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THE INFLUENCE OF VARIOUS EFFECTS ON THE ORDERING OF LIQUID CRYSTALS LOCATED ON NANORIBBON GRAPHENE

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Experiments on computer simulations of the behavior of polar nematic phenylpropargyl ethers of parachlorophylenes on the surface of graphene made it possible to reveal a number of regularities. The dynamics of molecules under the action of an electric field and temperature was investigated. As a method of investigation, the molecular dynamics method was used in the approximation of the liquid aggregate state. The simulation was carried out in an atomistic approach. A small effect of graphene type on the behavior of nematic liquid crystals (NLC) is shown. It should be noted that the NLC is highly ordered in the case of coincidence of the field directions and the flow of the NLC. It is found that with increasing electric field strength the ordering of the cluster grows nonlinearly. And the greatest growth is observed in the field of enlightenment. This allows us to assert that the primary role of graphene and the electric field is the self-organization of the NLC in the region of an isotropic liquid..

***Keywords*:** nematicliquid crystals, graphene, computer modeling

Introduction

Graphene has a great interest due to its electrical and thermoelectric properties. This allows us to obtain new nanocomposite materials [1-9] and to improve the performance of electronic devices [10-15] with graphene. These studies on changes in the electronic states of metal ions [1-2], photoelectrochemical response [3], absorption processes [4], the nature of the interaction [5], electrical [6-7] and temperature conductivity [8], phase transition temperatures [9] show the crucial role of graphene. The high mobility of the current carriers makes its use attractive as an electrode [10-11] in various devices [12], such as solar cells [13-14], lithium battery [15]. It is clear that for an effective use of graphene in devices there is need of understanding of the processes occurring in composite materials with graphene at the temperature and other influences.

The physical and chemical properties of the components definitely have significant effect on it. The widely used in electronics the liquid crystals are one of these materials by Wahle et al. [16]. As noted Divariet al. in [17], the ratio between length and width of the graphene has large impact on these properties. The founded effect of the flow of nematic liquid crystals (NLC) in [18] on the graphene surface at the temperature change had been experimentally confirmed [19].

Therefore, the understanding of influence of graphene size and its type on the properties located on the surface of such electronic products as the NLC must be considered when creating optoelectronic devices based on these compounds. In this regard, the aim of this study was to research the influence of the size and type of graphene, the effects of temperature and electric field on the dynamics of nematic liquid crystals based on the arylpropargyl ethers of phenols.

1. The methodology of the analysis

As a sample the nematic liquid crystal - phenylpropargyl ether of p-chlorphenol (PEC) [20], located on the graphene in a planar orientation was used. For the modeling of the behavior of these compounds we used the method of molecular dynamics based on the program GROMACS [21] version 3.3.1 approaching liquid state [22-24].

In the modeling the NPT ensemble is used, the modeling time at a given temperature was 10 ps. The radius of the cutoff of the Coulomb interaction and the dispersion was 2 nm. The successive annealing was carried out in the heating mode.

The input file for cluster formation was created, which took into account the distance between the molecules, in rows and layers of the cluster in the direction of XYZ. The grapheme sizes were varied by direction (OX), perpendicular to the director (OY). At the same time the sizes of the cluster and other side of graphene (OY) were unchanged. The direction of the electric field was set on the direction of the director.

The studies were carried out in the presence of the electric field parallel to the director. The sizes of the grapheme that were used in the modeling varied, with a ration of width (X) to the length (Y) - 1:1 (115Å: 115Å, 2:1 (230Å: 116Å), 3:1 (345Å: 116Å), 3,5 1 (401Å: 116Å).

In the study of the influence of some parameters the number of molecules of PEC was unchanged and they were oriented planar respectively to the graphene's plane. The structure of the graphene was chosen in the form of zigzag (Z) and armchair (A) [25]. The method of preparing and analysis of modeling results is presented in [22, 26].

2. Results and discussion

3.1 The effect of the grapheme type on the dynamic behavior of the NLC

In the first part of the studies of the influence of the grapheme type on the behavior of nematic liquid crystals for different directions of the electric field vector of $1x10^7$V/ m (along the x, y, z) were carried out. The cluster size was 14x14x3 molecules, the ratio of width to length of the grapheme was close to 1:2 for armchair and zigzag structures (112Å: 235Å) with a length of 1.4210Å. The results of these studies are shown in Fig.1-3.

