Polymer brush bilayer under steady state shear motion: Density functional theory, scaling theory and molecular dynamic simulation

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Abstract

In this article, polymer brush bilayer under steady shear motion is studied. The density functional theory and the molecular dynamic simulation reveal that in the nonlinear response regime the shear stress scales as $\dot{\gamma}^{1.46}$ in the absence of the hydrodynamic interactions. In the presence of the hydrodynamic interactions, theoretical method shows that the shear stress scales as $\dot{\gamma}^{0.8}$. Molecular dynamic simulation with implicit solvent and Langevin thermostat confirms $\dot{\gamma}^{1.46}$. However, molecular dynamic simulation with implicit solvent and dissipative particle dynamic thrmostat which takes the hydrodynamic interactions into account, does not detect power law $\dot{\gamma}^{0.8}$. The perpendicular stress remains constant under shear. In general, it turns out that the polymer brush bilayer could be a good lubricant exclusively in the presence of hydrodynamic interactions. Moreover, this study reveals that the so called blob picture in the works already published reflect a completely incorrect picture of this system.

Introduction

The building blocks of life are linear macromolecular structures which are called polymers.[1,6,20] Polymers consist of repeating atomic or molecular units which are called monomers.

Monomers are connected in the backbone of polymer chain through covalent bonds in which atoms share their valence electrons. Since, polymers in living tissues are suspended in interstitial water, the monomers undergo Brownian motion as a result of colliding with solvent molecules. The Brownian motion of each monomer gives rise to a collective fluctuation in polymer chain structure. If polymer chain is subject to equilibrium or steady state conditions, by long time measuring the length of chain one can obtain a chain extension. In polymer Physics, chain extension is measured by two quantities, the end-to-end distance R_e and the radius of gyration R_g.[1,6,20] Calculations show that in a polymer chain that its monomers are point-like particles with no internal structure, $R_e = aN^{1/2}$ and $R_g = 1/\sqrt{6}R_e$. Here, N is number of monomers or degree of polymerization and a is the monomer size or *Kuhn* length.[1,6,20] In this polymer model which is called freely-jointed-chain (FJC) model, the monomers distribution is Gaussian.[1,6,20] Therefore, in some literature it is called Gaussian chain model as well.[1,6,20] A more realistic polymer model is the one in which its monomers have internal structure. This model is called real polymer and the various calculations of polymer Physics including perturbation expansion theory, renormalization group theory, scaling theory, mean field theory and density functional theory (DFT) show that $R_e = (5/8\pi)^{1/5}a^{2/5}b^{1/5}N^{\nu}$. Where, b is the second Virial coefficient which contains information about interactions between monomers.[1,6,20] The exponent ν is called Flory exponent and it is equal to 3/5 and more precisely 0.588.[1,6,20] In Mathematical Physics, $1/\nu$ is called the fractal dimension.[3] In the real polymer model, monomers distribution is parabolic.[1,6,20] The chain extension is a sensitive function of molecular structure and interactions between them and solvent molecules. For instance, if chain is suspended in a good solvent like water, $b = 2.09a^3$ and if it is suspended in a θ solvent $b = 0$ and the Gaussian model holds.[1,6,20] In the case of a polymer suspended in a poor solvent like Alcohol, $b < 0$ and chain collapses i.e. $R_e \sim N^{1/3}$.[1,6,20]

Polymer brushes form when linear polymer chains are densely grafted to (from) a substrate.[2] In chemistry, grafted to means that polymer chains are formed when they are not

