DOI 10.31489/2022No3/18-22

UDC: 532.783; 541.1; 539.21; 535.37

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

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Experiments on computer simulation of the behavior of polar nematic phenylpropargyl ethers of parachlorophyllens on the surface of graphene nanoribbon made it possible to reveal a number of regularities. The dynamics of molecules is studied when the dimensions of graphene change under the action of an electric field and temperature. As a research method, the method of molecular dynamics was used in the approximation of a liquid state of aggregation. The simulation was carried out in the atomistic approach. It was shown that the graphene nanoribbon and electric filed defines the self-assembly of the nematic liquid crystals molecules in the biaxial state. These states appear at the variation of the graphene nanoribbon ratio of width to length. It was found that in the clearing area the ordering of the parachlorophyllens starts to grow when the value of the ratio of width to length is 3: 1.

Keywords: nematic liquid crystals, graphene nanoribbon, computer modeling

Introduction

Graphene has a great interest due to its electrical and thermoelectric properties. Research on changes in the electronic states of metal ions [1-2], photo-electro-chemical 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 performed experiments [10] on computer modeling of the behavior of the polar parachlorophyllens (PEC), located on the surface of graphene nanoribbon (GNR), 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 nanoribbon graphene and the electric field on self-organization of the NLC in the enlightenment region was shown. This allows stating that at least two processes are taking place under the influence of temperature and electric field: the 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.

It is clear that for an effective use of nanoribbon graphene in devices there is need of understanding of the processes occurring in composite materials with nanoribbon 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. [11]. As noted Divari et al. in [12], 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) by we in [13] on the graphene surface at the temperature change had been experimentally confirmed [14]. Therefore, the understanding of influence of nanoribbon graphene size 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 purpose of this work was to study the effect of nanoribbon graphene size on the dynamics of behavior molecules of nematic arylpropargyl esters of phenols with temperature and electric field changes.

1. The methodology of the analysis

As a sample the nematic liquid crystal - phenylpropargyl ether of PEC [15], located on the nanoribbon 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 [16] version 3.3.1 approaching liquid state [17-19]. In the modeling the NPT ensemble is used, the modeling time at a given temperature was 10 ps. The Coulomb and van der Waals interactions were used in the modeling of the dynamic dynamics method. The corresponding parameters for these options are specified in [16]. 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 graphene sizes 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) [18]. The method of preparing and analysis of modeling results is presented in [15, 19].

2. Results and discussion. Effect of the GNR`s size on the dynamic behavior of the NLC

In this study the GNR`s size that was used in the modeling varied by the ratio of width to length - 1:1 (1), 2-1 (2), 3-1 (3), 3.5:1 (4), but the number of the PEC molecules were kept same. The electrical intensity value was $1x10^7$ V / m, and it was directed by Y (Director). The research results are presented in Fig.1-7. The numbers are consistent with given ratios of width to length of the GNR and used in the figures.

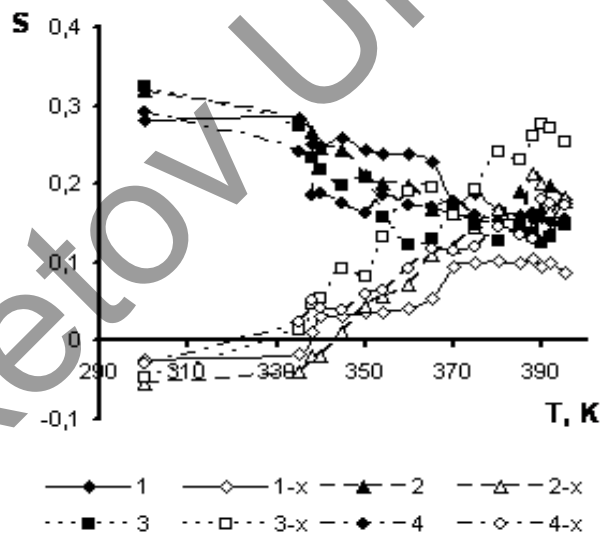

Fig.1. Temperature dependences of the ordering degree of the PEC at different GNR`s sizes (1, 2, 3, 4) and coordinates (x, y)

