Structure characterization of model tetra-poly(acrylic acid) gel

Caidric Gupit[1], Mitsuhiro Shibayama[1], Xiang Li[2]

[1]ISSP-NSL, Univ. of Tokyo, [2]Hokkaido Univ.

Polyelectrolyte gels are networks of charged polymers with macro-ions fixed on the polymer chains. This type of material is widely used in the industry, with applications in medicine, cosmetics, food, textile, packaging, agriculture, wastewater treatment, chemical separation, energy systems, and petroleum industries. A main attribute of polyelectrolytes is the strong interchain correlation both topologically and electrostatically. This is experimentally observed using light, X-ray, and neutron scattering techniques. Due to this strong correlation, the structure and properties of polyelectrolytes are complicated functions of multiple variables including polyelectrolyte concentration, pH, temperature, and degree of neutralization. It is even more complicated for polyelectrolyte gels due to the presence of crosslinks. Therefore, understanding of the structure-property relationship of polyelectrolyte gels remains limited. This is also partly due to the high degree of network heterogeneity and the poor control over the structure such as the chain length between neighboring crosslinks.

A model polyelectrolyte gel, tetra-poly(acrylic acid) (tetra-PAA) gel, was previously synthesized by end-linking tetra-arm polymers via click chemistry. However, small-angle scattering studies revealed a sharp upturn with decreasing scattering wave vector q in the scattering profile. This originates from heterogeneities in the network structure, presumably introduced by the crosslinking process and the solvation conditions of the polyelectrolytes. Recent studies by our research group achieved a more facile fabrication of a model, homogeneous neutral gel using the bond percolation scheme. To apply this scheme to tetra-PAA system, in this SANS study, we studied the solvation conditions of the tetra-PAA with different end-groups in D2O.

Due to the limited beam time, we only tested two solution samples. The SANS profiles of tetra-PAA solutions in D2O are shown in Fig. 1. While the profiles of tetra-PAA with N3 end-groups could be fitted with Orenstein Zernike (OZ) functions very well, the profiles of tetra-PAA MA showed a non-OZ type behavior, suggesting the presence of small aggregations. The upturn in the low-q limit ($q < 0.004$Å^{-1}) in tetra-PAA-N3 should be the artifact due to the incident beam. We will further perform the structure analysis on these prepolymers and found the proper solvation conditions to achieve the bond percolation.

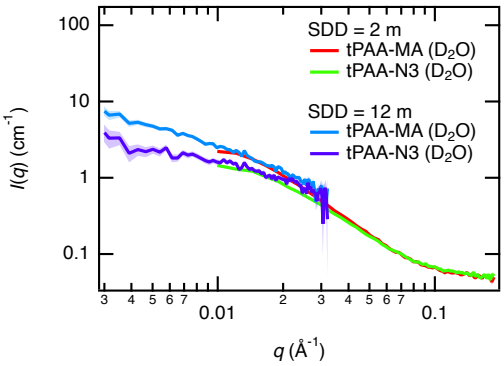

Figure 1. SANS profiles of tetra-PAA solutions with maleimide (MA) and azide (N3) end groups using D2O as solvent, at sample-to-detector (SDD) distances of 2 m and 12 m.