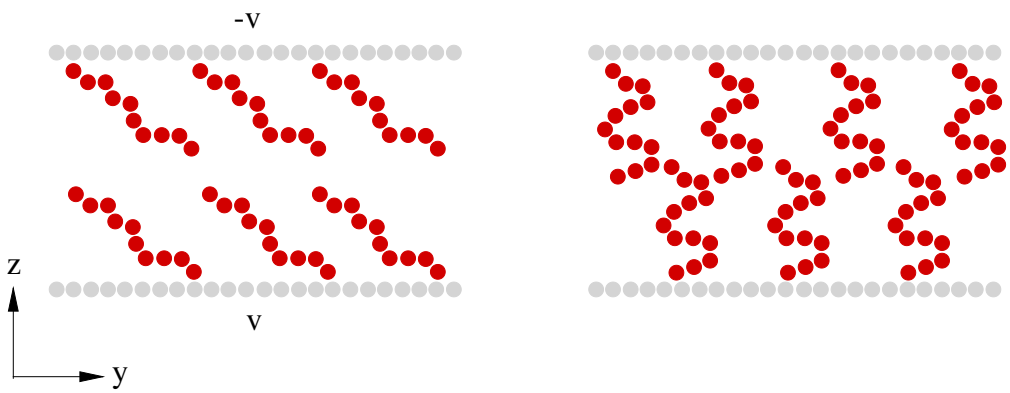

Figure 1: Schematic view of the model in equilibrium and steady state shear motion.

grafted and then by an experimental method the chain is grafted in one end to the substrate.[2] In grafted from method, the polymer brush forms by growing its chains on the substrate.[2] In any case, the steric repulsion between monomers stretch the chains in the perpendicular direction. Calculations of DFT show that mean perpendicular chain extension or brush height is $R_n = (a^2 b\sigma)^{1/3} N$ and the mean lateral chain extension is the same as single chain.[2?] The monomers in a brush have parabolic distribution in perpendicular direction.[2?] Polymer brushes could be found in so many biological systems such as as Glycol on the outside of the cell membrane and they play a key role in cells movement and interactions.[2]

When two opposing polymer brush covered surfaces are in a distance where two brushes are intermediately compressed over each other, the polymer brush bilayer (PBB) forms.[2,23–25] The PBB plays a key role as lubricant in human and other mammals.[2,23–25] For instance, the aggregans in synovial fluid of the mammalian joints are a similar structure.[2,23–25] In the last thirty years, there has been a competition in proposing a correct theory for PBBs in equilibrium and under steady state shear.[5,8–15] Also, there has been many experiments to measure the usefulness of the PBBs in friction reduction.[16–18] In this article, I tackle the problem of PBBs under steady state shear motion and I try to check if PBBs can reduce friction. I employ the DFT, scaling theory and molecular dynamic simulations to make sure that the results are reliable. In Fig. (1), a schematic view of the system in equilibrium and

in steady state shear could be seen.

Density functional theory framework

One of the methods to approach mechanics of a system is to calculate the Euler-Lagrange equation of that system and solve it under proper conditions. This method competes to other methods in mechanics like Newton's equation of motion and Hamilton-Jacobi method. The density functional theory is an efficient method to calculate the Euler-Lagrange equation in many body systems. It starts by writing down the grand potential functional of the system and then taking the variation of grand potential with respect to density of the system. The result of this variation is the correct Euler-Lagrange equation of the system. By solving the Euler-Lagrange equation under proper conditions, density and other Physical quantities could be calculated. In 1988, Hirz in his Master thesis applied the DFT method to PBBs.[7] In the case of PBBs the grand potential functional is given as follows,

$$\begin{aligned}\frac{\Phi[n(z),m(z)]}{k_{\mathrm{B}}T} &= \int_0^h \left(\frac{3z^2}{a^2N^2}n(z) + bn(z)^2 - \mu n(z)\right) dz \\ &+ \int_{D-h}^{D} \left(\frac{3(z-D)^2}{a^2N^2}m(z) + bm(z)^2 - \mu m(z)\right) dz \\ &+ b\int_{D-h}^{h} n(z)m(z)dz \end{aligned} \tag{1}$$

where $n(z)$ and $m(z)$ are the densities of bottom and up brushes, h is the brush height, μ is the chemical potential, σ is the grafting density and D is the distance between substrates. There are three Euler-Lagrange equations and one condition which are given as follows,

$$
\begin{aligned}
\frac{\delta\Phi[n(z),m(z)]}{\delta n(z)} &= 0 \\
\frac{\delta\Phi[n(z),m(z)]}{\delta m(z)} &= 0 \\
\frac{\partial\Phi[n(z),m(z)]}{\partial h} &= 0 \\
\int_0^h n(z) &= N\sigma
\end{aligned}
$$