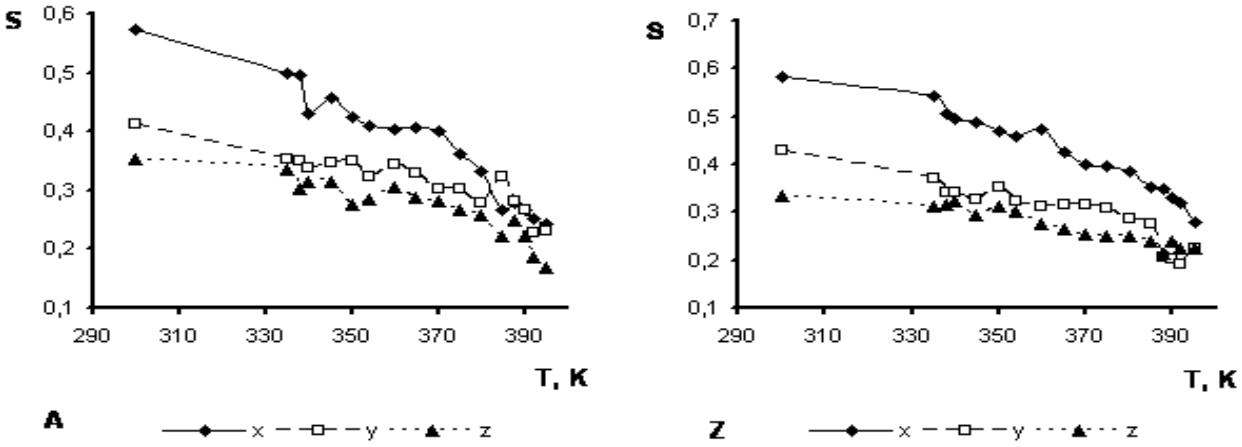


Fig.1. Temperature dependences of the degree of ordering of PEC at different orientations of the electric field (x, y, z) in case of graphene zigzag (Z) and armchair (A) structures

As seen in Figure 1, the type of graphene does not significantly affect to the nature of the curves S (T). In the area of disintegration of dimers (354-360K) [26] there is an excessive bend, after which there is a slight rise (Fig. 1). The higher values of the degree of ordering in the direction of X are largely due to the flow of the NLC in this direction.

The temperature dependences of information entropy (Fig. 2) are consistent with S (T) curves.

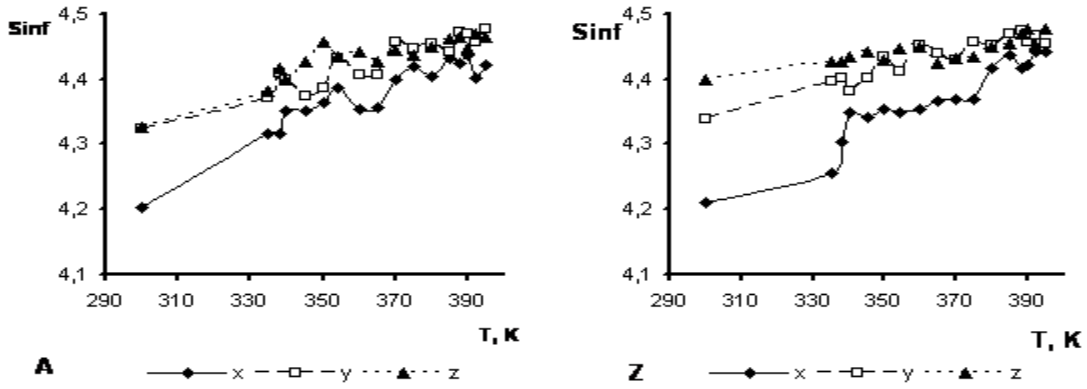


Fig.2. Temperature dependences of information entropy of the cluster with PEC at different orientations of the electric field in case of graphene zigzag (Z) and armchair (A) structures

