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SOME FEATURES OF THE BEHAVIOR OF LIQUID CRYSTALS IN NANOSYSTEMSAgelmenev M.E.¹, Bratukhin S.M.², Polikarpov V.V.², Bektasova G.S.¹, Sadenova M.A.¹,
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In this work the results of research of the effect of nanosystems of different configurations on the behavior of liquid crystals at the temperature effect is presented. It was found that in case of T-shaped arrangement of nanotubes here is a stabilization of the LC molecules on the surface of the tube at the effect of temperature. It was shown that in other configurations, there is a movement of the LC molecules on the surface of nanosystems. The specific features of the dynamics of the flow of molecules depending on the structure of systems were established. These results show the importance of the nanotube orientation controlling in a matrix liquid crystals. Such influence nanocomposite topology represents a new technological method.

Keywords: nanotubes, graphene, liquid crystals, molecular dynamics.

Introduction

Carbon nano materials – nanotubes and graphenes – have the unique properties and wide area of possible applications [1-4]. One of the applications of these nano materials is a creation of new nano composite materials using them. Single-walled carbon nanotubes (SWNTs) possess a wide range of biological applications from the biomedical sensors to drug delivery. This leads to investigation of the interactions between biological molecules and carbon nanotubes [5-14]. A polymer chain changes from three-dimensional (3D) direction to two-dimensional direction of polymers adsorbed on surfaces have received much more attentions [15-22]. The understanding of the nature of interactions between the surface of nano compounds and different materials – metals, ion liquids, organic compounds, allows modify their properties of self-diffusion [23-25], electrical resistance [26], absorption [27-30], ionic stacking and distributing [31-33]. The existence of different configurations of nanotubes has been experimentally [2] and theoretically [34-37] determined. They are more thermally and mechanically stable [38-41], the absorption of hydrogen of nanofluid tubes [43] is higher than in corresponding straight CNT [44-55]. The combinations of graphenes and nanotubes are also being used in the process of creation of new electrical materials. It is embodied in today's researches. Liquid crystals in such kind of systems are able to increase their practical relevance.

It is not a coincidence that in the research of such systems the significant influence of nanostructures on the properties of liquid crystals, such as electro-physical properties [56-57], switching speeds [58-59], electro-optic memory [60], space distribution [61-63] are observed.

The existence of liquid-crystalline properties in nanotubes themselves were mentioned in [64] and were considered two approaches:

- 1) liquid crystalline behavior of carbon nanotubes in solution, and
- 2) inclusion of CNTs in lyotropic or thermotropic LCs. The research of composite matters with the participation of nematic liquid crystals (LC) and carbon nano-plates – graphenes – made it possible to determine the fact that flowing of molecules on bases is connected with the rise of temperature [65].

The issues of fluid transport (flow) in carbon nanotubes are being studied very intensively [66]. Furthermore, a great amount of works is devoted to water flow [67-71]. It has been determined [67] that the effects of carbon surface curvature on the behavior of water molecules near the CNT surface are negligible in tubes with diameters larger than 10 nm. The water molecules form two oppositely polarized chains [68-69]. The density of water close to the nanotube walls is lower compared to the density in the center of the nanotube [70]. The results of [71] show the presence of a thin, interfacial water layer whose microscopic structure and thickness are independent of the distance between confining layers of single-wall carbon nanotubes and graphene sheets.

It is clear that flow pattern of liquid crystals on surface, which is a combination of one-wall nanotube and nano-plates, will have more complex dynamics than water flow. The binding of nano structures can have different combinations that must be considered when creating on their basis the nano-composite materials. Therefore, it is important to understand the influence of the geometry, relief on the properties of these compounds. In this regard, the aim of this study was to find the influence of the configurations of combination of various nano structures on the dynamics of the LC at the effect of temperature in the presence of an external electric field.