As seen in Fig. 1, the difference in the ordering degree values in two coordinate axes is observed before the temperature of decay of the dimers as in the previous section. The ordering degree values relative to the axes X and Y are changing in opposite direction with increase of temperature: along X increases, along Y reduces. In case 1 this value is higher in the clearing area than the value relative to the X-axis. In cases 2 and 4 the ordering degree values with respect to X and Y are equal. In case 3, there is a matching value at the decomposition temperature of dimers (354 K). The ordering degree along X exceeds this value with respect to Y with further increase in temperature; only at the temperature of 370 K they become equal. Biaxial state develops in varying ordering degrees in the OX and OY axis at melting temperature.

As seen in Figure 2, for case 3 the highest increase in the ordering at the clearing area is typical, less in case 2. This is the exact ratio, which significantly changes the electrical properties of the GNR [12]. The curves of the temperature dependences of the bond energy for all cases (Fig. 3) show the increase of its value with the increase of a temperature. The most rapid growth occurs in case 3. The smaller increase is observed in cases 2 and 4. This is consistent with the considered temperature dependences of the ordering degree and information entropy.

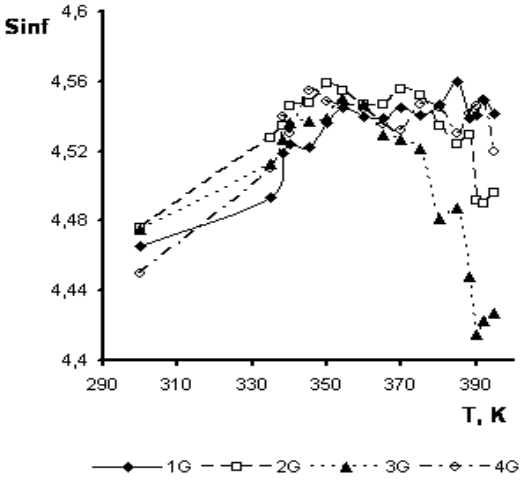

Fig.2. Temperature dependences of the information entropy for different GNR`s sizes (1, 2, 3, 4).

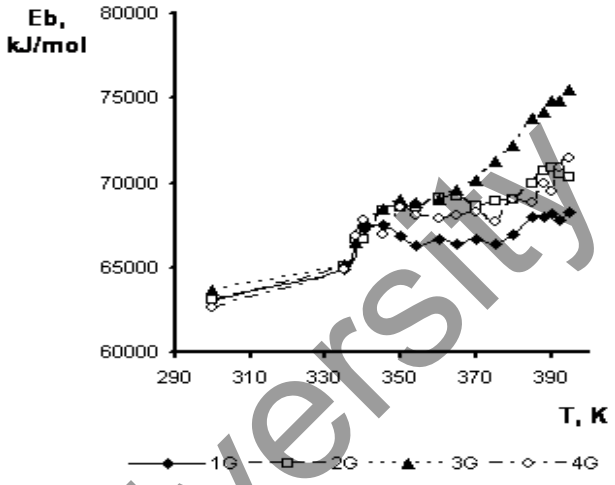

Fig.3 Temperature dependences of the bond energy for different GNR`s sizes (1, 2, 3, 4)

As shown on snapshots of clusters in various phase states (Fig. 4-7), the thickness of clearing becomes smaller with increasing ratio of width to length of the GNR. This is obviously due to the flow of the PEC molecules with increasing of temperature and surface of the GNR area.