By solving these equations simultaneously and one can obtain $n(z)$, $m(z)$, h and μ that are primarily unknown quantities. The solutions of the above set of equations are given as follows,

$$
\begin{aligned}
n(z) &= \frac{N^2a^2\mu + 3D^2 - 6Dz - 3z^2}{3a^2bN^2} \\
m(z) &= \frac{N^2a^2\mu - 6D^2 + 12Dz - 3z^2}{3a^2bN^2} \\
h &= \frac{1}{2}\left(\chi_0^{1/3} + D\left(\frac{D}{\chi_0^{1/3}} - 1\right)\right) \\
\mu &= k_{\mathrm{B}}T\frac{3\left(4D\chi_1 + D^3\chi_0^{1/3} + 2\chi_1\chi_0^{1/3} - 5D^2\chi_0^{2/3} - D^4\right)}{4a^2N^2\chi_0^{2/3}}
\end{aligned}
$$

where χ_0 and χ_1 are defined as follows,

$$
\begin{aligned}
\chi_0 &= \left(\sqrt{6a^2bN^3\sigma\left(6a^2bN^3\sigma - 2D^3\right)} + 6a^2bN^3\sigma - D^3\right) \\
\chi_1 &= \left(2\sqrt{3a^2bN^3\sigma\left(3a^2bN^3\sigma - D^3\right)} + 6a^2bN^3\sigma - D^3\right)
\end{aligned}
$$

It turns out that h scales as molecular parameters as follows,

$$h \sim \frac{a^{2/3} b^{0.4} \sigma^{0.4} N}{D^{0.05}} \tag{2}$$

By putting all calculated quantities back into Eq. (1), and recalling the Gibbs-Dohem relation $\Phi = -PV$, It's straightforward to calculate pressure or the equation of state of PBB just as $P = -\Phi/D$. Note that the grand potential is already written in the form of energy per surface area. The resulting equation of state is given as follows,

$$\begin{aligned} P &= \frac{k_{\mathrm{B}}T}{240\, a^4\, b\, N^4\, D^4}(435\, D^8 + 720\, a^2\, b\, D^5\, N^3 \sigma - 187\, D^7\, \chi_0^{1/3} - 192\, a^2\, b\, D\, N^3 \sigma \chi_1 \chi_0^{1/3} \\ &+ 187\, D^6\, \chi_0^{2/3} - 600\, a^2\, b\, N^3\, \sigma\, \chi_1\, \chi_0^{2/3} + 2\, D^4\, \chi_0^{1/3}\, \chi_2 + 4\, D^3\, \chi_0^{2/3}\, \chi_3) \end{aligned}$$

where the following quantities are defined,

$$\begin{aligned} \chi_2 &= (-351\, a^2\, b\, N^3\, \sigma + 151\, \sqrt{3\, a^2\, b\, N^3\, \sigma\, (3\, a^2\, b\, N^3\, \sigma - D^3)}) \\ \chi_3 &= (-558\, a^2\, b\, N^3\, \sigma + 169\, \sqrt{3\, a^2\, b\, N^3\, \sigma\, (3\, a^2\, b\, N^3\, \sigma - D^3)}) \end{aligned}$$

Looking more carefully at the equation of state, one can realize that this somewhat big formula simply indicates the following similarity relation,

$$P \sim (k_{\mathrm{B}}T) a^{1.3} b^{1.7} \sigma^{2.7} \left(\frac{N}{D}\right)^4 \tag{3}$$

