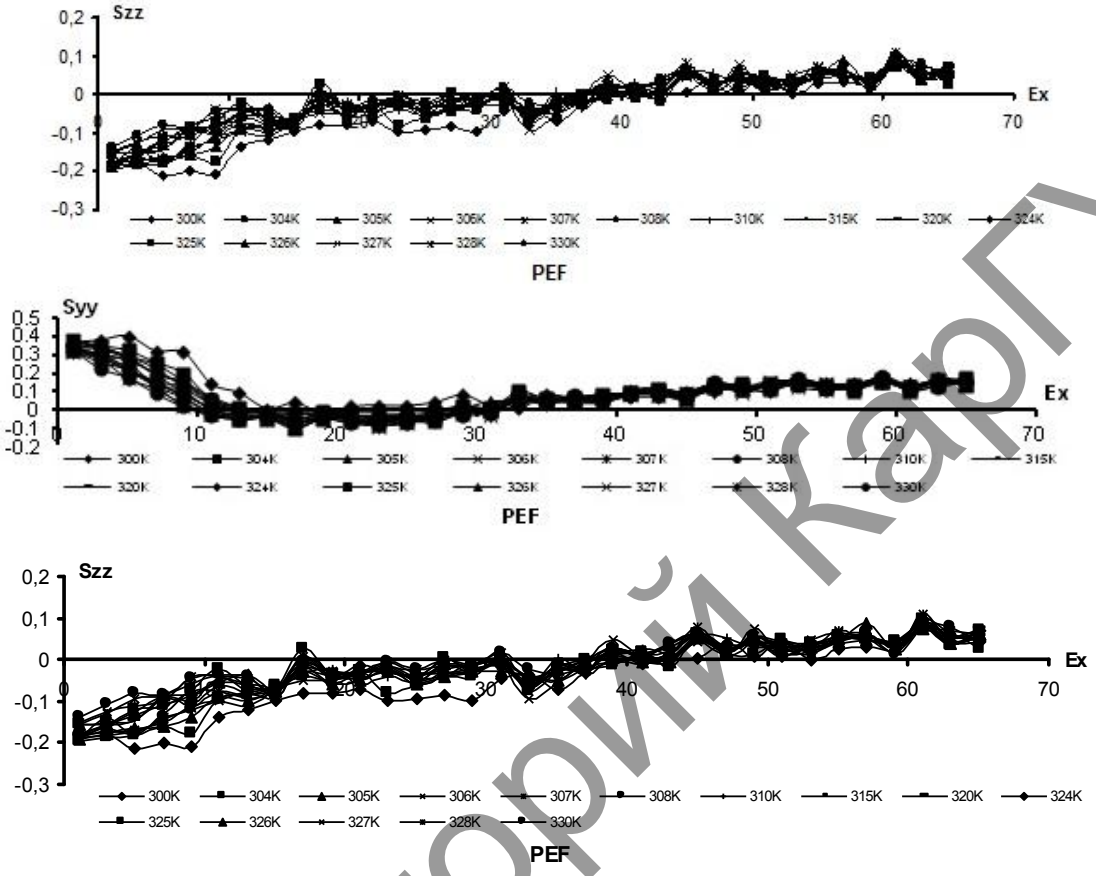


Fig.10. Dependence of the PEF ordering degree on the intensity at different temperatures. Intensity vector is E||OX. [E] = 1,0x10^7 V/m