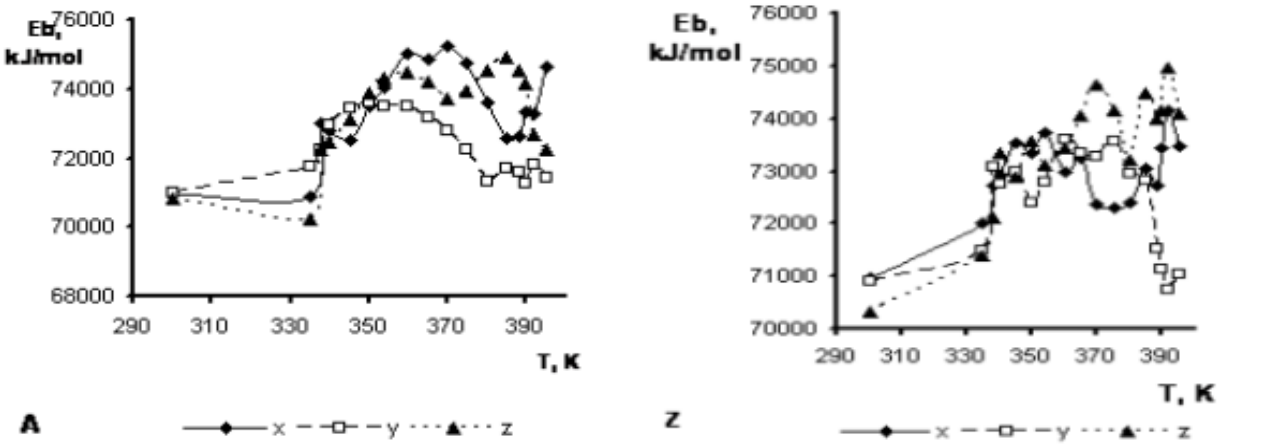


Fig.3. Temperature dependences of bond energy of the cluster with PEC at different orientations of the electric field in case of graphene zigzag (Z) and armchair (A) structures

As seen in Figure 3, there is some rise of bond energy in case of direction Z and X. The bond energy of the area of mesophase increases rapidly from the moment of melting. The minimum values of bond energy are observed at the orientation of the field along Y.

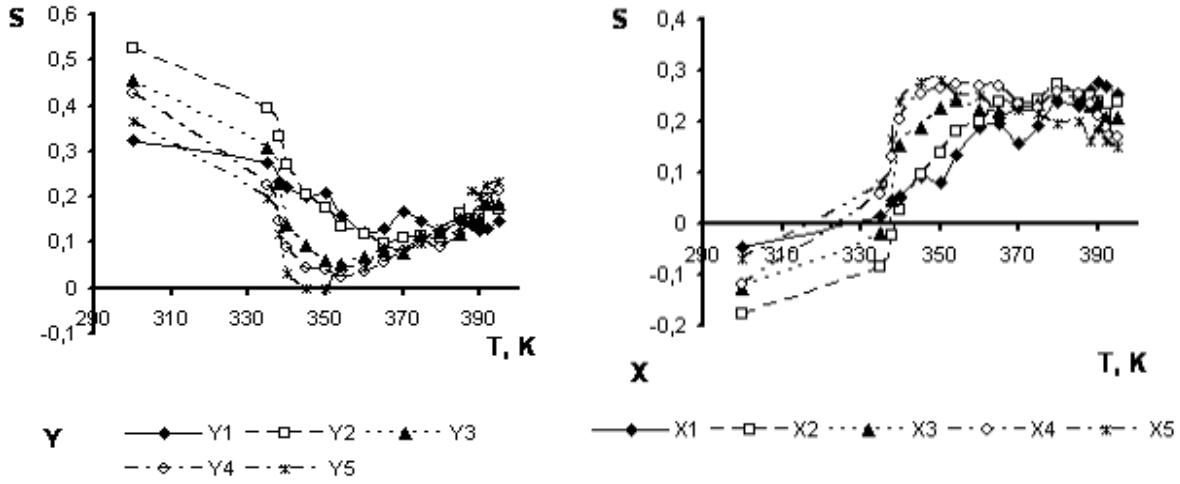
Thus, the small effect of the graphene type on the behavior of the NLC can be stated when the field direction coincides with the direction of flow the higher degree of order should be noted.