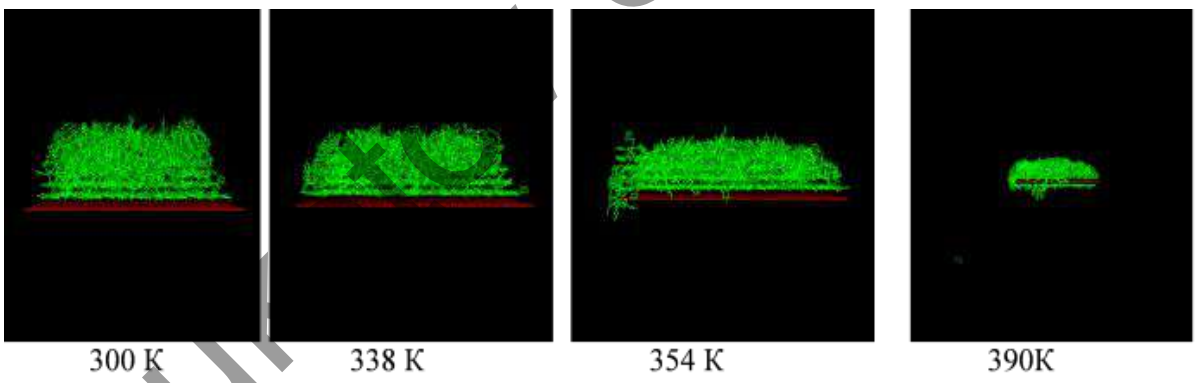

Fig.4. Snapshots of clusters in XOZ plane at the ratio of width to length (1)

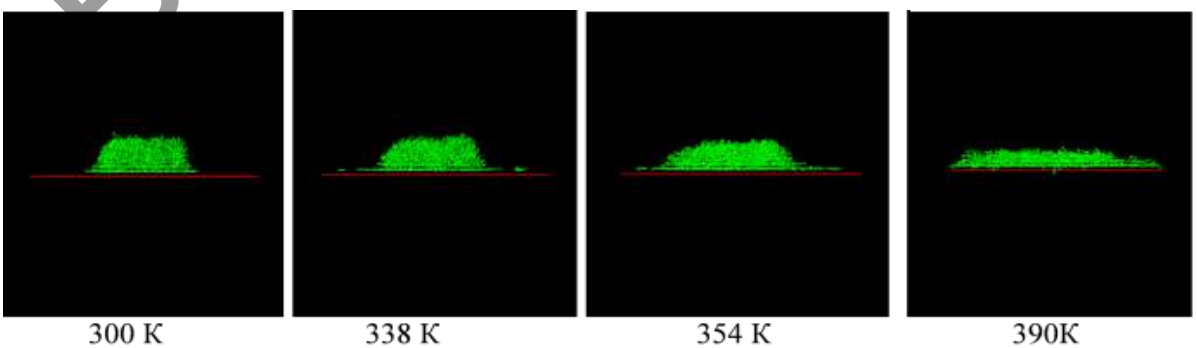

Fig.5. Snapshots of clusters in XOZ plane at the ratio of width to length (2)

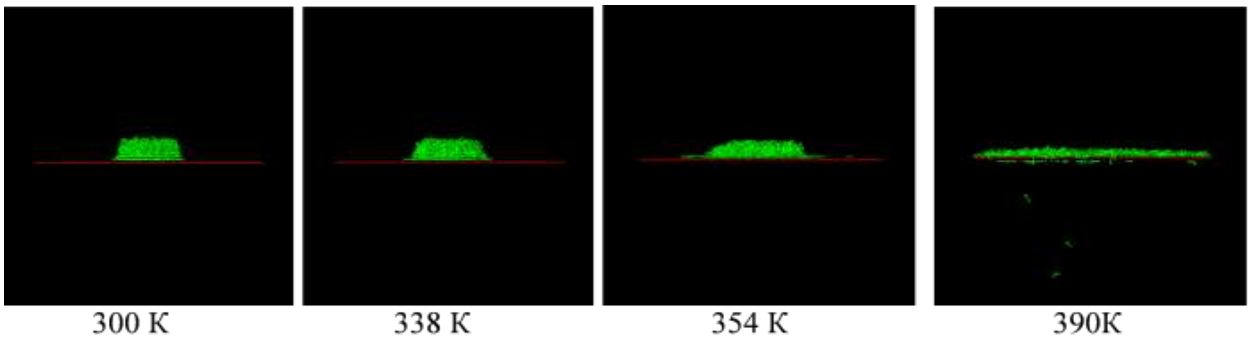

Fig.6. Snapshots of clusters in XOZ plane at the ratio of width to length (3)

