

Computer simulation of the process of absorption of electromagnetic field by liquid crystal systems

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Abstract. The behavior of LC systems in alternating external fields is investigated; hysteresis curves are calculated. The dependencies of the area of the hysteresis curves on the frequency of the external field, at various values of temperature, amplitude of external field and of intermolecular interactions constants are discussed. The position of maximum and the peak height depending on the temperature and the of interactions constants are investigated.

1. Inrtoduction

Liquid crystal (LC) materials are of high potential for use in modern chemical and medical industry, instrument-making and machine-building. Therefore, currently they synthesize new low molecular LC and intensively research their properties by various theoretical and experimental methods. Besides, polymer systems are synthesized, which successfully combine unique properties of both low-molecular liquid crystals, and high molecular compounds with their ability to form films, fibers and coatings. Such polymers include a wide range of homologues of poly-n-acrylates, poly-n-acryl methacrylates, simple and complex poly-n-acryl-vinyl esters, poly-n-alkyl-styrenes, etc.[1-5].

The main features of physical characteristics of low molecular and polymer LC are associated primarily with geometrical anisotropy of structural units (molecules, fragments of polymeric chains, etc.) of these systems, as well as with the values of intra- and intermolecular orientational interactions. Therefore taking into account similar molecular structure of such systems, the processes occurring in them can be investigated via similar models and methods.

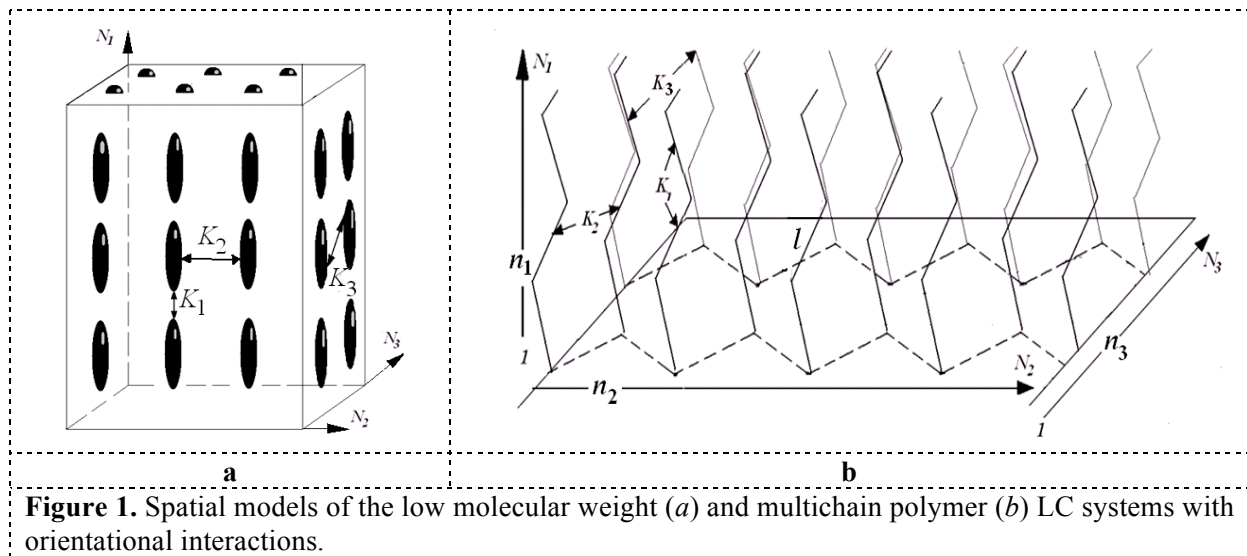
Under the influence of electric fields physico-chemical properties of LC systems change [6], such as color, transparency and the ability to rotate the plane of polarization of the transmitted light. This, in turn, determines the wide range of applications of LC materials in optoelectronics and optical information processing systems, laser physics, medicine, thermography, etc. [7, 8].

The aim of this research is the theoretical study of the absorption of external alternating electric field by ordered low molecular weight and polymer LC systems within a unified model via the Monte Carlo method. For this, we calculated the dependencies of the areas of hysteresis curves on the frequency of the external field at different values of temperature and constants of the model.