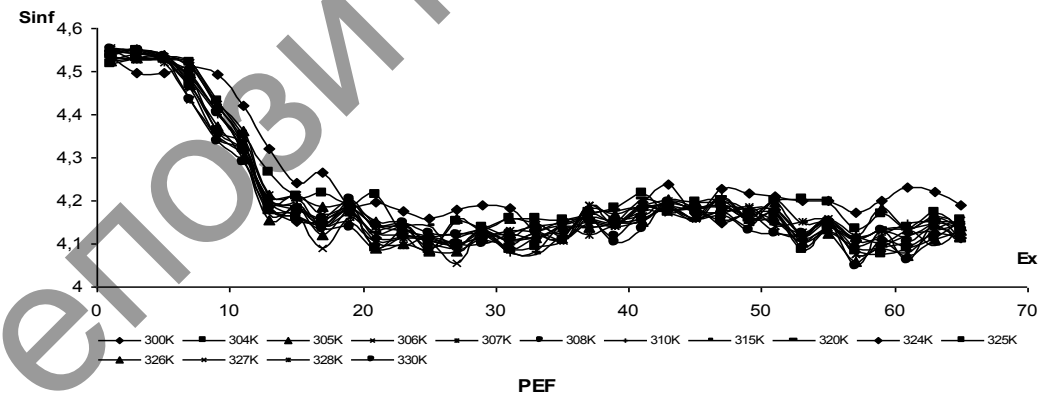


Fig.11.Dependence of the PEF informational entropy on the intensity at different temperatures. Intensity vector is E||OX. [E] = 1,0x10^7 V/m

At all orientations of the electric intensity vector from some value of E entropy is decreasing (see Figure 13). At E||OY the entropy decrease in the range from 7 to 21 x10^7 V/m. Further small monotonous growth is observed.

The evolution of the curves shape of the distribution functions of molecular pairs at both field orientations (Figures 14 and 15) shows the tendency of ordering improvement. However, compared with the case of PEK, there is a significant presence of molecular pairs; the angle between them is 90^0.

