



Conformations and dynamics of single flexible ring polymers in simple shear flow



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ABSTRACT

The conformational, orientational and dynamical properties of single flexible ring polymers under simple shear flow are studied by a hybrid multiparticle collision dynamics simulation method. We found that contributing to the continuous stretching and constant alignment in the tank-treading motion, ring polymers undergo weaker deformation and orientation in the gradient direction, and show similar behaviors in the vorticity direction compared with their linear analogues. We also present the mechanisms of both tumbling and tank-treading motions based on the time trajectories of relative deformation and orientation. Furthermore, the simulation results reveal that the special structures and unique dynamics of ring polymers in simple shear flow have an obvious influence on rheological properties, which are qualitatively different from the properties of linear polymers.

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1. Introduction

Ring polymers as one of the common forms have now been discovered in bacteria, plants and animals, such as plasmid, genome, actin, and polyose [1–5]. It is believed that the absence of end groups results in all monomers in a ring polymer are identical and the whole polymer prefers special conformations and dynamics [6]. This is not the case for linear polymers since the translational invariance along the chain is suddenly interrupted due to the terminal ends [1,7]. The rather extensive studies have been devoted to investigate the conformational and dynamical properties of linear polymers under shear flow [8,9], while the flow-induced behaviors of ring chains are still poorly understood. A deep insight into the basic conformational and dynamical properties of ring polymers in simple shear flow is highly needed in a wide range of biophysical fields, e.g. segregation of the cyclic genome from bacteria [4], migration of a cyclic DNA in a nanochannel [10] and ejection of viral DNA into the host [5].

The conformations as well as dynamics of individual linear polymers have been comprehensively understood in theories

[11–14], experiments [15–19] and simulations [20–24]. It is a well-known fact dating back to 1974 that De Gennes described the coil-stretch transition of linear polymer chains in shear flow [11]. The theory predicted that when a certain critical value of the velocity gradient is reached, the fluid viscous forces are greater than the entropic elastic retraction forces and the chain is stretching. Traditional experiments involving optical techniques such as birefringence and light and neutron scattering have sought average structural information of linear polymers in shear flow [25,26]. Chu and his co-workers have shed light on the conformations and dynamics of an individual DNA via fluorescence microscopy [17,27,28]. They observed directly that DNA molecules indeed substantially stretch and continually undergo end-over-end tumbling motion as reflected in large conformational fluctuations. More recently, Steinberg groups studied the orientation angles of λ -DNA relative to the shear plane by particle image velocimetry measurements [19]. They found that the strong deviation of the probability distribution functions of the orientation angles from Gaussian distribution is in good accord with theory. Besides experiment and theory, Larson et al. studied the deformations and tumbling dynamics of individual polymer chains in shear flow via Brownian dynamics (BD) simulations [23,29]. They found that the decrease in chain stretch ceases at sufficiently large flow shears. Furthermore,

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the knowledge of the flow-induced conformational information can be used to calculate rheological properties such as shear viscosity [30,31]. Doyle et al. used BD to simulate rheological properties by conformational properties such as shear viscosity and normal stress differences [31].

The flow-induced behaviors of ring polymers are generally related to separation required for identification, quantification, purification, and fractionation [32–36]. Zheng and Yeung separated circular ϕ X174 RF DNA from λ DNA, based on their radial migration in capillary electrophoresis with applied hydrodynamic flow [36]. Cramail and his coworkers purified the synthesis macrocyclic polystyrenes from the residual linear precursor and byproducts by liquid chromatography [34]. Although the flow-induced behaviors are very important in separation processes, the conformations as well as dynamics of single flexible ring polymers in shear flow have still remained elusive. Cifre et al. studied the stretching behaviors of ring polymers in simple shear flow by BD simulation and demonstrated that the shear dependence of the average extension of ring polymers is analogous to that of linear polymers [37]. Recently, our groups studied the dynamics of individual ring polymers in simple shear flow by the multiparticle collision dynamics (MPCD) method [38,39]. The results revealed that individual ring polymers exhibit two primary types of motion, continually end-to-end tumbling like linear polymers and tank-treading like fluid droplets and capsules. Frey and his co-workers also found the two types of motion and used the time evolution of the orientation angle to distinguish these motions [40]. Though various novel behaviors of ring polymer in shear flow have been revealed, qualitative and quantitative studies on how the conformation and orientation of single flexible polymer chains response to shear flow are still far from clear.

Computer simulation plays an important role in studying instantaneous dynamics of a single polymer in shear flow since simulation can provide a bridge between theory and experimental observation [41,42]. In this work, we present the detailed simulation results of the conformational, dynamical, and rheological properties of single flexible ring polymers in steady shear flow. We apply a hybrid simulation approach, combined MPCD method describing the solvent with molecular dynamics simulation (MD) for the polymers [43,44]. As has been shown, the MPCD method has the virtue of taking into account hydrodynamic interactions and thermal fluctuations, which is suited to study the non-equilibrium properties of polymers under shear flow [45–50].

