

Structure and dynamics of polyrotaxane in solution investigated by neutron scattering

Koichi Mayumi, Hitoshi Endo, Noboru Osaka, Hideaki Yokoyama, Mitsuhiro Shibayama, Kohzo Ito

Graduate School of Frontier Sciences, University of Tokyo and Institute for Solid State Physics, University of Tokyo

Supramolecular chemistry has developed novel polymer architectures composed of two or more molecules connected by non covalent bonds. One of the most fascinating supramolecules is polyrotaxane (PR), in which a linear polymer chain threads into cyclic molecules. Because of the unique molecular structure, PR has been applied to various nano materials [1]. Recently, a novel type of advanced polymer gels, called "slide ring (SR) gel", has been developed. By cross linking the ring molecules on different PRs, the linear polymers are connected by dimmers of the cyclic molecules. When SR gels are deformed, the linear polymers move through the crosslinked rings and chain lengths between the crosslinks are adjusted freely to minimize the local stress in the gels. The polymer dynamics through the crosslinks gives rise to remarkable mechanical properties of SR gels.

We investigated the structure of PR in solution by means of small angle neutron scattering (SANS). We calculated static partial scattering functions for PR solutions based on the scattering function of worm like chains. By analyzing the scattering functions of PR measured by SANS, we evaluated quantitatively the distribution of CDs along PEG and conformation of PEG in PR [2]. We also studied the monomer diffusion of PR by using neutron spin echo (NSE) technique [3]. NSE determined the monomer diffusion constant of PR in solution to be about one third as small as that of free PEG without CDs.

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