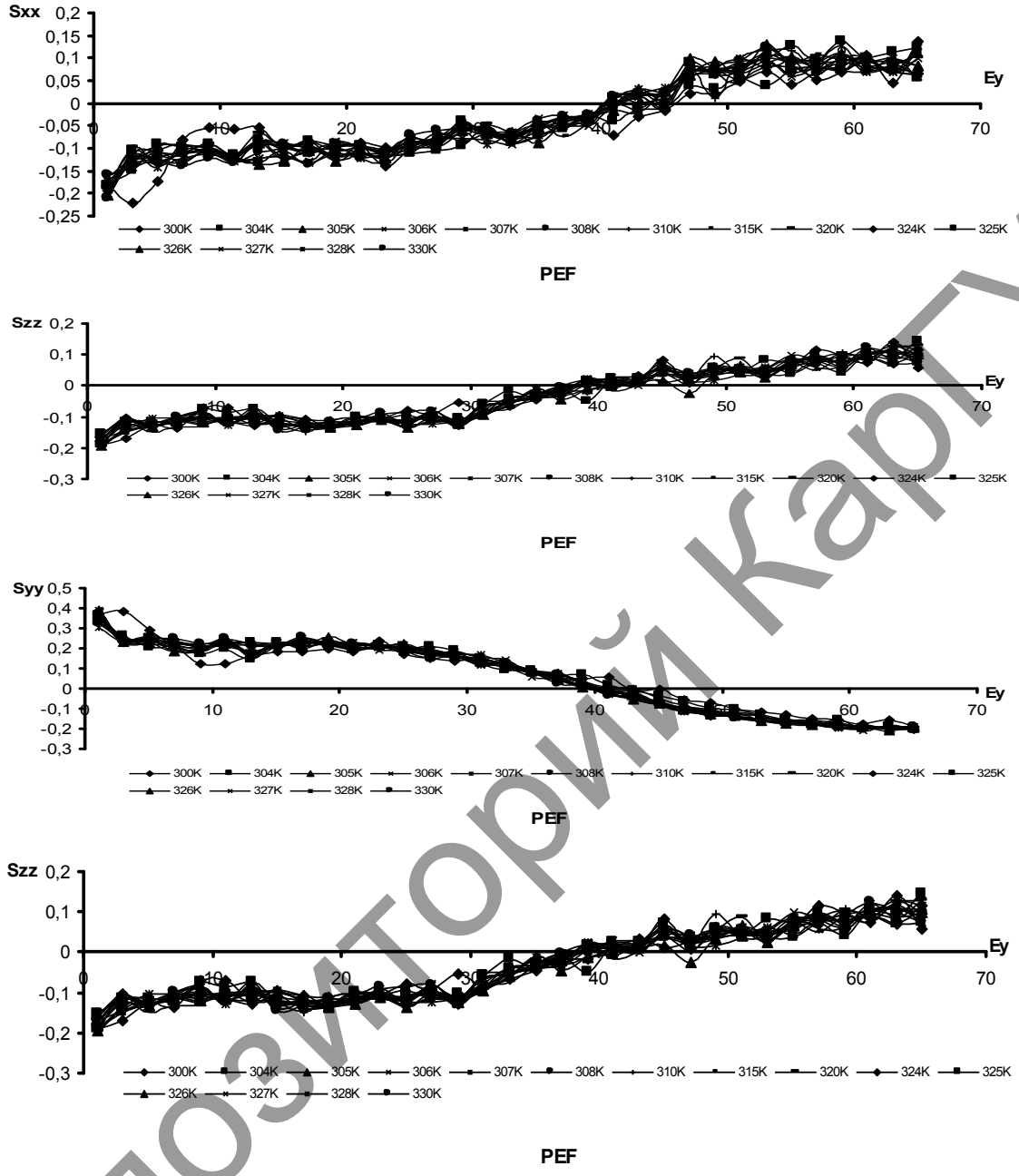


Fig.12.Dependence of the ordering degree of PEF with CNT on the intensity at different temperatures. Intensity vector is E||OY. [E] = 1,0x10^7 V/m.