3.2 The effect of the electric field on the dynamics of the NLC

For this study the cluster of the NLC with size of 14x7x6 molecules with the ratio of width to length 3:1 (345Å: 116Å), and the direction of the electric field along the OY axis, coinciding with the direction of the director was used. The magnitude of the electric voltage had the following values: $1x10^7$V/ m (1), $2x10^7$ V/ m(2), $3x10^7$V/m(3), $4x10^7$V/ m (4), $5x10^7$ V / m (5). The graphene had the structure of armchair.

The research results are presented in Fig.4-12. As seen in Figure 4, the ordering in the Y direction after some decrease, which is until the temperature of decomposition of the dimers (354 K), further is increasing as the temperature begins to rise.

The nonlinear dependence on the magnitude of intensity occurs mainly in the area of decline, in the enlightenment area values are close to each other. The similar character of changes observed for the ordering in the direction of the X axis. The difference is that the decrease and growth of the Y axis corresponds to the growth and decay of X, respectively. One of the explanations may be a flow, at which the molecules begin to move along the X axis.



a) b)

Fig.4. Temperature dependences of ordering degree of the PEC along Y (a) and X (b) directions at different values of the electric field

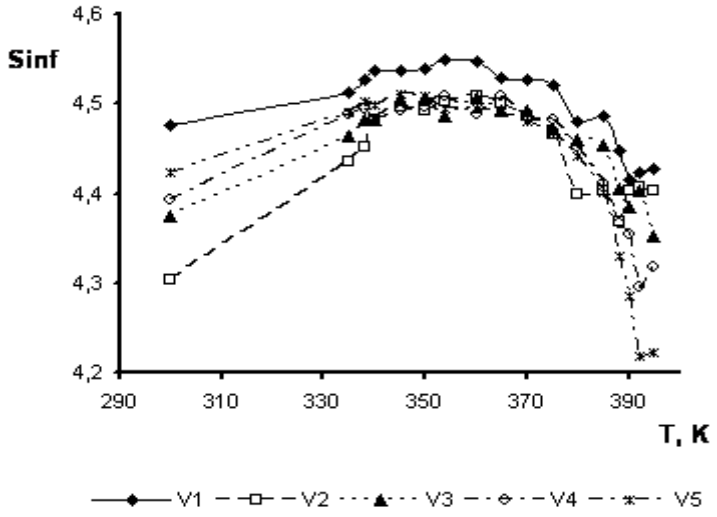


Fig.5. Temperature dependences of the information entropy of PEC at different values of electric field

The curves of the information entropy (Fig. 5) confirm this pattern. In this case it is clear that increasing the size of the fields' intensity leads to increase of ordering. For larger fields (V4, V5) the ordering in the area of enlightenment is considerably higher than the ordering in the initial state (300 K) and this trend is typical of other field values. This is may be due to both the orienting influence of graphene, and the effect of crystallization under normal substrates [27]. It should be noted that the difference in the values of entropy between the initial state and the area of enlightenment is much higher in this case as compared to [27]. It can be argued that this is due to the presence of the graphene as a substrate.

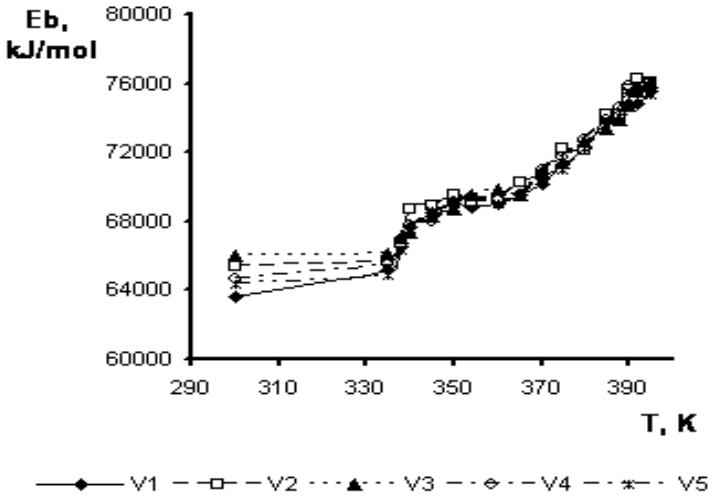


Fig.6. Temperature dependences of the bond energy of clusters' molecules at different values of the electric field

The bond energy for all values of intensity changes the same way, with a characteristic inflection in the area of disintegration of dimers (Fig. 6). The growth of the bond energy with increasing temperature indicates the predominance of processes of ordering over chaotic processes due to thermal motion. The similar values of the bond energy for all values of the field intensity, apparently, can be related to the determining role of the graphene. The free flowing of the molecules on the surface of graphene, and self-organization of polar molecules under the electric field contributes to this fact.