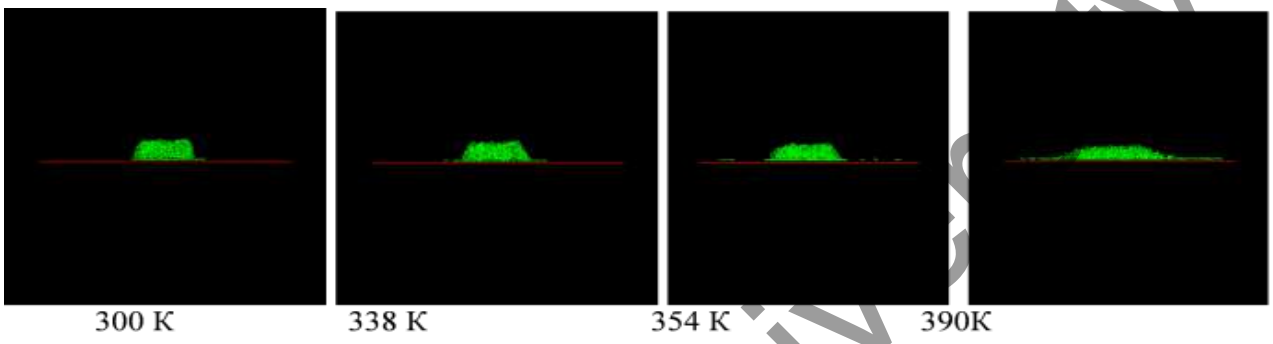

Fig.7. Snapshots of clusters in XOZ plane at the ratio of width to length (4)

Taking into account that the main flow X direction is perpendicular to the initial of molecules Y location the existence of 2 processes in clusters can be assumed. These processes occur simultaneously with increasing of temperature, which are most agreed from the moment of the dimer disintegration (354 K).

The first process is “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, since the PEC dipole moment [15] has an angle of 50^0 relative to the longitudinal axis of the molecule in its initial state. The ratio of width to length as 3:1 should lead to the maximum universal conductivity of the GNR near the Dirac [13] point and at the ratio of 1:3 leads to the minimum value. However, the molecular dynamics method does not account quantum properties of the GNR. However, the carried out studies allow us to state that the nematic liquid crystals dynamics depends on the size of the GNR. The ratio of width to length of 3:1 leads to noticeable changes in the ordering in the clearing area.

Thus, on the basis of these studies it was found that the value of the ratio of width to length of 3 / 1 the ordering of the NLC begins to rise in the clearing area. This may be due to the possibility of a larger movement of molecules on the front surface, also due to the distribution of electron density of the GNR atoms.

Conclusion

It’s identified a some of dependences by the performed computer modeling experiments on the polar PEC behavior located on the GNR surface. It was shown that the GNR and electric filed [10] defines the self-assembly of the NLC molecules in the biaxial state. These states appear at the variation of the GNR ratio of width to length. It was found that in the clearing area the ordering of the NLC starts to grow when the value of the ratio of width to length is 3: 1.

This helps to state that at least two processes are taking place under the influence of temperature and electric field: first one is the "flow" of the molecules in the direction of X, and the second one is the molecule rotation in the direction of this axis. The second process may be due to the molecule reorientation relative to the electric field. An isotropic phase and nematic phase coexist when NLC is on the prepared exfoliated graphene oxide platelets [20]. This is consistent with our results. Formation of this composite requires controlling of the GNS size.

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Article accepted for publication 15.06.2022