Scaling theory

In Physics, it is possible to obtain relations between quantities of a system by using phenomenological arguments. Scaling theory is a powerful method which can solve the Physics problems that are difficult to handle by other methods. To solve the problem of PBB under

steady state shear, the phenomenological argument is as follows. When the PBB is sheared, at some critical moment the shear forces dominate the steric repulsion between monomers and the chains stretch in the shear direction. This situation is similar to the equilibrium situation but now chains stretched in the shear direction. So the shear stress and perpendicular stress swap their N power laws. Using this argument and introducing a scaling function in form of $\Xi(\dot{\gamma}) = \dot{\gamma}^{\alpha}$ with $\dot{\gamma} = 2v/D$ the shear rate and v the relative velocity of substrates, one can calculate α. To do so one needs to know both shear and perpendicular components of stress tensor at the regime of low shear rates (linear response regime). In equilibrium, the stress tensor components are the same but once the shear motion started, they become different. The perpendicular stress remains as before but the shear stress obtained by multiplying the shear viscosity and shear rate. Calculation of the shear viscosity needs information about what really happens at molecular scale. Every monomer travels freely until it gets a kick by either solvent molecules or other monomers. This distance is called mean-free-path λ and its duration is called mean-free-time τ. It's known that $\lambda = 1/4\sqrt{2}\pi a^2 n$ with n density of the system. For PBBs $n = 2N\sigma/D$ so the mean-free-path for PBBs is given as follows,

$$\lambda = \frac{D}{8\sqrt{2}a^2 N\sigma}$$

The mean-free-time could be calculated as $\tau = \lambda/v_{rms}$ with v_{rms} the root-mean-squared velocity of monomers. Since monomers undergo Brownian motion, their movement is diffusive and not ballistic. Therefore, $v_{rms} = \lambda/D_G$ with D_G the diffusion constant of the center of mass monomer. Here, I assume that every monomer diffuses with D_G.

Since, hydrodynamic interactions (HIs) are very important in biological systems, I describe the scaling theory in two cases of with and without the HIs.

PBB under steady state shear without the HIs

As the shear rate increases, at some critical moment the chains start to stretch in the shear direction. This critical moment is $\tau_c^R = \xi\, a^2\, N^{2\nu+1}/3\pi^2\, k_{\rm B}T$ which is the longest relaxation time of monomers. Therefore, the quantity $W = \tau_c^R \dot{\gamma}$ is unity at critical moment.

The chain extensions at linear response regime are given as follows,

$$\begin{aligned} R_s^R(W \ll 1) &= \left(\frac{5}{8\pi}\right)^{1/5} a^{2/5}\, b^{1/5}\, N^{3/5} \\ R_n^R(W \ll 1) &\sim \frac{a^{0.88}\, b^{0.4}\, \sigma^{0.38}}{D^{0.5}} N \end{aligned} \tag{4}$$

The diffusion constant of monomers in the Rouse dynamics with excluded volume interactions is $D_G^R = k_{\rm B}T/N\xi$.[20] So, the mean-free-time in this situation is given as follows,

$$\tau^R = \frac{D^2 \xi}{128\pi^2 a^4 \sigma^2 N k_{\rm B} T}$$

The viscosity in linear response regime is $\eta = P\tau^R$. By using the viscosity, the shear stress at low shear rate is given as follows,

$$\begin{aligned} \Pi_s^R(W \ll 1) &\sim \left(\frac{3k_{\rm B}T}{128}\right) \frac{b^{1.7}\sigma^{0.7} N^{2(1-\nu)}}{a^{4.7} D^2} W \\ \Pi_n^R(W \ll 1) &\sim (k_{\rm B}T) b^{1.7} \sigma^{2.7} a^{1.3} \left(\frac{N}{D}\right)^4 \end{aligned} \tag{5}$$

When shear rate gets higher that critical shear rate, the shear extension must scale as N. This argument determines the scaling function $\Xi = W^{1/5}$ for shear extension and $\Xi = W^{-1/5}$ for perpendicular extension.

$$
\begin{aligned}
R_s^R(W \gg 1) &= \left(\frac{5}{8\pi}\right) a^{2/5} b^{1/5} N^{3/5} W^{1/5} \\
R_n^R(W \gg 1) &\sim \frac{a^{0.88} b^{2/5} \sigma^{0.38} N}{D^{1/2}} W^{-1/5}
\end{aligned} \tag{6}
$$

