SUMMARY OF Ph.D. DISSERTATION

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Title

Orientational order and transport properties of nematic liquid crystals confined in nano-space: A molecular dynamics simulation approach

Abstract

Recently, several nano-processing techniques have been developed and a device with nano-sized pores has been fabricated Molecules confined in such nano-space show various properties different from the ones in the bulk system, which have been extensively researched. Currently, liquid crystals (LCs) are investigated as suitable molecules to be confined in nano-space. LCs can orientationally order under electric field and the mechanism has been widely applied to LC displays. It has been recognized that the orientational order of LCs depends on temperature and pressure. It is also expected that the orientational order of the LCs in nano-space will diverge from that of the ones in the bulk system especially when LCs are exclusively confined in nano-space.

In this thesis, the transport properties and the system size dependence of the orientational order of the nematic LCs in nano-slit are thoroughly investigated using the classical molecular dynamics simulation. It is found that the rotational transport coefficient is an important factor in the evaluation of LC display. Additionally, to inspect the existence of the system size dependence provides basic information to molecular simulation.

In Chapter 1, the introduction and the purpose of the thesis are demonstrated. In Chapter 2, the general aspects of the shape and the phase diagram of nematic LCs are comprehensively reviewed. In Chapter 3, the general scheme of the classical molecular dynamics simulation is explained. In Chapter 4, several general but unique methods of the thesis are introduced: the Gay-Berne (GB) particle is modeled as a nematic LC molecule, the interaction between a GB particle and a wall of the slit is established to make the GB particle parallel to the wall, and finally, the integration algorithm and the definitions of physical quantities are mentioned.

In Chapter 5, the self-diffusion and the self-rotation coefficients are calculated, and the transport properties of LCs in the nano-slit are discussed. The profiles of the transport coefficients show that GB particles easily diffuse and rotate in the plane parallel to the slit, while hardly do so in the plane perpendicular to the slit upon approach to the wall. Furthermore, the velocity and the angular velocity auto-correlation functions and their Fourier spectra are analyzed. It is found that the transport properties of GB particles are closely related to the characteristic frequencies of the Fourier spectra.

In Chapter 6, the system size dependence of the orientational order is investigated at several temperatures. It is revealed that the orientational order parameter depends on the system size while no region behaves as bulk in the nano-slit, and that the system size dependence has a threshold. The value of the order parameter converges when the system size is larger than the threshold. In order to examine the mechanism of the system size dependence, the mutual orientational correlation function (MOCF) is introduced. As a result, it is found that the system size dependence of the order parameter converges when the system is so large that MOCF decays to zero.

Finally, the conclusion follows in Chapter 7.