A NEW SIMULATION METHOD OF INTERACTION BETWEEN A LIQUID CRYSTALLINE POLYMER AND TWO SERRATED WALLS

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ABSTRACT

This paper presents a new molecular model to define the interactions of a liquid crystalline polymer (LCP) flowing between two serrated walls. The wall is modeled by a rough atomic serrated wall. The roughness characteristics are given by the space and height of the serrated wall. Molecular model of the liquid crystalline polymer is described by an improved model that consists of GB (Gay-Berne) sites as rigid segments and LJ (Lennard-Jones) sites. There are two nonlinear springs each connecting from a GB site to a LJ site that situate between two GB sites as flexible segments. This improved model is newly developed to reduce the computational cost from that of the hybrid GB/LJ model, which has provided an effective way to investigate the boundary problems and flowing behaviors of LCPs at nano-scale. The molecular dynamics (MD) simulation using this reduced computational cost method to study the effect of boundary conditions on alignment and rheological properties of the LCP is shown in the result.

1. INTRODUCTION

Liquid crystalline polymers are a relatively new class of materials that have received considerable scientific attention. Compared with traditional polymers, LCPs have high performances, good flowability and excellent dimensional stability. Due to their unique characters, LCPs have become ideal materials for fabricating micro devices or components by micro injection molding. However producing parts from thermotropic LCPs through injection molding still has its problems. The major problem is that the polymer flows through the micro channels in the mold are dominantly shear flows which cause direct tumbling and disrupt the molecular orientation. Another intractable problem is that the contacting boundary conditions become important factors that influence the orientation and rheological properties of LCPs in the nano-channel. The key to resolving such problems is an understanding of the relationship between the material structure and the flow. Though there have been studies in micro flowing behaviors in recent years, there are few studies using LCPs as fluid due to the anisotropic structures as well as the complication and variety of mesogenic behaviors of LCPs.

2. SIMULATION METHOD

In the MD simulation, a semiflexible main chain LCP is assumed to be subject to planar shear in \(\hat{x}\) direction (shown in Fig.1) in a nanometer channel by moving the upper and lower walls in opposite directions. The improved model reduces greatly the total number of elements to represent a LCP molecule when compared with the original
The simulation is done with the upper and lower walls of the shear cell each consisting of 1920 atoms distributed between two (111) planes of a fcc (face-centered-cubic) lattice. The position of the wall particles on the wall in the Z direction is displaced by $\Delta z$ given:

$$\Delta z = \begin{cases} \frac{2A}{P} (x - a - P) & x - a - P \leq \frac{P}{2} \\ \frac{2A}{P} ((a + 1) - P - x) & x - a - P > \frac{P}{2} \end{cases}$$

where $a = \text{integer}(x / P)$. Where, A and P, that characterize the roughness, are the amplitude and period of the serrated wall respectively. Each atom on the wall is attached to its lattice position by a stiff spring. The wall springs have a potential of the form $V_{ws} = \phi_s R^2$, where, $\phi_s$ is the spring stiffness, and $R$ is the distance of the wall atom from its lattice site. The interaction between LCP molecules and atoms on the wall is modeled as shifted LJ potential with the energy scale $\varepsilon_{gb} = 2\varepsilon_{gb}$ and the length scale $\sigma_{gb} = \sigma_{gb}$. The entire simulation cell measures $38.1 \times 6.0 \times 12.8 \text{ nm}^3$ and the liquid crystalline polymer fluid is confined in a gap width of $h = 12.8 - 2A \text{ nm}$. Periodic boundary conditions are enforced in $\hat{x}$ and $\hat{y}$ directions. The simulation system configuration is shown in Fig. 1.

The equations of motions are integrated using a form of leap-frog algorithm suitable for anisotropic systems [1]. Initial calculations are carried out only for LCP molecules to form the liquid crystalline phase of fluid molecules ignoring the wall particles. Actual simulations of shear flow are conducted in constant temperature ensemble (NVT) at $T=350K$ using Anderson thermostat in all three directions of the wall and fluid particles. The time step used in the simulation is 2fs. An equilibrium run of 100,000 time steps is performed followed by another 200,000 time steps to collect the results. Physical variables of the rheology of LCPs are computed from the Kirkwood relation [2]. The orientational order parameter is quantified by diagonalizing the order tensor [3].

The relationships between the amplitude of roughness $A$, the period of roughness $P$ and orientational order parameter $S$, the shear viscosity $\eta$, normal stress $\sigma_{zz}$, first normal stress difference $\Delta N_1$ are presented here. As shown in Fig 2 and Fig 3, the amplitude of roughness has a dramatic effect on shear viscosity, orientation of LCP molecules and normal stress differences on fluid properties. The viscosity and normal stress increase with the increase of the amplitude of roughness. The rheological variables of the LCP show some peak and valley values with the increase of the period of roughness. The largest peak value appears when the period is comparable with the distance of two adjacent GB sites. According to above results, we can design suitable boundary conditions making for LCPs flow at nano scale.

Figure 2. Viscosity against the amplitude of roughness (The shear rate is $10^3 \text{ s}^{-1}$ and the period of roughness $P = 1.347 \text{ nm}$).

Figure 3. Orientation order parameter against the period of roughness (The shear rate is $10^3 \text{ s}^{-1}$ and the period of roughness $P = 1.347 \text{ nm}$).

3. RESULTS AND DISCUSSION

The relationships between the amplitude of roughness $A$, the period of roughness $P$ and orientational order parameter $S$, the shear viscosity $\eta$, normal stress $\sigma_{zz}$, first normal stress difference $\Delta N_1$ are presented here. As shown in Fig 2 and Fig 3, the amplitude of roughness has a dramatic effect on shear viscosity, orientation of LCP molecules and normal stress differences on fluid properties. The viscosity and normal stress increase with the increase of the amplitude of roughness. The rheological variables of the LCP show some peak and valley values with the increase of the period of roughness. The largest peak value appears when the period is comparable with the distance of two adjacent GB sites. According to above results, we can design suitable boundary conditions making for LCPs flow at nano scale.