Also, $\Xi = W^{(2\nu+2)/(2\nu+1)}$ for shear stress.

$$
\begin{aligned}
\Pi_s^R(W \gg 1) &\sim \left(\frac{3k_{\mathrm{B}}T}{128}\right) \frac{b^{1.7}\sigma^{0.7}N^{2(1-\nu)}}{a^{4.7}D^2} W^{(2\nu+2)/(2\nu+1)} \\
\Pi_n^R(W \gg 1) &\sim (k_{\mathrm{B}}T) b^{1.7}\sigma^{2.7}a^{1.3} \left(\frac{N}{D}\right)^4
\end{aligned} \tag{7}
$$

The kinetic friction coefficient at nonlinear response regime is given as follows,

$$
\mu^R(W \gg 1) \sim \left(\frac{3}{128}\right) \frac{D^2}{a^6\sigma^2N^3} W^{(2\nu+2)/(2\nu+1)} \tag{8}
$$

PBB under steady state shear with the HIs

In the presence of HIs, the Zimm dynamics is governed. In this dynamics, the diffusion constant of the monomers is $D_G^Z = k_{\mathrm{B}}T/\eta_s N^\nu a$ and the relaxation time of chains is $\tau_c^Z = \eta_s N^{3\nu} a^3/k_{\mathrm{B}}T$. The same calculations for the Zimm dynamics show that the mean-free-time with HIs is given as follows,

Table 1: Universal power laws of phyiscal quantities at nonlinear response regime ($W \gg 1$).

Quantity	Power	Quantity	Power	Quantity	Power
R_s^R	1/5	Π_s^R	1.46	μ^R	1.46
R_n^R	-1/5	Π_n^R	0	μ^Z	0.8
R_s^Z	0.23	Π_s^Z	0.8	η^R	0.46
R_n^Z	-0.23	Π_n^Z	0	η^Z	-0.2

$$\tau^Z = \frac{D^2 \eta_s}{128\pi^2 a^3 \sigma^2 N^{2-\nu} k_{\rm B} T}$$

For the shear chain extension $\alpha = 2/15\nu$ and for the perpendicular extension $\alpha = -2/15\nu$.

$$\begin{aligned} R_s^Z(W \gg 1) &\sim \left(\frac{5}{8\pi}\right)^{1/5} a^{2/5}\, b^{1/5}\, N^{3/5}\, W^{2/15\nu} \\ R_n^Z(W \gg 1) &\sim \frac{a^{0.88}\, b^{2/5}\, \sigma^{0.38}\, N}{D^{1/2}}\, W^{-2/15\nu} \end{aligned} \tag{9}$$

The shear stress at linear response regime is given as follows,

$$\Pi_s^Z(W \ll 1) \sim (k_{\rm B}T) \frac{b^{1.7} \sigma^{0.7} N^{(2+\nu)/3\nu}}{128\pi^2 D^2 a^{4.7}}\, W \tag{10}$$

$$\tag{11}$$

For the shear stress $\Xi = W^{2(1-2\nu)/3\nu}$ which leads to the following solution,

$$\begin{aligned} \Pi_s^Z(W \gg 1) &\sim (k_{\rm B}T) \frac{b^{1.7} \sigma^{0.7} N^{(2+\nu)/3\nu}}{128\pi^2 D^2 a^{4.7}}\, W^{(2-\nu)/3\nu} \\ \Pi_n^Z(W \gg 1) &\sim (k_{\rm B}T) b^{1.7} \sigma^{2.7} a^{1.3} \left(\frac{N}{D}\right)^4 \end{aligned} \tag{12}$$

The kinetic friction coefficient for the nonlinear response regime with HIs is given as follows,

$$\mu^Z(W \gg 1) \sim \frac{D^2}{128\pi^2 a^6 \sigma^2 N^{(13\nu-2)/3\nu}}\, W^{(2-\nu)/3\nu} \tag{13}$$

Table (1), summarizes universal power laws in nonlinear response regime.