2. Model

To describe the LC the lattice model is used, a single one for low molecular weight (Figure 1a) and polymer (Figure 1b) systems. Each lattice node $\vec{r} = (n_1, n_2, n_3)$ has anisotropic elongated particle - rotator having rotational (orientational) degrees of freedom. Orientation of the rotator in a spherical coordinate system is defined by the angles θ_{n_1, n_2, n_3} and ϕ_{n_1, n_2, n_3} . In this model, it is assumed that the potential of orientational interactions $U_{\vec{r}, \vec{m}}$ between rotators located in the lattice nodes \vec{n} and \vec{m} depends only on their mutual orientation, i.e. the spatial angle $\Phi_{\vec{n}, \vec{m}}$ between their axes.



Quadrupole interaction energy of two nonpolar particles not possessing the electric dipole moment decreases with the increase of distance R proportionality $1/R^5$, while the energy of interaction of dipole moments, set due to their mutual polarizability, changes depending on the distance in proportion $1/R^8$. Therefore, the quadrupole interaction is dominant. To describe the orientational interactions between non-polar molecules capable of forming typical liquid crystal structures they usually apply quadrupole potential of interaction [9].

Therefore, in this study it is assumed, that potential energy of interaction of rotators with external electric field has the form:

$$U = - \sum_{n_1, n_2, n_3} K_1 \cos^2(\Phi_{n_1, n_2, n_3, n_1+1, n_2, n_3}) - \sum_{n_1, n_2, n_3} K_2 \cos^2(\Phi_{n_1, n_2, n_3, n_1, n_2+1, n_3}) - \sum_{l, j, k} K_2 \cos^2(\Phi_{n_1, n_2, n_3, n_1, n_2, n_3+1}) - f q E \sum_{n_1, n_2, n_3} \cos^2(\varphi_{n_1, n_2, n_3}) \quad (1)$$

where $\Phi_{n_1, n_2, n_3, n'_1, n'_2, n'_3}$ is the angle between the rotators located in the nodes n_1, n_2, n_3 and n'_1, n'_2, n'_3 of the lattice, q is the module of the quadrupole moment of the rotator, E is intensity of the external electric field, φ_{n_1, n_2, n_3} is the angle between the direction of orientation of the rotator and the vector of field intensity, f is coefficient of proportionality.

Energy constants characterize different types of interactions, depending on the considered chemical compound. For low molecular weight systems the constants K_i can be estimated by the multipole expansion of the interaction energy of two identical quadrupoles. For polymers energy constant K_1 along the longitudinal curved direction n_1 of the lattice describes intrachain orientational interactions

and is associated with the chain bending rigidity, which determines the elastic properties of the individual chain. Its value can be estimated from the relation $K_1 = A \cdot k_B T / 4$, where A is Kuhn segment length (in numbers of rotators), T is temperature. The constants K_2 and K_3 characterize the orientational interactions between adjacent rotators (links) in different chains, in “transverse” directions of the lattice.

As a long-range quadrupole order parameter the Tsvetkov’s factor is used:

$$S = \frac{3\langle \cos^2 \theta \rangle}{2} - \frac{1}{2} . \quad (2)$$

where θ is the angle of orientation of the rotator relative to the preferred direction.