Two simplifications were used in this work. The atoms on nanostructures were frozen which is allowed considering them as carrying bases for nematic liquid crystals. Reference [72] shows that the amount of H₂ adsorption is strongly influenced by the applied temperature, and that the adsorption energy is higher for nanotubes with smaller diameters. The adsorption of hydrogen on carbon nanotubes as a function of temperature, in all cases SWCNTs undergo deformations in the presence of adsorbed hydrogen and these deformations increase with increasing temperature. Because of this reason in order to minimize the process of absorption in this work we used nanotubes with long radiuses.

1. Model and computational details

As the object of the study one-component, single-layer clusters, that has the LC of phenyl propargyl ether of p-chlorophenol (PEC) [73], located on the carbon nanotube or graphene, which is neighboring to other nanotube («g-t» - LC molecules that in the initial state are located on graphene, «t-g» - LC molecules that in the initial state are located on the nano tube, «t-t» - T-shaped arrangement of two nanotubes) were selected.

For modeling of the behavior of these compounds the method of molecular dynamics based on the program GROMACS [74] version 3.3.1 in the approximation of liquid state [75-77] was used. In the modeling NPT ensemble was used, the modeling time at the given temperature was 10 ps. The radii of the cut off of the Coulomb interaction and the dispersion were 2 nm. The successive annealing was carried out in the heating mode.

The structure of graphene and nanotubes was chosen as a zigzag (Z) [2, 4]. The method of preparation and analysis of modeling results is presented in [75, 78]. The input files, defining the geometry and force field of these compounds was created.

The length of the nanotubes was 230.202 Å, radius - 18 Å. The width of the graphene was equal to 113,083 Å, and length - 230.202 Å. The gross formula of nanotubes and graphene was C₁₀₀₄₄H₃₀₈, distance of C-C is equal to 1.421 Å. The number of molecules of the LC: 2618. The distances between the planes (OZ) was 0.4 nm, OY - 1.6 nm, OX - 0.7 nm. The direction of the electric field vector is overlapped with the normal to the plane in which there is a layer of the LC molecules.

2. Results and discussion

As seen in Figure 1, the character of curves variation of temperature dependences of the degree of ordering for all studied cases is complex. It should be noted that, despite this, the ordering does not fall to zero in the studied temperature range.

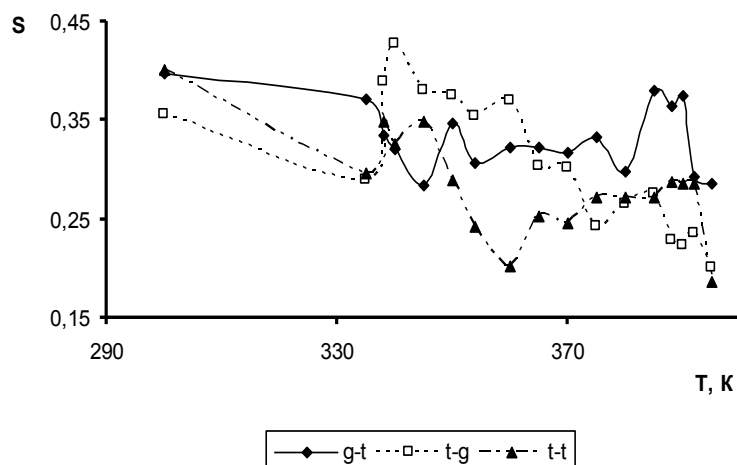


Fig.1. Temperature dependences of the degree of ordering of the LC

At the same time, the curves of the temperature dependences of information entropy (e.g. Figure 2) show that the ordering is higher in case of g-t, where the initial cluster is located on graphene. This is due to the fact that the bond energy between the molecules in this case has the highest value (e.g. Figure 3).