Table 2: Numerical values of the simulation parameters.

Quantity	Value	Quantity	Value	Quantity	Value	Quantity	Value
dt	2×10^{-3}	T	1.68	r_c^{LJ}	$2^{1/6}$	b	2.09
N	30	ϵ	1	r_0	1.5	η_s	5
σ_g	10^{-1}	σ	1	k	30	D	20
ξ	5	a	1	r_c^{DPD}	2.5	ν	0.588

Molecular dynamic simulation

Another method to approach dynamical systems is to solve Newton's equation of motion. Molecular dynamic simulation is a numerical method based on solving Newton's equation of motion for every particle in the system. In this study, I employ the Leap-Frog algorithm to discrete the equations of motion. The Leap-Frog algorithm calculates the half-step velocities from old and current positions and then it calculates the current velocities from half-step velocities and current forces, and, in the final step it calculates future positions from current positions and velocities. The system is composed of two walls located at $z = 0$ and $z = D$ that are made arranging atoms in a 2D simple cubic lattice. The size of the wall is $L_x = 10\sigma$ and $L_y = 20\sigma$. The linear polymer chains are grafted to randomly chosen wall atoms. The periodic boundary conditions (PBC) is applied to the system to mimic the bulk properties. To mimic the shear motion, the bottom wall atoms move in the $+y$ direction and the top wall atoms move in the $-y$ direction with speed $v/2$. There are two types of conservative forces in the system as follows, The Lennard-Jones potential which mimics hard-core excluded volume interactions between particles,

$$U_{\mathrm{LJ}}(r) = 4\epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right) + C \qquad\qquad (r \leq r_c)$$

And the finitely-extensible-nonlinear-elastic (FENE) potential which connects monomers in the backbone of chains,

