Molecular Dynamics of Stretched Polymer Chains

Koichi MAYUMI, Kosuke AOMURA

Institute for Solid State Physics,

The University of Tokyo, Kashiwa-no-ha, Kashiwa, Chiba 277-8581

The segmental dynamics of polymer chains is the molecular origin of the entropic elasticity of polymeric materials [1]. When polymer chains are stretched, the molecular dynamics of polymer chains is restricted, and chain tension is increased with stretching. In this study, we have performed full-atomistic molecular dynamics simulations of stretched polymer chains in water.

A polyethylene glycol (PEG) chain consisting of 42 monomers was placed in a simulation box filled with 68,000 water molecules. The MD simulations were performed with GROMACS version 2021.1. The PEG chain was stretched at 0, 5, 10, 30, 70, 100, and 210 kJ/(mol nm). Fig.1 shows the intermediate scattering functions of PEG in the unstretched and stretched states (0 and 10 kj/(mol nm)). The segmental motion of the stretched chain becomes slow in the stretching direction (z-direction), while the chain dynamics in the directions perpendicular to stretching (x and y directions) is accelerated by stretching. This simulation result is consistent with our quasi-elastic neutron scattering results on the segmental motion of polymer chains in stretched PEG gels [1].

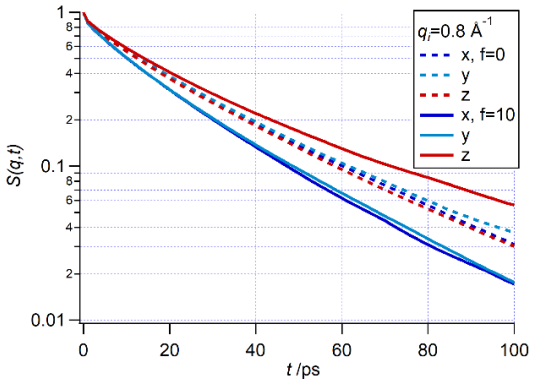

Fig. 1: Simulated intermediate scattering function of unstretched and stretched single PEG chain in water.

References

[1] M. Rubinstein, R. H. Colby, “Polymer physics”, Oxford university press (2003).

[2] K. Aomura, Y. Yasuda, T. Yamada, T. Sakai, K. Mayumi, Soft Matter, **19**, 147 (2023).