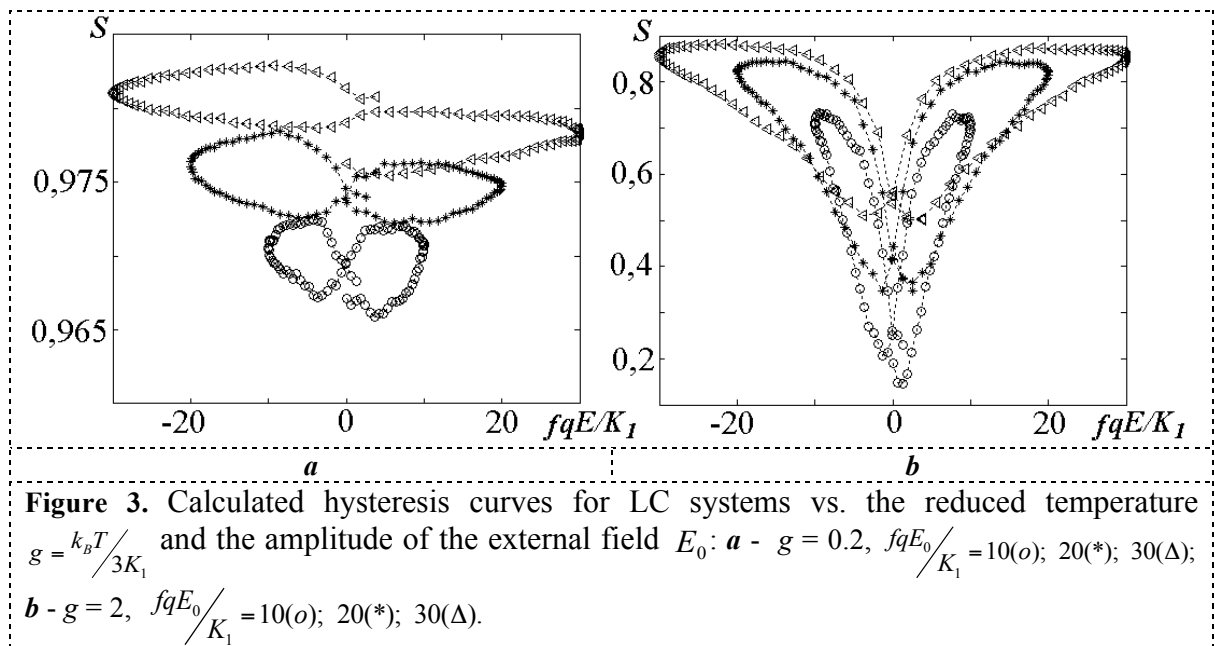
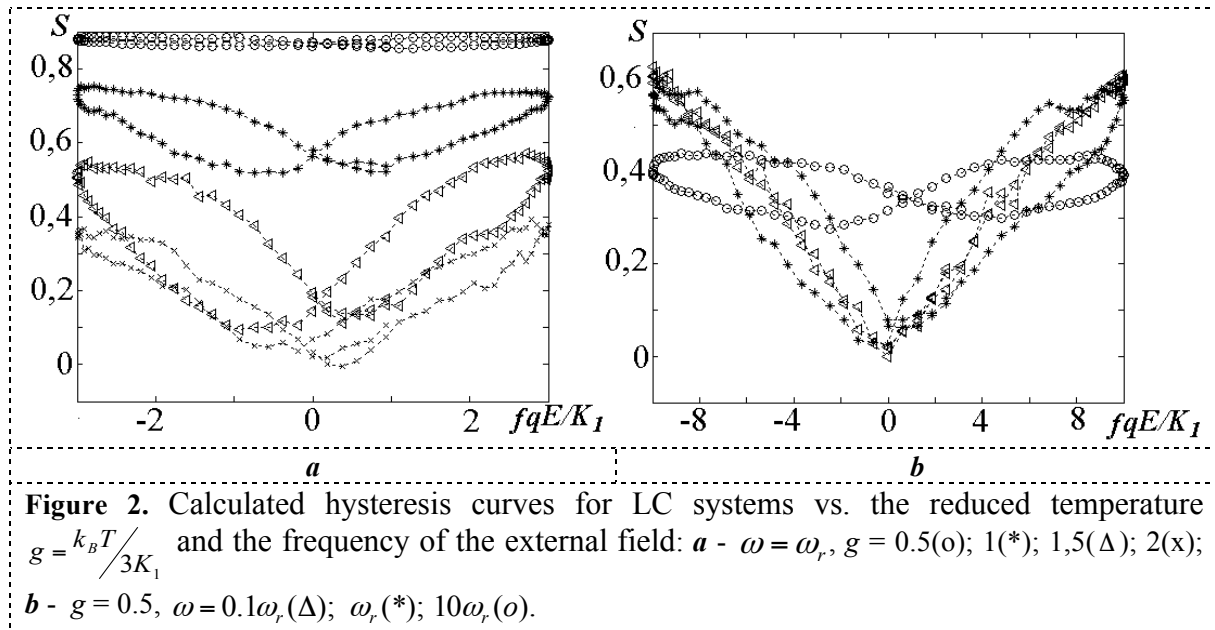
The absorption of the energy of electromagnetic field in the liquid crystal system occurs due to periodic change of the molecular orientational order. Molecular mechanisms of formation of quadrupole order in the nematic phase in electric fields are associated with the turn of the rod-shaped molecules around the long and short axes [1]. The forces of intermolecular interactions are responsible for this type of long-range orientational order prevent such turns.