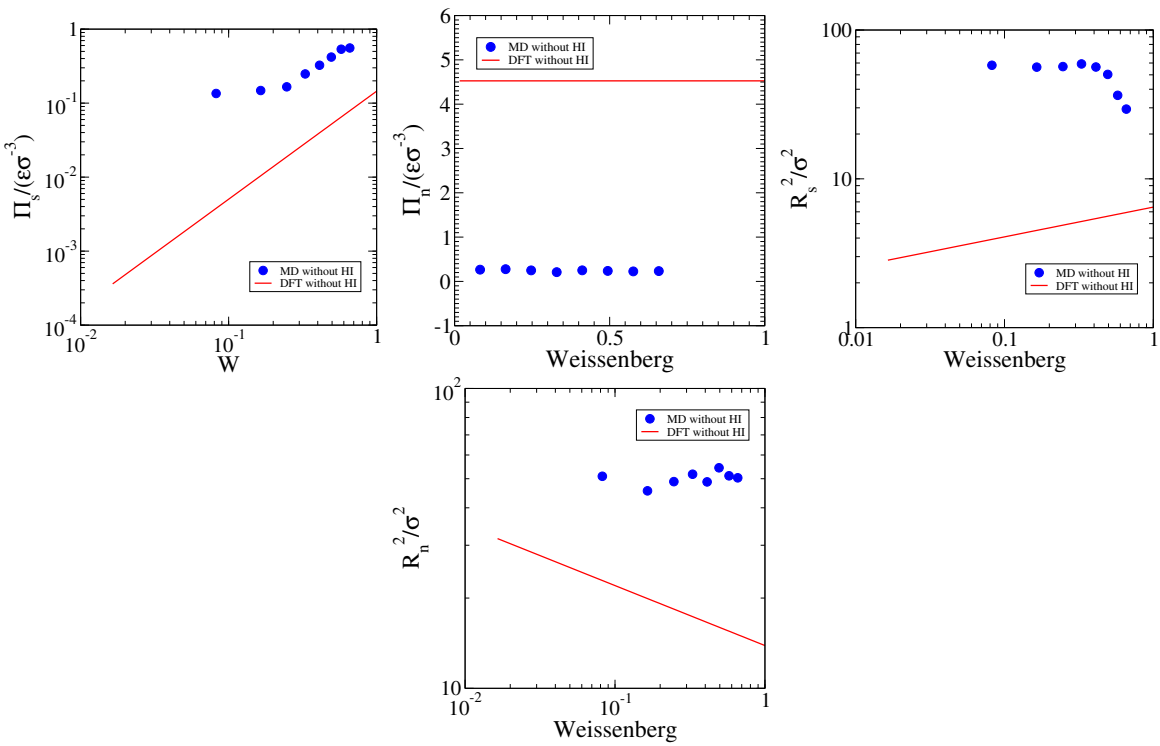

Figure 2: The shear and perpendicular stress and the shear and perpendicular extension as functions of Weissenberg number for MD and DFT calculations in the absence of HIs.

$$U_{\mathrm{FENE}}(r) = -\frac{1}{2}kr_0^2 \log\left(1 - \left(\frac{r}{r_0}\right)^2\right) \qquad (r \leq r_0)$$

For the systems without HIs, the Langevin thermostat is given as follows,

$$\begin{aligned} \boldsymbol{f}^D &= -\xi \boldsymbol{v} \\ \left\langle \boldsymbol{f}^R(t) \cdot \boldsymbol{f}^R(t') \right\rangle &= 2k_{\mathrm{B}}T\xi\delta(t-t') \end{aligned}$$

And for the systems with HIs, the dissipative particle dynamics (DPD) thermostat is given as follows,

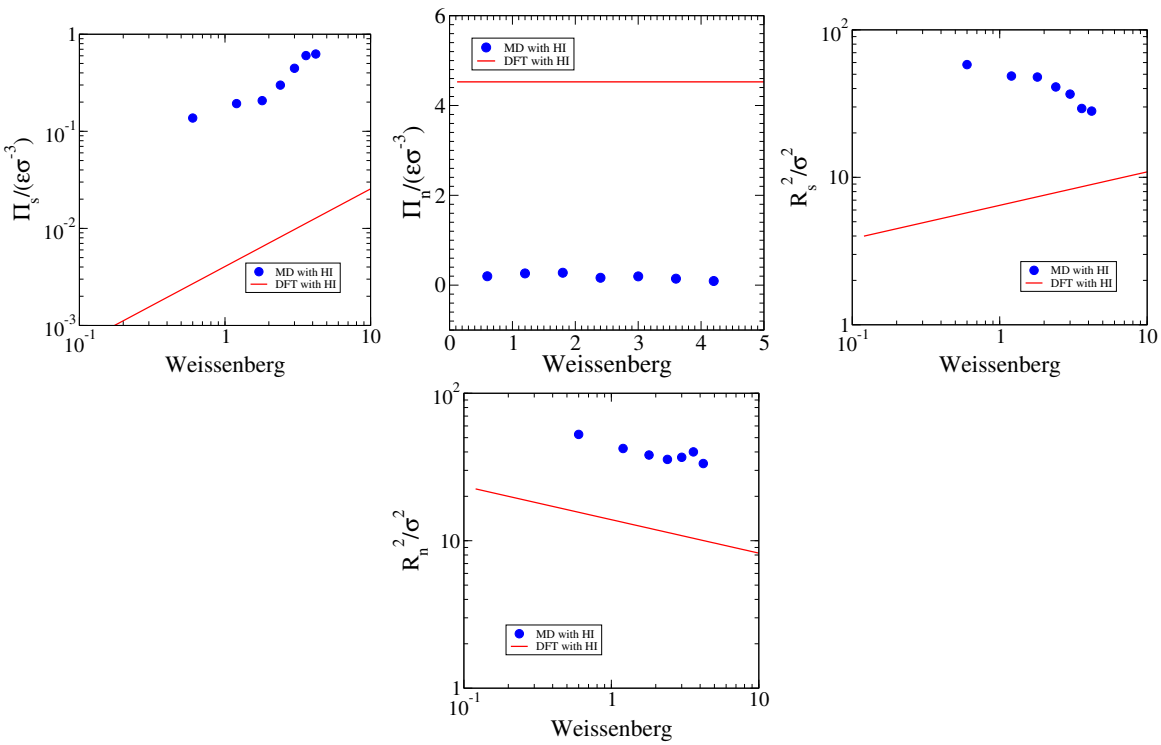

Figure 3: The shear and perpendicular stress and the shear and perpendicular extension as functions of Weissenberg number for MD and DFT calculations in the presence of HIs.