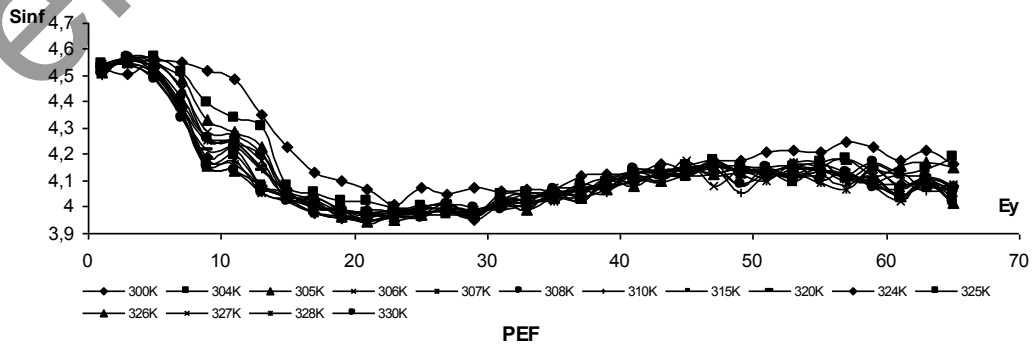
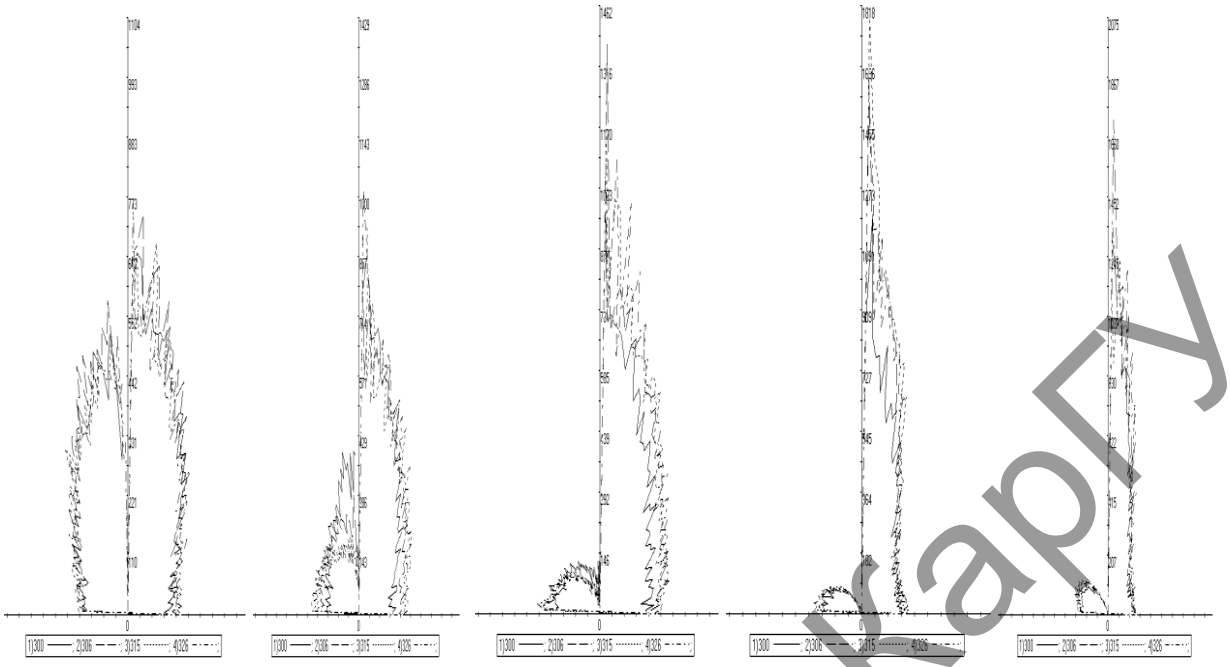
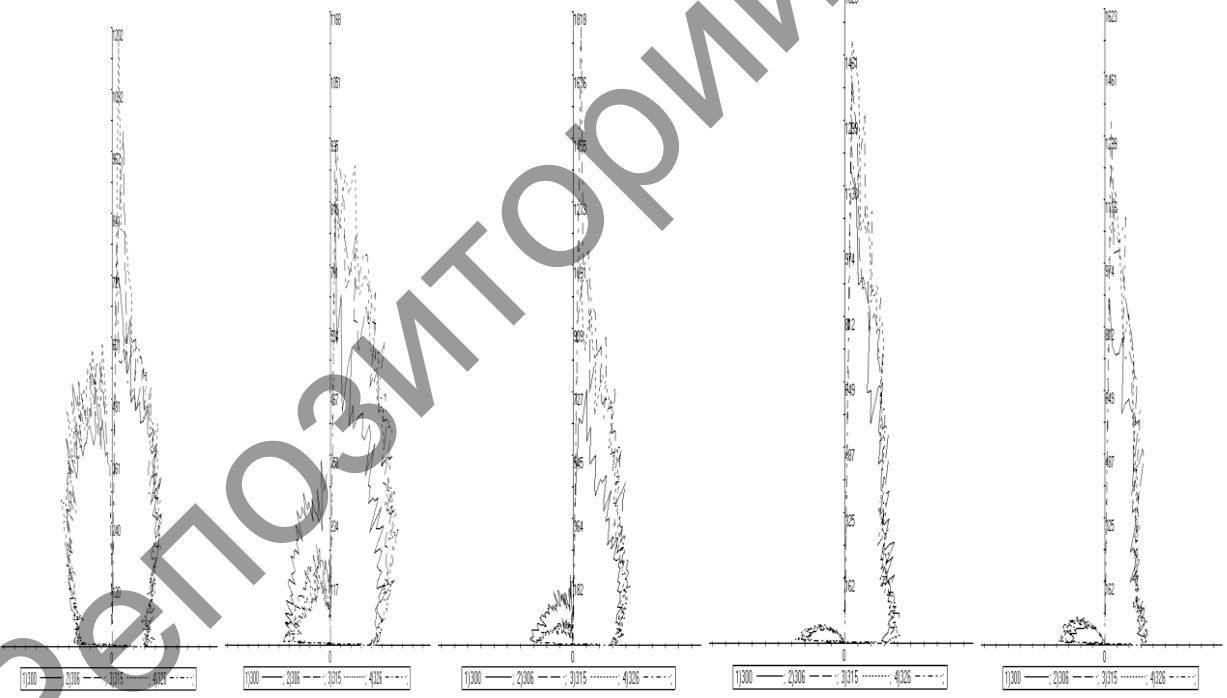


Fig.13. Dependence of the PEF informational entropy on the voltage at different temperatures. Intensity vector is E||OY. [E] = 1,0x10^7 V/m



E = 1 7 11 31 39

Fig.14.Distribution functions of D pairs of molecules in crystalline phase at the temperature of melting, mesophase and enlightenment. Intensity vector is E||OX. [E] = $1{,}0x10^7$ V/m



E = 1 7 11 31 39

Fig.15.Distribution functions of D pairs of molecules in crystalline phase at the temperature of melting, mesophase and enlightenment. Intensity vector is E||OY. [E] = $1{,}0x10^7$ V/m

The analysis of clusters images shows the lack of clear orientation of molecules relative to the CNT axis. At the same time, more symmetrical picture of detached molecules location is observed at the E||OY.