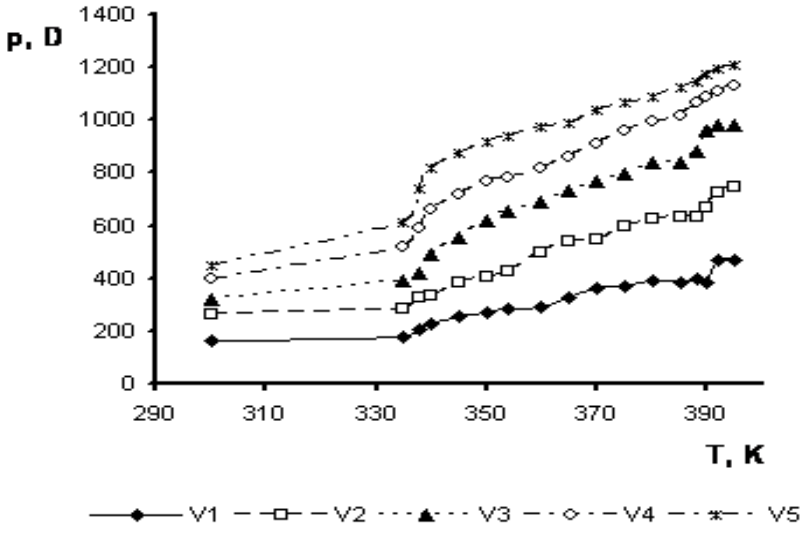


Fig.7. Temperature dependences of the total dipole moment of cluster's molecules at different values of the electric field

The discussed above the curves of temperature dependencesof the degree of ordering, the information entropy and the total dipole moment cluster also are comply with it (Fig. 7).

As seen in Figure 7, with increasing of field the total value of the dipole moment of the molecules in the cluster also increases. This behavior may be associated with sensitivity of the electric field to the influence of the PEC polar molecule and with the polarizability of the molecules with increasing of field intensity.

It is not difficult to see from Fig. 8-12 that increased intensity leads to the significant reversal of the cluster in the plane of graphene in the melting area (338 K). In the area of the mesophase (354 K) there is a noticeable movement of individual molecules on the surface of graphene. At the point of enlightenment (390 K) the molecules of cluster are distributed over its surface, flowing over the edge.

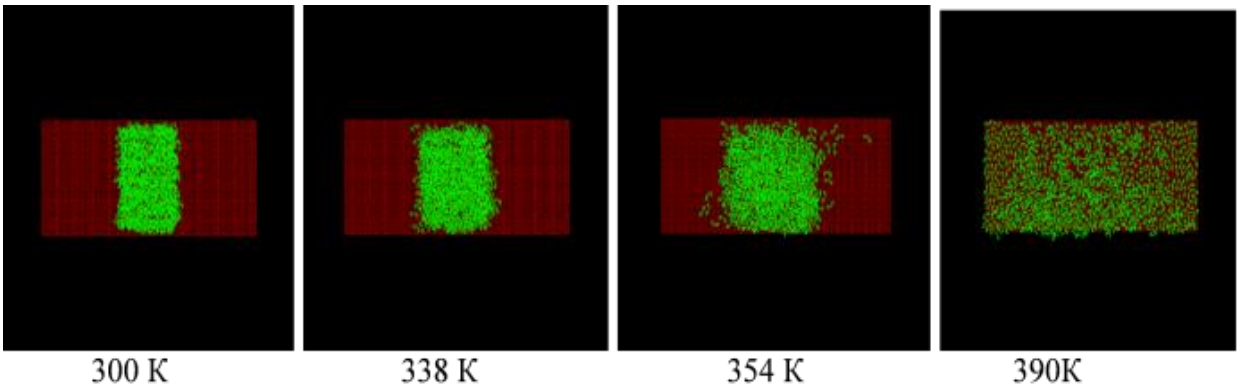


Fig.8. Cluster's view in the XOY plane at the value of electric field of $1x10^7$V/m