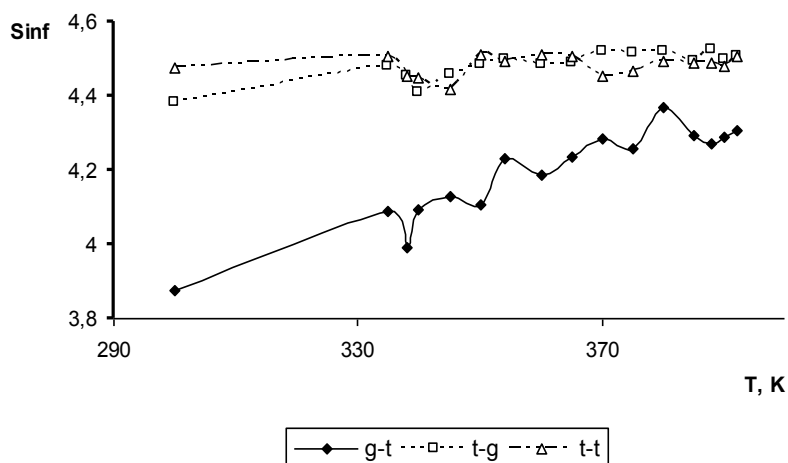


Fig.2. Temperature dependences of the information entropy of the LC

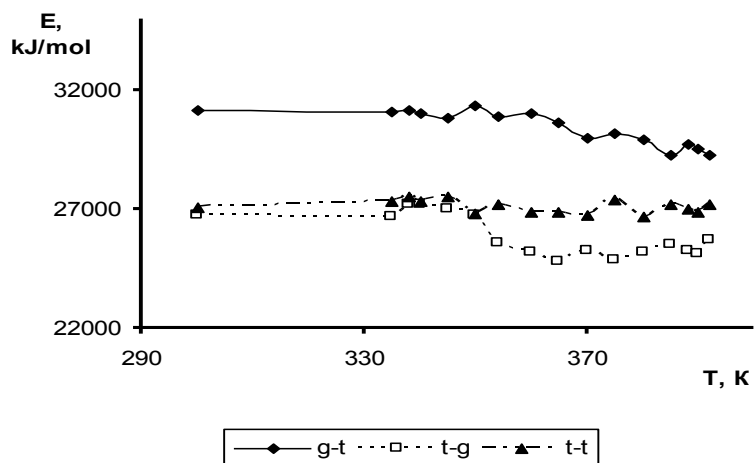


Fig.3. Temperature dependences of the bond energy of the LC

Apparently, the flowing of the initial cluster with the LC along the plane contributes to better maintenance of ordering and to more intense intermolecular interaction. The lowest bond energy is observed in case of t-g, when the original cluster is located on the nanotube. Moreover, the difference of the bond energy in case of t-t and t-g case starts from the temperature of decomposition of the dimers [79]. This non-obvious difference becomes clearer at the studying of clusters' snapshots. All paragraphs must be indented. All paragraphs must be justified alignment. With justified alignment, both sides of the paragraph are straight.

As can be seen from the snapshots of clusters at different temperatures (e.g. Figure 4-7), there is no molecules flow in the t-t system. In two other cases there is a flow of molecules to the empty nano structure.