$$\boldsymbol{f}^D(r) = -\xi\omega^D(r)(\hat{\boldsymbol{r}}\cdot\boldsymbol{v})\hat{\boldsymbol{r}}$$
$$\boldsymbol{f}^R(r) = 2k_{\mathrm{B}}T\xi\omega^R(r)\boldsymbol{\Theta}$$

Where Θ is a random matrix with the following properties and $\omega^R(r)$ is a weight function as follows,

$$\langle\Theta_{ij}(t)\Theta_{kl}(t`)\rangle = (\delta_{ij}\delta_{jk}+\delta_{il}\delta_{jk})\delta(t-t`)$$
$$\omega^R(r) = (1-\frac{r}{r_c}), \qquad (r\leq r_c)$$

Note that in my simulation $\omega^D(r) = \omega^R(r)^2$. This type of simulation integrates over all quantum mechanical degrees of freedom and it's called Kremer-Grest model.[21,22] The

simulations without HIs have run for 10^5 time steps and the simulations with HIs for 2×10^5 time steps. Table (2), lists the numerical values of simulation parameters.

Results and conclusions

In this research, I tackle the PBBs under steady state shear by considering whether the HIs are present between the monomers or not. I develop a theory based on the DFT and scaling theory (phenomenological arguments) and compare its results with a MD simulation which is developed by myself. The results of this research is shown in Fig. (reffig:langevin) and (reffig:dpd). In each figure, the shear and perpendicular stress as well as the shear and perpendicular chain extension is shown. In Fig. (2), both simulation and theory show a perfect agreement on the shear and perpendicular stress. However, they differ in calculating chain extensions. The reason for this disagreement is the fact that I measure the end-to-end-distance which is highly fluctuating. It's plausible that by measuring the radius of gyration, this difference is removed. In Fig. (3), the simulation with implicit solvent and DPD fails to reflect the properties of the system in the presence of HIs. I also, separately, performed a simulation with DPD and explicit solvent (with total density 0.9) to check out if it can show the sub-linear regime in high Weissenberg number. Unfortunately, this simulation shows nothing meaningful and the shear stress does converge. This high fluctuation in stress tensor is certainly due to filling up the system by such big solvent molecules. My study reveals that the shear stress power law $W^{0.54}$ that is calculated by using the blob picture and MD in,[5] and any sub-linear regime presented in,[5,13–15] does not exist. In conclusion, I strongly reject the results presented in,[5,13–15] either theory or simulation and I would confidently say that these authors[5,13–15] are engaged in some sort of scientific fraud. Generally speaking, the only way to capture the effect of HI is to employ the Ossen's tensor in the simulation as well as in theory. Alternatively, if someone is interested in using explicit solvents to mimic the HIs, he/she has to use very small solvent molecules and very large number of them. In small

scales, the low Reynolds number conditions hold which means that the HIs are so strong that they dominate both gravity and inertia forces. Therefore, HIs have a key role in the dynamics at small scales which is the focus of this work. This opens a door to perform MD simulations with the Oseen's tensor which would be very very time-consuming task. Despite its difficulty, I would try to do that in the near future to reach the power law $W^{0.8}$ for shear stress.

Acknowledgments

This is my great honor to thank the Cold Spring Harbor Laboratory (CSHL) and the Regeneron Pharmaceuticals Inc. for financial support, Wolfram Research for Mathematica, the GNU for gfortran compiler, the Red hat Inc. for Fedora Linux, Tecplot Inc. for Tecplot visualization software, Weizmann Institute of Science for XMGrace.

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