Computer Simulation of Phase Transition Isotropic Fluid - Lyotropic Liquid Crystal

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By using the methods of molecular dynamics and Monte-Carlo, based on the lattice model of charged ends of dipole fragments of amphiphilic molecules, new phase transitions of lyotropic liquid crystals have been studied depending on the incidence angle of the dipole molecule fragments to the surface of lamella.

With an increase of the incidence angle of the dipole fragments of phospholipid molecules, the density of bilayer was decreased and a thickness of lamella – increased. This could be explained by the increase of electrostatic repulsion force and decrease of Van der Waals attraction force with an increase of the incidence angle. As a results of equilibration of those forces, the molecules in the lamella are distanced from each other, leading to a decrease in density and increase of the lamella's thickness. The number of molecules in lamellas is also increased due to its hydrophobicity.

Existence of the upper and lower critical angles of incidence to the lamella's surface ϑ_c^T and ϑ_c^L has been shown. Under the incidence angle $\theta > \vartheta_c^T$, lamella is destroyed, while under $\theta < \vartheta_c^L$ transformed into a crystal state. The latter is followed by separation of phases: a new free water phase and crystal domains with characteristic domain boundaries.

It has been shown that if a lyotropic liquid crystal consists of phospholipid molecules, then creation of micelle structures does not take place. This might be explained by stronger repulsion forces near concentration of micelle formation, compared to attraction ones. The equilibrium between those forces has been achieved when dimmer or trimers are formed. Under high concentrations of phospholipids, lamellas are formed. Intermediate variations such as formation of vesicles and liposomes (lipid vesicles) is also possible.

The obtained data allow to calculate a swelling coefficient of a lamella, which is an important parameter of phospholipid bilayer.