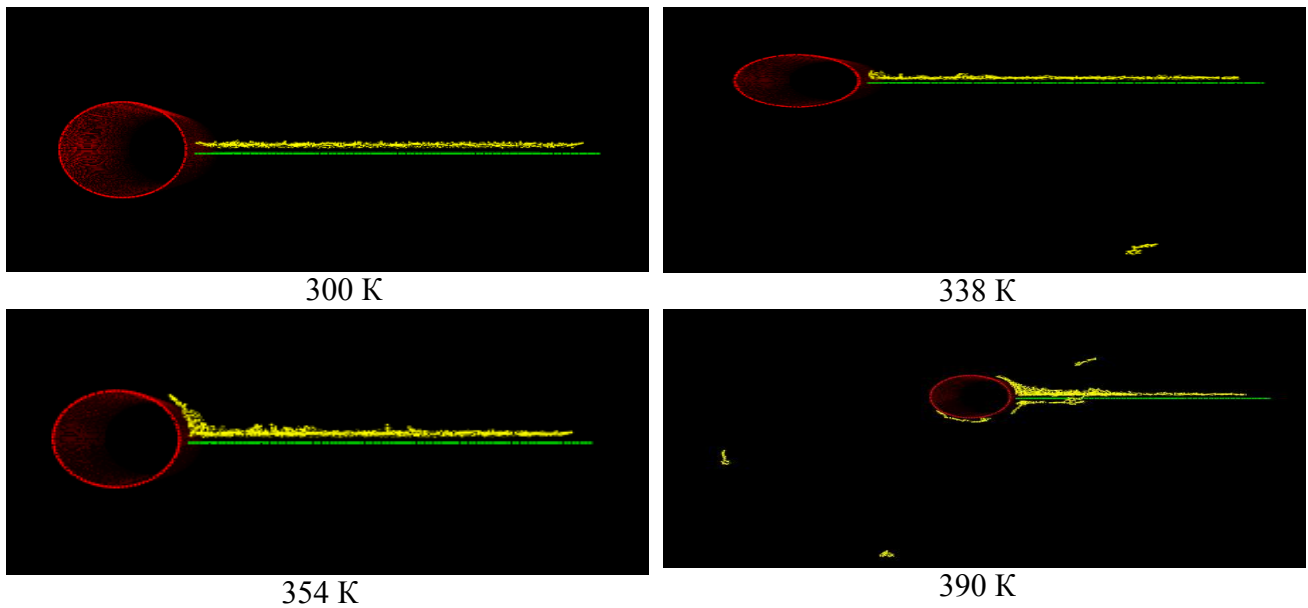


Fig.4. Snapshots of the g-t nanosystem with PEC in the XOZ plane in the crystalline state, melting, mesophase and enlightenment

As seen in Figure 5, in the mesophase (354K) there is a noticeable flowing of the molecules on both sides of the graphene.