The outline of the paper is as follows: In Section 2, we describe the model and simulation approach. In Section 3, the conformational and orientational properties of flexible ring polymers under simple shear flow are presented. Then a deep research is given for tumbling and tank-treading motions. We also discuss the contribution of ring polymers to the rheological properties. In Section 3.3, we generalize our studies and give a conclusion.

2. Model and simulation method

In our model system, flexible ring polymer chains consist of N_{se} beads of mass M each [51,52], which are connected by the finitely extensible nonlinear elastic (FENE) potential U_{FENE} ,

$$U_{FENE}(r) = \begin{cases} -\frac{1}{2}KR_0^2 \ln \left[1 - \left(\frac{r}{R_0} \right)^2 \right] & r \leq R_0 \\ \infty & r > R_0 \end{cases} \quad (1)$$

where R_0 is the maximum bond length and K is the spring constant.

The excluded-volume interactions between beads are taken into account by a truncated and shifted Lennard-Jones potential U_{LJ} :

$$U_{LJ} = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] + \epsilon & r \leq r_{cut} \\ 0 & r > r_{cut} \end{cases} \quad (2)$$

where $r = |\mathbf{r}_i - \mathbf{r}_j|$ denotes the spatial distance between beads i and j located at \mathbf{r}_i and \mathbf{r}_j . The parameters ϵ and σ are taken as the units of energy and length, respectively. The short-range, purely repulsive interactions are taken into account by choosing $r_{cut} = 2^{1/6}\sigma$. The velocity Verlet algorithm with time step h_p is used to integrate Newton's equations of motion of beads.

The explicit solvents are simulated by the MPCD method, which consists of streaming and collision steps [43,44]. Solvents are modeled as N_{st} point-like particles of mass m . In the streaming step, the solvent particles propagate ballistically and their positions are updated according to [53].

$$\mathbf{r}_i(t+h) = \mathbf{r}_i(t) + h\mathbf{v}_i(t) \quad (3)$$

where $i = 1, \dots, N_{st}$ and the collision time h is the time interval between collisions. In the collision step, the particles are sorted into cubic cells with length a , and their relative velocities, with respect to the center-of-mass velocity of each cell $\mathbf{v}_{cm}(t)$, are rotated by an angle α around a random axis $\mathbf{R}(\alpha)$ [43], i.e.

$$\mathbf{v}_i(t+h) = \mathbf{v}_{cm}(t) + \mathbf{R}(\alpha)[\mathbf{v}_i(t) - \mathbf{v}_{cm}(t)] \quad (4)$$

where $\mathbf{v}_i(t)$ is the velocity of particle i at time t and the center-of-mass velocity

$$\mathbf{v}_{cm}(t) = \frac{1}{N_{st}^c} \sum_{j=1}^{N_{st}^c} \mathbf{v}_j(t) \quad (5)$$

N_{st}^c is the total number of solvent particles within the collision cell.

The solute-solvent coupling is achieved by taking the solute into account in the collision step, and velocities of the center-of-mass are [43,44].

$$\mathbf{v}_{cm} = \frac{\sum_{i=1}^{N_{st}^c} m\mathbf{v}_i(t) + \sum_{j=1}^{N_{se}} M\mathbf{v}_j(t)}{mN_{st}^c + MN_{se}} \quad (6)$$

where N_{se}^c denotes the number of monomers in the cell. Mass, momentum, and energy are conserved in the collision step. In addition, a random shift is performed to ensure Galilean invariance at every collision step [54].

Lees–Edwards boundary conditions are applied for the solvent particles and the solute beads in order to impose shear flow [55]. The velocity field is given by

$$v_x = \dot{\gamma}y, \quad v_y = 0, \quad v_z = 0 \quad (7)$$

The schematic representation of a flexible ring polymer in simple shear flow is shown in Fig. 1. A local Maxwellian thermostat is used to maintain the temperature of the system at the desired value [56].

All simulations are performed with the rotation angle $\alpha = 130^\circ$, $\sigma = 1.0$, $a = \sigma$, $\epsilon = 1.0$, $k_B T/\epsilon = 1$, where T is the temperature and k_B is the Boltzmann constant. The collision time $h = 0.1\tau_p$, MD time step $h_p = 0.005\tau_p$, with $\tau_p = \sqrt{ma^2/(k_B T)}$. Small collision time h and large rotation angle α are used to obtain large Schmidt numbers required for fluid-like behaviors [53,57]. The average number of solvent particles per collision cell $\rho = 10$, and $M = \rho m$. The maximum bond length $R_0 = 1.5\sigma$ and the spring constant $K = 30\epsilon/\sigma^2$. The viscosity of solvent fluid [58] is $8.7(\epsilon m)^{1/2}/\sigma^2$. The chain

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