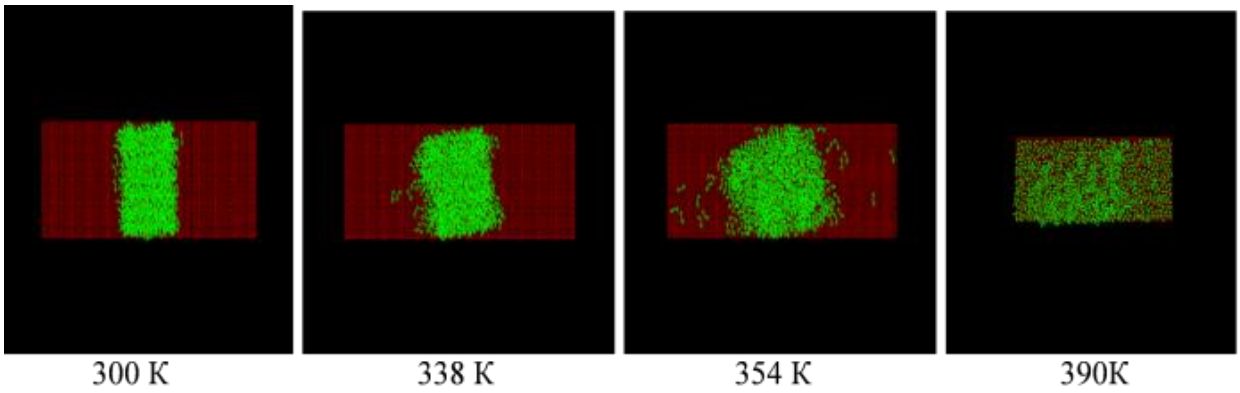


Fig.9. Cluster's view in the XOY plane at the value of electric field of $2x10^7$V/m

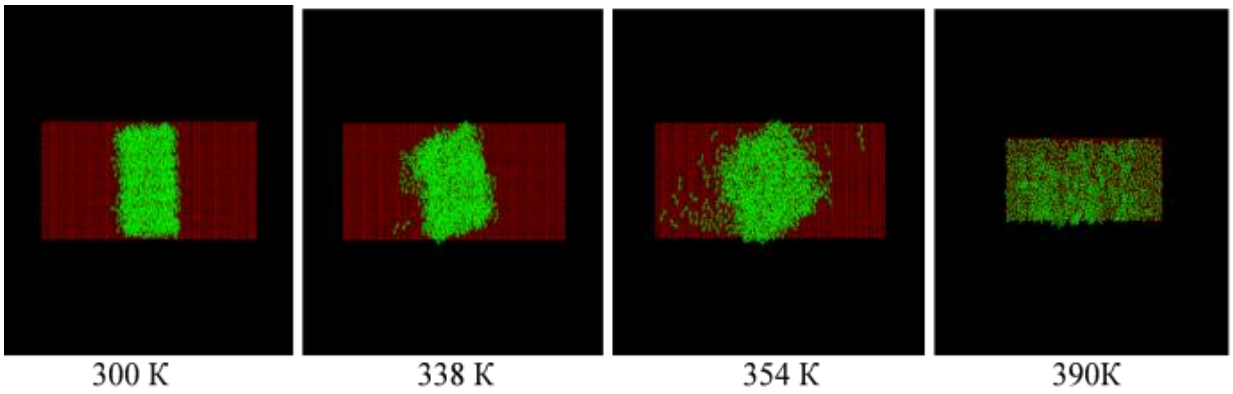


Fig.10. Cluster's view in the XOY plane at the value of electric field of $3x10^7$V/m