The complication of the process of molecular reorientation, apparently, caused by the increase of the intermolecular interaction effect. It leads to loss of the dominance of interaction between the field and molecules.

c**)** phenylpropargyl ether of p-chlorophenol (PEC)

No less complicated situation is observed in the study of PEC. The dependence of the information entropy from the field represents the curves where the entropy starts decreasing monotonically from $3x10^7$ V/m to $31x10^7$ V/m at E||OX and to $17x10^7$ V/m at E||OY. The subsequent growth of E does not lead to significant changes in entropy. Figures 18-19 present the components of the ordering degree with positive values for the cases of both orientations. The nature of the observed changes is different from the picture, previously observed for molecules of PEK, PEF. In the case of E||OY we find the lack of biaxial states, and for E||OX - the disappearance of order in OY-direction in the range of field values within 7-15 $x10^7$ V/m at different temperatures and the appearance of positive component in OX-direction. By evaluating the interaction energy between the PEC molecules and the CNT wall, the value of the ordering of 1,6-3,5 eV is obtained, which is comparable with the values for the PEK molecule.

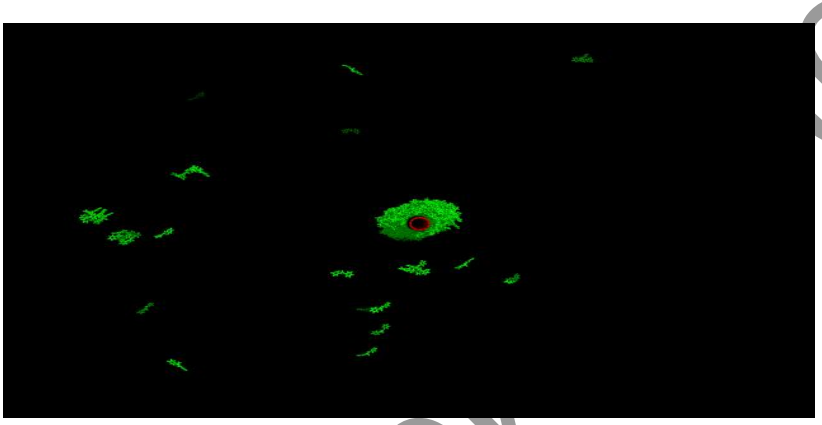


Fig.16. Image of cluster with PEF in the XOZ plane in the mesophase (345K).
Intensity vector is E||OY. E = $59x10^7$ V/m

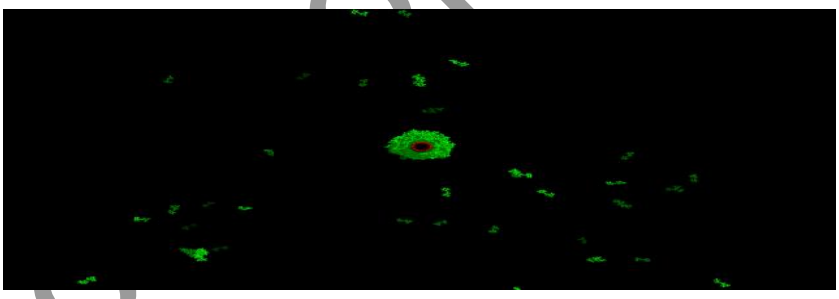


Fig.17. Image of cluster with PEF in the XOZ plane in the mesophase (315K).
Intensity vector is E||OY. E = $39x10^7$ V/m

