Neutron Diffraction Study of Hydrogels

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Hydrogels are unique materials that can contain a large amount of water in their three-dimensional polymer chain networks. The water content varies from a dry state to nearly 98 wt% [1,2]. Because of characteristic properties of water, hydrogels are widely used as biomedical materials. The structure of water is thus an important factor governing the chemical and physical properties of hydrogel materials.

We used neutron diffraction to probe the structure of D_2O in poly-*N*,*N*,-dimethylacrylamide (PDMAA) hydrogel. Two PDMAA hydrogels with high and low D_2O-content W (W = 0.9 and 0.5) were prepared. The neutron diffraction measurements were performed using the Wide Angle Neutron Diffractometer (WAND) [3] at the High Flux Isotope Reactor in Oak Ridge, USA. The samples were rapidly cooled using liquid nitrogen, and then heated from 10 to 300 K.

The neutron diffraction profiles of the high D_2O-content PDMAA gel (W = 0.9) have strong sharp peaks below 270 K that are similar to diffraction patterns of hexagonal ice Ih. At 300 K, the profile has a broad liquid-like diffraction feature. The profile of the gel at W = 0.5 has a broad band in the 2θ range from 20°–28° below 230 K that are similar to diffraction pattern of glassy water. Sharp peaks are observed in the profile at 230 K. The feature of the profile is similar to that of cubic ice. The profile at 260 K has ice Ih-like strong peaks.

Our neutron diffraction results show the existence of ice in hydrogels and that the structure of ice depends on the water content of the hydrogel. The structural changes of ice in hydrogels might have important implications in the interpretation of hydrogel properties, for both biological tissues and synthetic gel materials

References

[1] Y. Sekine, and T. Ikeda-Fukazawa, J. Chem. Phys. **130**, 034501 (2009).
[2] Y. Sekine, and T. Ikeda-Fukazawa, J. Phys. Chem. B **114**, 3419 (2010).
[3] S. Katano *et al.* Physica B **241**, 198 (1998).