Confirmation of stress-overshoot phenomena under biaxial elongational flow of ring-linear mixtures

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Recently, we have studied (linear-rich) ring-linear mixtures [1,2] using Kremer-Grest (KG) [3] bases coarse grained molecular dynamics (CGMD) simulations. To study linear-chain penetrations into rings, we performed topology analyses based on the Gauss linking number (GLN) for all pairs of linear and ring polymers. The probability distributions of the number of linear chain penetrations per ring (n_P) were evaluated. We have investigated the possibility of increase of n_P by some conditions in order to make rings to work as a movable cross-linkers.

In the preliminary simulations at the last year, we discovered the increase of n_P under biaxial elongational flows [4]. Here, we used our extended uniform extensional flow (UEF) method [5]. We also discovered the stress overshoot under the biaxial elongational flows. Although the stress overshoot under uniaxial elongational flows were reported, that under biaxial elongational flows had been not. Thus, we proposed the D-Class project to publish a paper as quickly as possible.

In the proposed D-Class project, we started systematic preparation of ring-linear blends. Here, we treated uncatenated rings and ring complexes such as catenanes and bonded-rings consist of two or three rings per complex as shown in Fig. 1. We studied the cases with ($N_{\rm linear}$, $N_{\rm ring}$) = (160,40), (160,80), (160,120), (160,160), (40,160), (10,160) and ring fraction was fixed to be about 0.1. Here, $N_{\rm linear}$ and $N_{\rm ring}$ denotes number of beads per a linear chain and a ring, respectively. To keep enough statistical precisions, we used large system sizes with approximate 0.7 M beads. As the initial relaxation run, we performed a tun with 10^9 MD steps for each system. As the MD solvers, we used LAMMPS [5] for preparations at the ISSP supercomputer. At later we also used HooMD-bule [6] on the GPUs for continuous product runs.

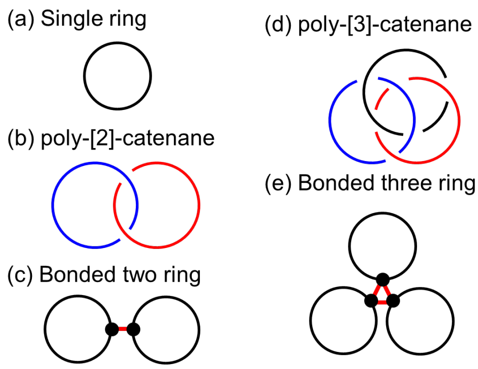

Fig. 1: Schematics of single ring, bonded-rings, poly-catenanes and ring-linear mixture.

In the present project, we developed a method to estimate n_P by using GLN. Here, the ends of linear chains are virtually connected to each other, but we prepared an extra linear chain and connected it to the original linear chain to form a cyclic chain as explained in our work [1,2]. For computation of GLN among cyclic chain and ring polymer, we used the Topoly Python package [7]. Figure 2 shows the probability distributions of linear chains penetrating into a single ring with (N_{linear}, N_{ring}) = (160,40), (160,80), (160,120), (160,160).

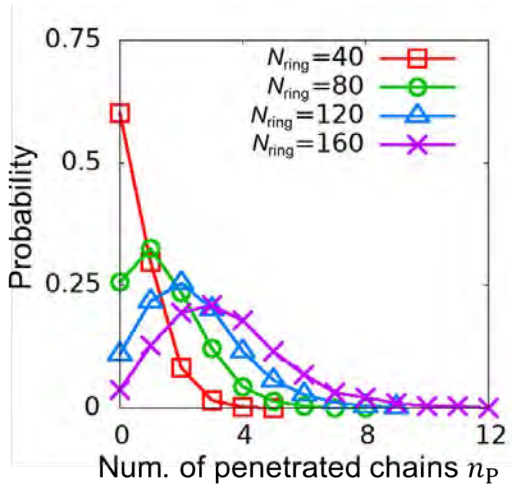

Fig. 2: Probability distributions of linear chains penetrating into a single ring with (N_{linear}, N_{ring}) = (160,40), (160,80), (160,120), (160,160).

In this project, we also performed deformed simulations with the deformation rate of 0.001 in order to grub preliminary results. As results, we obtained the key result for biaxial elongational flows as shown in Fig. 3.

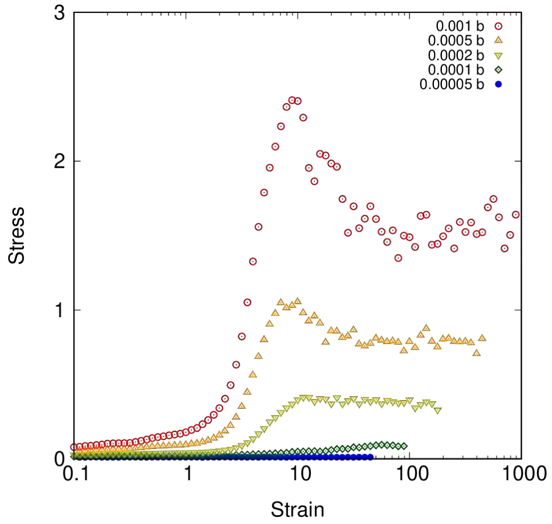

Fig. 3: Stress overshoot under biaxial elongational flows. (N_{linear}, N_{ring}) = (160,40)

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