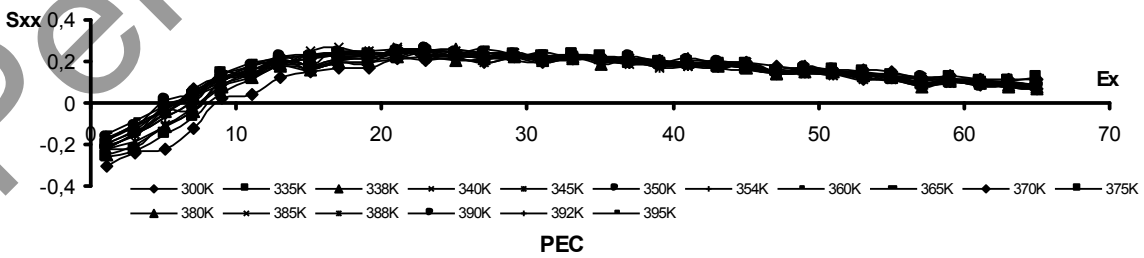


Fig.18.Dependence of the PEC ordering degree on the intensity at different temperatures.
ntensity vector is E||OX. [E] = 1,0$x10^7$ V/m

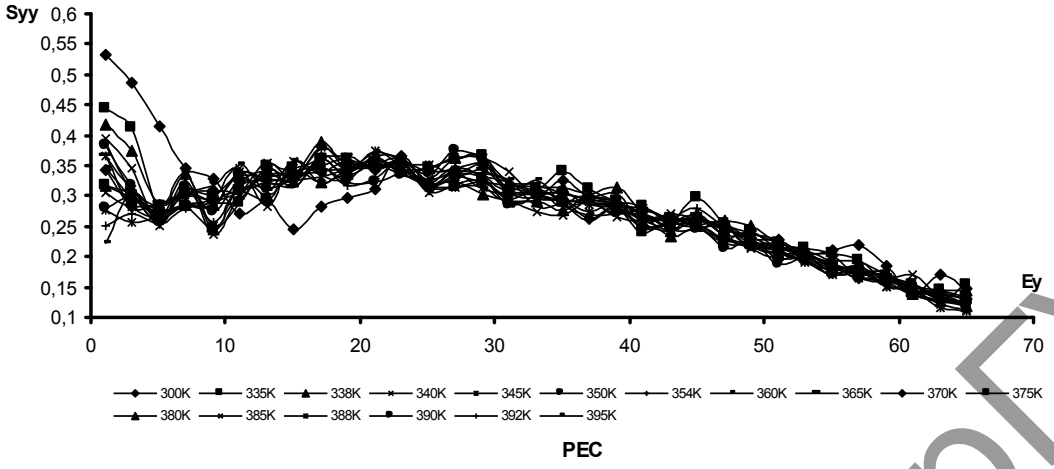


Fig.19. Dependence of the PEC ordering degree on the intensity at different temperatures. Intensity vector is E||OY. [E] = 1,0x10^7 V/m

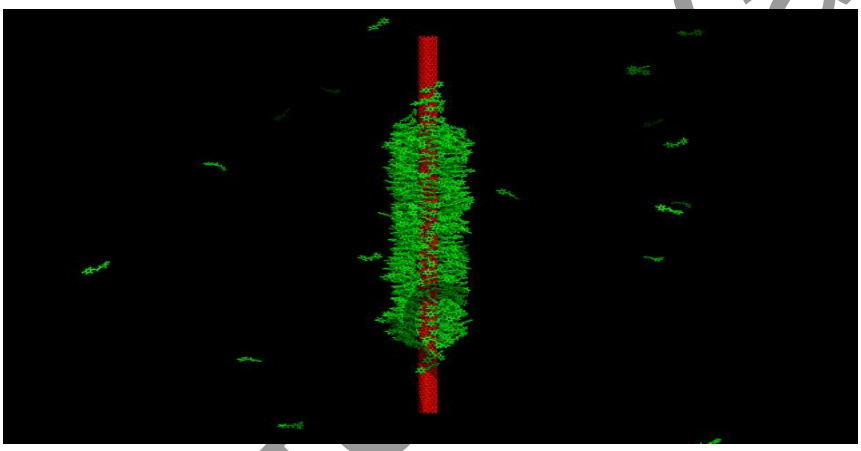


Fig.20.Image of cluster with PEC in the XOY plane in the mesophase (385K). Intensity vector is E||OX. E = 23x10^7 V/m

The reduction of the substituent electronegativity - chlorine atom – by changing the intermolecular interaction leads to inversion effect, when the effect of the field is no longer dominant. It leads to the fact that the molecules are arranged exactly opposite to conclusions [19-21]. As can be seen from Figure 20, at E||OX molecules are located along the field, although the dipole moment is perpendicular to the longitudinal molecule axis.