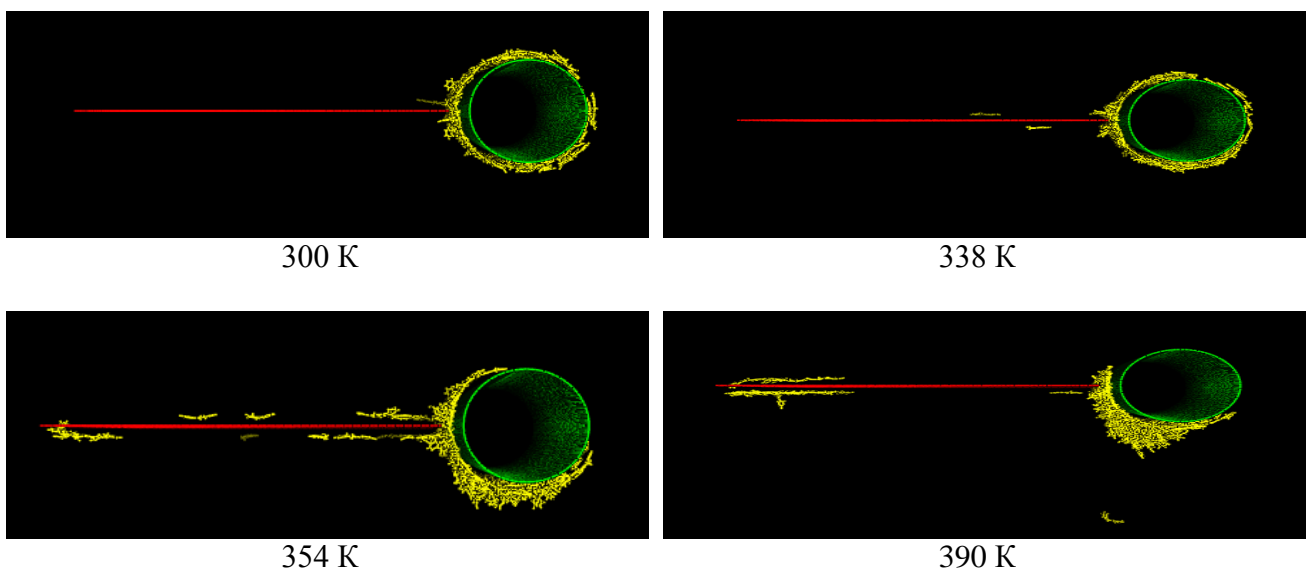


Fig.5. Snapshots of the t-g nanosystem with PEC in the XOZ plane in the crystalline state, melting, mesophase and enlightenment

In the region of enlightenment (390 K) molecules are concentrated at the edge of graphene and nanotubes. At the same time on the nanotube, they accumulate on the border area. The conducted additional experiments showed that flow continue when the nanotubes are arranged parallel relative to each other (e.g. Figure 7). In case of g-t the molecules flow on the nanotube surface, accumulating in the main border area of graphene and nanotubes. The more noticeable movement of the molecules occurs in case when the initial cluster is located on the nanotube t-g. As for the t-t case, it is necessary to emphasize the stability of arrangement of the molecules under the influence of temperature (e.g. Figure 6). This is can be seen clearly on the snapshots which are taken in different projections (e.g. Figure 7).

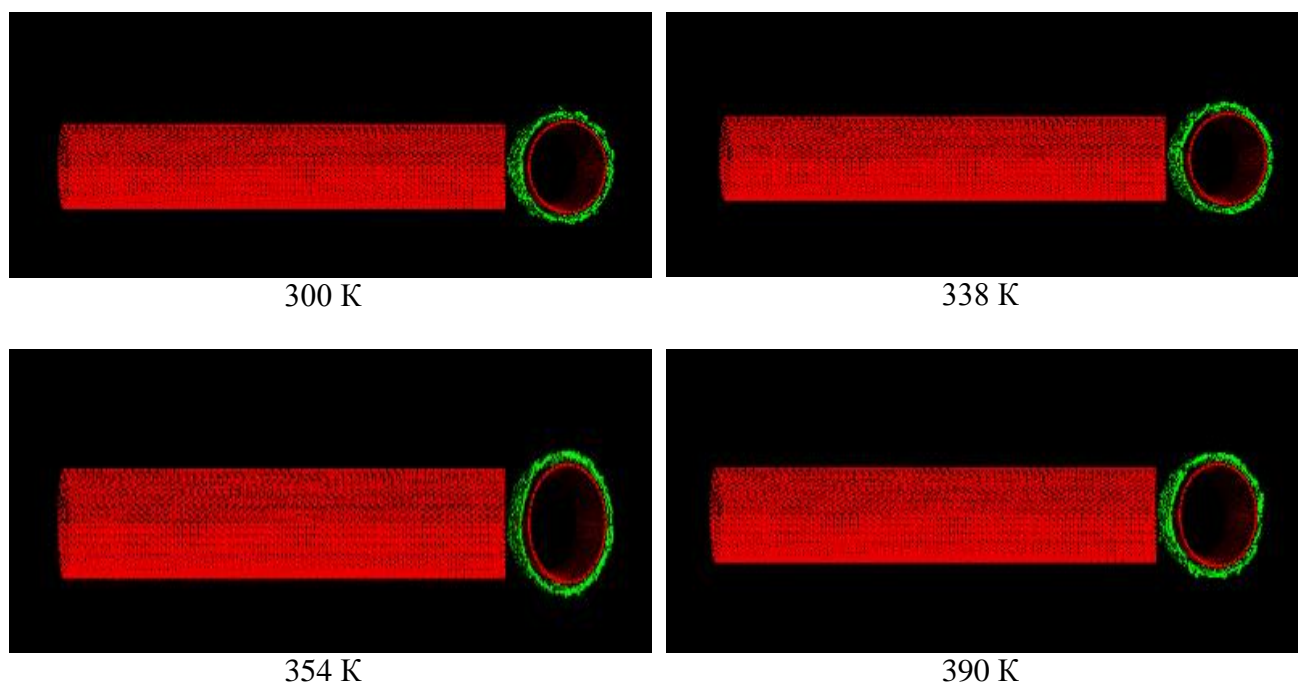


Fig.6. Snapshots of thet-tnanosystem with PEC in the XOZ plane in the crystalline state, melting, mesophase and enlightenment

