Understanding Conformational and Dynamical Evolution of Semiflexible Polymers in Shear Flow

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Supporting Information

Fig. S1. The introduction of the contact matrix and the shortest path for a linear polymer.
Fig. S2. (a) the largest eigenvalue $G_1$, (b) the intermediate eigenvalue $G_2$, (c) the smallest eigenvalue $G_3$, and (d) the elongation ratio $G_1/G_3$ in the gyration tensor as a function of $Wi$ for polymer chains with increased rigidities $L/L_p = 20.0, 6.9, 4.4, \text{ and } 2.0$ respectively.
Fig. S3. A typical evolution of $R_g^2$ vs simulation time is shown in (a), (b-e) show the distribution of $R_g^2$, $R_g\text{Max}$ and $R_g\text{Min}$ of polymer chains with different rigidities as a function of $Wi$. The right profile in (a) is the normalized probability density function (PDF) of $R_g^2$. $R_g\text{Max}$ (10%) and $R_g\text{Max}$ (20%) are the cutoff values that cover largest 10% and 20% of the square radius of gyration $R_g^2$, accordingly, $R_g\text{Min}$ (10%) and $R_g\text{Min}$ (20%) are the cutoff values that cover the smallest side. Four sub-processes are defined according to $R_g\text{Max}$ and $R_g\text{Min}$: the collapse process is between adjacent $R_g\text{Max}$ and $R_g\text{Min}$, the stretching process is between adjacent $R_g\text{Min}$ and $R_g\text{Max}$, the align & flip process represents the motions between two neighboring $R_g\text{Max}$, and the tumble represents the motions between two neighboring $R_g\text{Min}$. 
Fig. S4. The evolution of the square radius of gyration $R_g^2$, the normalized Wiener index $W/W_0$, and the orientation angle $\phi$ for polymer chains with different rigidities in intermediate shear flow.
Fig.S5. Cross-correlation functions $C_{xy}$ against reduced time scale for polymer chains at different Weissenberg numbers.
Fig.S6. The differential contact maps for (a) the collapse and (b) the stretching processes of polymer chains in intermediate shear flows.
SUPPLEMENTAL MATERIAL

See supplementary material for videos of flexible and semiflexible polymer chains in shear flow: Video 1, $L/L_p=20.0$, $Wi=12.1$; Video 2, $L/L_p=4.4$, $Wi=13.3$; Video 3, $L/L_p=20.0$, $Wi=121.4$; Video 4, $L/L_p=4.4$, $Wi=132.6$. 