Conclusion

Thus, on the basis of the carried out researches, it was found that the behavior of non-polar PEK molecule corresponds to Fredericks transitions. It is shown that the CNT enhances the LC ordering, and the interaction energy of the LC and the CNT is comparable to [18]. At E||OY orientation appearance of biaxial states is observed. The LC polarity significantly complicates the process of reorientation due to the increase of contribution of intermolecular interaction. By decreasing the electronegativity the inversion of influence of electric field on this process is possible.

REFERENCES

1 Kaur S, Singh S.P., Biradar A.M., Choudhary A., Sreenivas K. Enhanced electro-optical properties in gold nanoparticles doped ferroelectric liquid crystals. *Appl Phys Lett.*, 2007, Vol. 91, pp. 023120 (1–3).

2 Prakash J., Choudhary A., Kumar A., Mehta D.S., Biradar A.M. Nonvolatile memory effect based on gold nanoparticles doped ferroelectric liquid crystal. *Appl Phys Lett*., 2008, Vol. 93, pp. 112904 (1–3).

3 Shivakumar U., Mirzaei J., Feng X., Sharma A., Moreira P., Hegmann T. Nanoparticles: complex and multifaceted additives for liquid crystals. *Liq Cryst*., 2011, Vol. 38, pp. 1495–1514.

4 Kumar A., Prakash J., Mehta D.S., Biradar A.M., Haase W. Enhanced photoluminescence in gold nanoparticles doped ferroelectric liquid crystals. *Appl Phys Lett*., 2009, Vol. 95, pp. 023117 (1–3).

5 Holt L.A., Richard B.J., Stephen E.D., Andrew B., Gordon S. A 106-fold enhancement in the conductivity of a discotic liquid crystal doped with only 1% (w/w) gold nanoparticles. *J. Appl Phys*., 2008, Vol. 103, pp. 063712.

6 Qi H., Hegmann T. Multiple alignment modes for nematic liquid crystals doped with alkylthiolcapped gold nanoparticles. *Appl Mater Inter*., 2009, Vol. 1, pp.1731–1738.

7 Joshi T., Kumar A., Prakash J., Biradar A.M. Low power operation of ferroelectric liquid crystal system dispersed with zinc oxide nanoparticles. *Appl Phys Lett*., 2010, Vol. 96, pp. 253109 (1–3).

8 Bisoyi H.K., Kumar S. Carbon-based liquid crystals: art and science. *Liq Cryst.*, 2011, Vol. 38, pp.1427–1449.

9 Prakash J., Choudhary A., Mehta D.S., Biradar A.M. Effect of carbon nanotubes on response time of ferroelectric liquid crystals. *Phys Rev E.*, 2009, Vol.80, pp. 012701 (1–4).

10 Iijima, S. Helical microtubules of graphitic carbon. *Nature*, 1991, Vol. 354, pp.56–58.

11 Lee W., Wang C.Y., Shih Y.C. Effects of carbon nanosolids on the electro-optical properties of a twisted nematic liquid-crystal host. *Appl Phys Lett*., 2004, Vol. 85, pp. 513 (1–3).

12 Gupta S.K., Kumar A., Srivastava A.K., Manohar R. Modification in dielectric properties of SWCNT doped ferroelectric liquid crystals. *J Non-Cryst Solids*, 2011, Vol. 357, pp. 1822–1826.

13 Park HG, Jeong HY,Kim YH,Kim BY,Kim JH,Yoon H, Seo DS. Electrooptical properties of single-walled carbon-nanotube mixed liquid-crystal cells with rubbed and ion-beam-treated alignment layers. *J Display Tech.*, 2011, Vol. 7, pp. 644–648.

