Molecular dynamics simulations of polymer liquid crystals

J. Ilnytskyi

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine, E–mail: iln@icmp.lviv.ua

Recent developments in computing facilities (especially availability of affordable workstation clusters) enable to focus attention on a new kind of problems that were impossible to simulate a decade ago. One of such examples are various effects that take place in polymeric liquid crystals. These systems combine the features of both the polymer and liquid crystal, enable fine-tuning on the stage of synthesis and found a numerous practical applications (high strength plastics, displays, optical data storage).

We present some recent developments in molecular dynamics simulations of such systems. *Liquid crystalline dendrimer* is studied in isotropic, nematic and smectic A solvent and we concentrate on orientational relaxation of the macromolecule and its equilibrium shape depending on the phase of the solvent and the way the terminal mesogens are attached to the dendritic core. The results are discussed in terms of the connection between molecular shape and its bulk phase.

The second problem addresses the origin of photo-induced deformations in *azobenzene-containing polymer films*. We reproduced the opposite sign of the deformations under uniform linearly polarized light in liquid crystalline and amorphous films, respectively. The simulations revealed underlying microscopic mechanisms of these deformations depending on the details of molecular architecture.

The third problem is the memory effects in *liquid crystalline elastomers* that are potentially attractive for the application as artificial muscles. In our molecular dynamics simulations we reproduce the reversibility of the shape of lightly crosslinked melt of polymer liquid crystal when driven via the smectic–isotropic transition.

The examples presented demonstrate the potential of molecular dynamics simulations in clarification of the microscopic mechanism behind various effects and are a starting point for simulation driven predictions of the properties of new materials.