Radiation from Relativistic Electrons in Periodic Structures "RREPS-23" & Electron, Positron, Neutron and X-ray Scattering under External Influences "Meghri-23"

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The Molecular Mechanism of Smectisation and Regulation of Polymorphism in Nematic Liquid Crystal Systems

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This study explores the application of catastrophe theory to describe the molecular mechanism of smectisation and the regulation of polymorphism in nematic liquid crystal (NLC) systems that are based on polar liquid crystals, whose molecules have a large dipole moment directed along the long axis of the mo¬¬le¬cule .We have identified a relationship between the control variables of cusp catastrophe and the smectic order parameter η of NLC systems.

Thus, we conducted thermodynamic potential ϕ minimization not only in terms of structural degrees of freedom, but also in terms of the molecular composition of NLC systems, in order to better understand the role of various types of intermolecular interactions in the process of polymorphism. Then for ϕ we finally get the expression: ϕ=1/(4) x^4+1/2 〖ax〗^2+bx which becomes the characteristic equation for the cusp catastrophe. This equation makes the study of structural transitions in NLC system possible using the analysis of the critical points of ϕ(x;a,b) function. As the control (a,b) variables vary, a local minimum can disappear and the internal variable can suddenly jump to a different equilibrium state. Also the state (x;a,b) will be forced to jump to the other sheet when it crosses the fold curve. The bi¬furcation set is the critical image of the projection (x;a,b) from the equilibrium surface onto the control space (a,b).

On the other hand, the equilibrium state of Sm phase at given temperature and pressure ultimately determined by the equilibrium constants K_1, K_2 (control variables) of the DA and D_2 A type CTC. Thanks to the catastrophe theory it was possible to evaluate the area of K_1,K_2 change which allows system to remain in sustainable state. That is by controlling the value of K_1, K_2 it is possible to regulate the process of polymorphism in NLC systems. An important circumstance is the role of the control variables, a smooth change of which can lead to a jump-like change in the functionality of the system. The catastrophe theory at a sufficiently high level allows determining the scope of changing control variables and thereby ensure the operability of the device.

Author: Dr BEZHANOVA, Liana (Institute of Applied Problems of Physics of the National Academy of Sciences of the Republic of Armenia)

Co-authors: ATANESYAN, Armen; VASILYAN, Marianna

Presenter: Dr BEZHANOVA, Liana (Institute of Applied Problems of Physics of the National Academy of Sciences of the Republic of Armenia)

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