14 Mitroova Z., Tomasovicova N., Timko M., Koneracka M., Kovac J., Jadzyn J., Vavra I., Eber N., Toth-Katona T., Beaugnon E., Chaude X., Kopcansky P. The sensitivity of liquid crystal doped with functionalized carbon nanotubes to external magnetic fields. *New J Chem*., 2011, Vol.35, pp. 1260–1264.

15 Srivastava A.K., Pozhidaev E.P., Chigrinov V.G., Manohar R. Single walled carbon nano-tube, ferroelectric liquid crystal composites: excellent diffractive tool. *Appl Phys Lett*., 2011, Vol. 99, pp. 201106 (1–3).

16 Sood N., Khosla S., Singh D., Bawa S.S. Dielectric investigations of pure and carbon nanotube-doped deformed helix ferroelectric liquid crystals. *Liq Cryst*., 2012, Vol. 39, pp. 1169–1174.

17 Dierking I., Scalia D.G. I., Morales P. Liquid crystal-carbon nanotube dispersions. *J. Appl. Phys*., 2005, Vol. 97, pp.044309-11.

18 Park K.A., Lee S.M., Lee S.H., LeeY.H. Anchoring a liquid crystal molecule on a single-walled carbon nanotube. *J Phys Chem C*., 2007, Vol. 111, pp. 1620–1624.

19. Blinov L.M. *Electro- and magneto-optics of liquid crystals*. Moscow, Nauka, 1978.-384 p.

20 Friederiksz V.K., Zolina V.V. About the application of a magnetic field to measure the forces which orients anisotropic liquid in a thin homogeneous layers. *RPCAJ phys*., 1930, V. 62, No. 5, pp. 457-464.

21 Freedericksz V.K., Zolina V.V. Forces causing the orientation of an anisotropic liquid. *Trans. Faraday Soc*. 1933, Vol. 29, No. 9, pp. 919-928.

22 Amoddeo A., Barberi R., Lombardo G. Nematic order and phase transition dynamics under intense electric fields. *Liquid Crystals*, 2013, Vol. 40, No. 6, pp. 799–809.

23 Agelmenev M.E., Muldakhmetov Z.M., Bratukhin S.M., Polikarpov V.V., Pak V.G. The electric field effect on the distribution of polar mesogenic molecules. *Chemistry Journal of Kazakhstan*, 2009, No.4, pp. 189-195 (Russian).

24 Agelmenev M.E., Muldakhmetov Z.M., Bratukhin S.M., Pak V.G., Polikarpov V.V., Yakovleva O.A. The Dynamics of Some Nematic Liquid Crystals. *Mol. Crys. Liq. Cryst.* , 2008, Vol. 494, pp. 339–352.

25 Agelmenev M.E., Bratukhin S.M., Muldakhmetov Z.M., Polikarpov V.V. Modeling of mesogenic system in the liquid aggregative state. *Russ.J. phys. chem*., 2010, Vol. 84, No. 7, pp. 1158–1162.

26 Agelmenev M.E. The modeling with free boundary. *Mol. Cryst. Liq. Cryst.*, 2011, Vol.545, No. 1, pp. 190-203.

27 Muldakhmetov Z.M, Agelmenev M.E. Sovetov E.S. Substituent effect on the mesomorphism acetylenic compounds. *Russian J. phys. chem*., 1999, Vol. 73. No. 11, pp. 1881-1882.

28 Agelmenev M. E., Bazhikov K.T., Muldakhmetov Z. M., Sizykh M.Yu. Effect of the Nature of Halogen on the Acetylene Compounds. *Russian journal of physical chemistry*, 2002, Vol. 76, No. 10, pp. 1713-1714.

29 Van der Spoel D., Lindahl E., Hess B., van Buuren A. R., Apol E., Meulenhoff P. J., Tieleman D. P., Sijbers A. L. T. M., Feenstra K. A., van Drunen R. and Berendsen H. J. C., *GROMACS User Manual version 3.3.1* , www.GROMACS.org

Article accepted for publication 05.09.2014