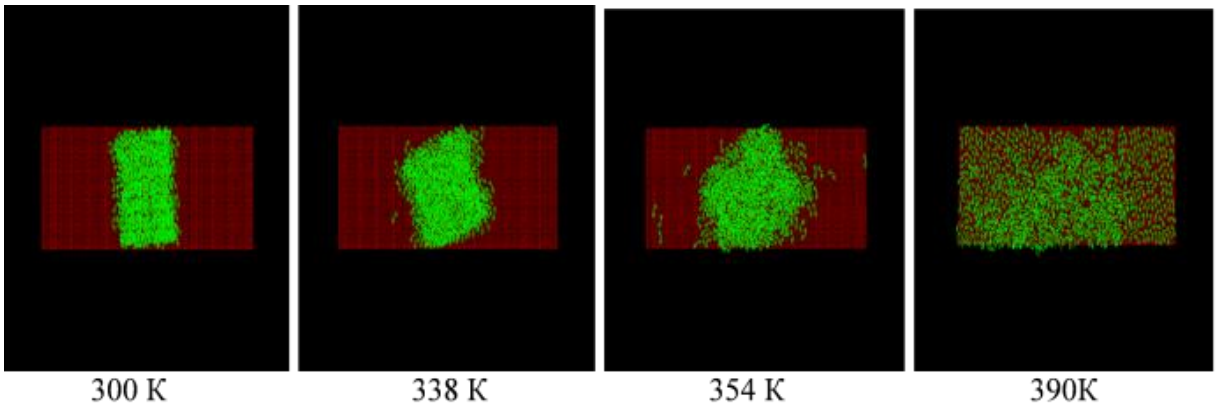


Fig.11. Cluster's view in the XOY plane at the value of electric field of $4x10^7$V/m

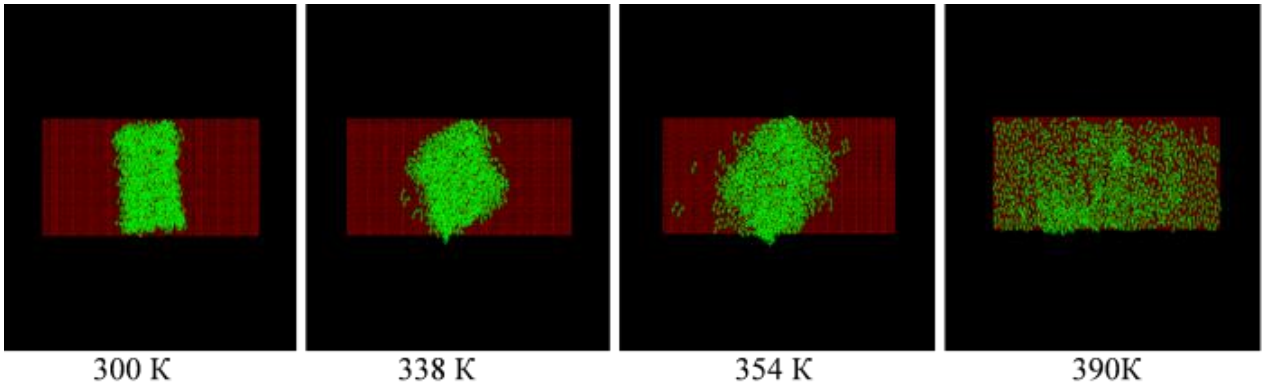


Fig.12. Cluster's view in the XOY plane at the value of electric field of $5x10^7$V/m

Thus, on the basis of the performed studies it was shown, that with increasing of the electric field intensity the ordering of clusters increases nonlinear. The greatest increase was in the area of enlightenment. Based on this fact it can be stated that graphene and electric field take a dominant role on the self-organization of the NLC in the area of the isotropic liquid.

Conclusion

The performed experiments on computer modeling of the behavior of the polar PEC, located on the surface of graphene, allowed identifying a number of laws. The little effect of the graphene type on the behavior of the NLC was shown. It was established that the ordering of nematic liquid crystals increase non-linear with increasing of the electric field. The determining role of graphene and the electric field on self-organization of the NLC in the enlightenment region was shown.

It was found that in the area of enlightenment the ordering of the NLC starts to grow when the value of the ratio of width to length is 3: 1. This allows stating that at least two processes are taking place under the influence of temperature and electric field: First - "flow" of the molecules in the direction of X, the second - the rotation of the molecule in the direction of this axis. The second process may be due to the reorientation relative to the electric field of the molecules.

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