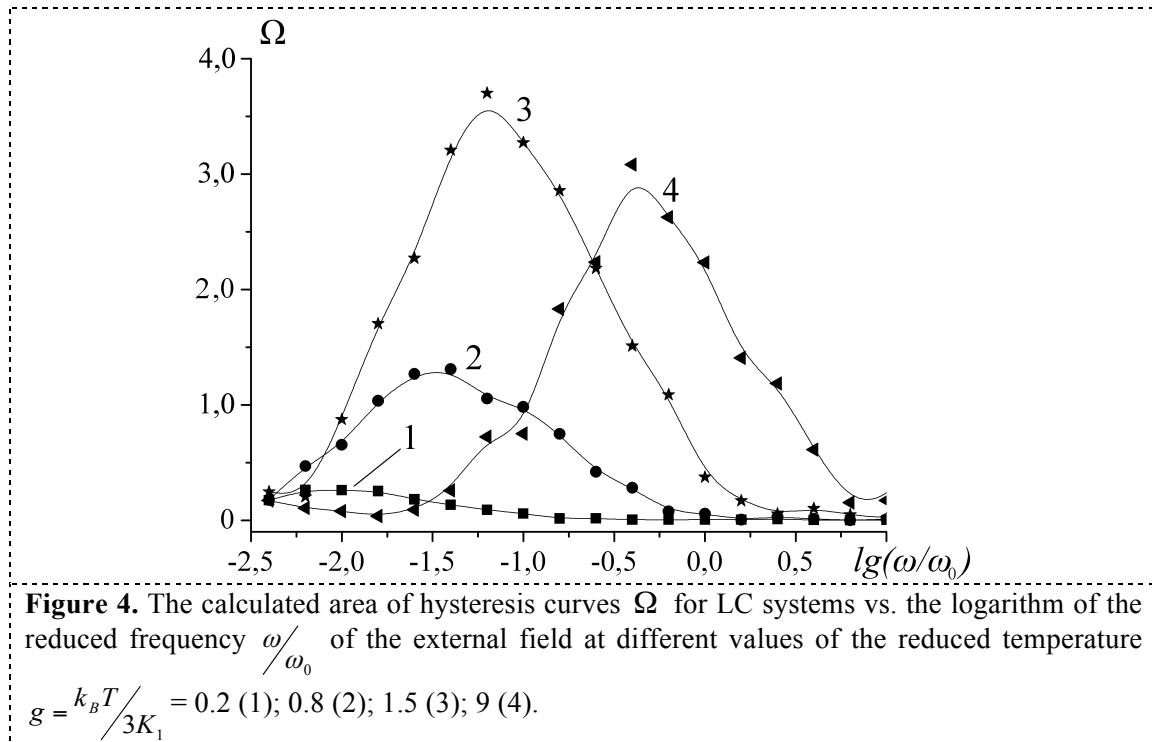
3. Results and discussion

In this work we calculated the dependencies of the order parameter (the Tsvetkov’s factor S) in LC systems on the value of external harmonic electric field $E = E_0 \cdot \sin \omega t$ at different values of internal and external parameters. When simulating by the Monte Carlo method, the interaction potential was selected in the form (1) and dynamic interpretation of this method is given to averaging in the Markov process, i.e., the number k of successive configurations of the system is associated with the definite timescale, which allows to explore various dynamic characteristics of the system. Therefore, the frequency was selected inversely proportional to the number of Monte Carlo steps N_{MK} . We analyzed the behavior of LC systems in external alternating electric fields. As the standard we adopted the frequency value corresponding to the number of Monte Carlo steps $N_{MK} = 10^3$ when simulating 8,000 of rotators under periodic boundary conditions.

The calculated hysteresis curves for LC systems are asymmetric (Figure 2-3), their form is determined by the temperature, the value of the interaction constants, amplitude and frequency of the external field. The order parameter varies near its equilibrium value, which increases with the rise of amplitude of the external field.

The main characteristic of the hysteresis curve is its area, which is proportional to the energy expended on the periodic change of orientation order in the system. It is seen that with the increase of the amplitude of the external field E_0 at low and high temperatures the area of the hysteresis curve increases. It was found that the form of the hysteresis curve and its area is dependent on interaction constants of the model and temperature. Figure 4 shows the dependencies of the area of hysteresis curves (Ω) on the logarithm of the reduced frequency of the external field ($f q E / 3 K_1$) at various temperatures.





4. Conclusion

At a certain frequency of the external field the phenomenon of resonance occurs and the maximum of hysteresis curve area is observed. The peak position and its value depend on the temperature and interaction constants and is defined by the relation $g = \frac{3k_B T}{K_1 + K_2 + K_3}$. With the increase of the value g the peak of the area of hysteresis curve is shifted towards higher frequencies. Moreover, with the increase of the reduced temperature the maximum value of the function $\Omega\left\{\lg\left(\frac{\omega}{\omega_0}\right)\right\}$ first increases, then decreases.

Acknowledgments

The reported study was funded by Russian Science Foundation; according to the research project No.15-19-10008.

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