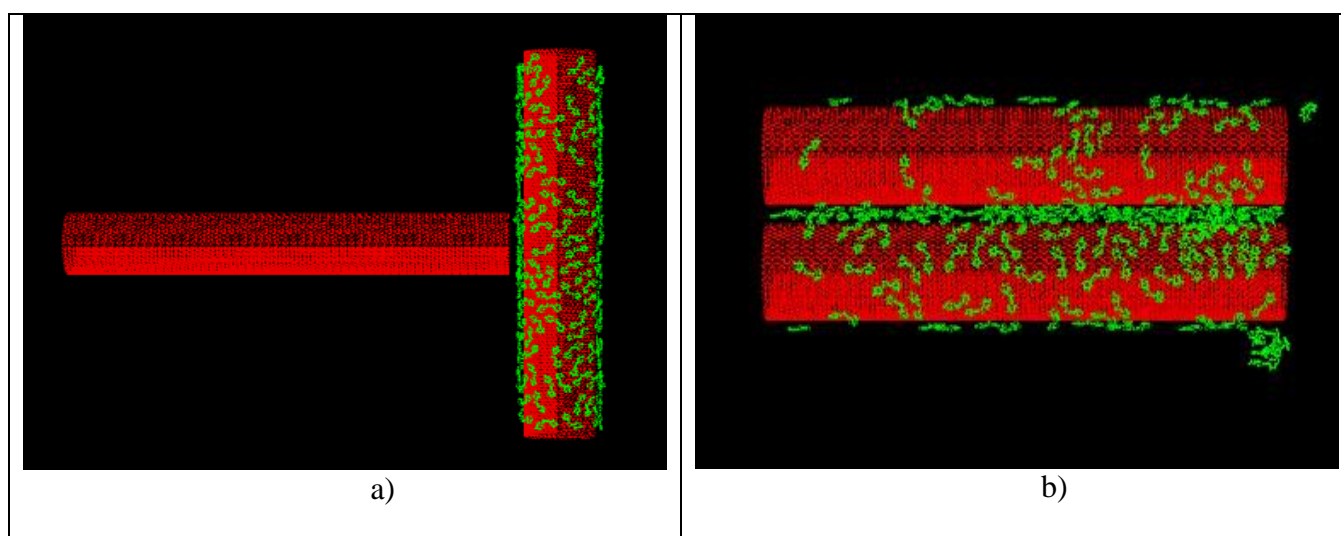


Fig.7. Snapshots of thet-t nanosystem with PEC in the XOY plane at the enlightenment:
a - t-t (390K); b - Parallel nanotubes (390K)

The additional research of 3 layers LC-clusters in case of t-t show the absence of flow of the molecules. Therefore it can be stated that the determining factor in the stabilization of the molecules is T-shaped arrangement of the nanotubes.

Conclusion

Thus, these studies have discovered that as a result of thermal annealing in the initial configuration - graphene + (LC)-nanotube and nanotube + (LC)-graphene—flowing of the LC molecules on the appropriate empty nanostructure is observed. In that case in the state of enlightenment the LC molecules are located on the both side of the graphene and nanotube, they are located on the neighboringside of graphene. It was found that in case of T-shaped arrangement of nanotubes there is a stabilization of the LC molecules on the surface of the initial tube and there is no ‘uncovering’ of any part of it. The analysis of the temperature dependences of the degree of ordering, information entropy, bond energy shows in general a better ordering in the system of graphene + (LC)-nanotube compare with the other two cases.

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