Structure of Water and Ice in Poly-N,N,-dimethylamide Hydrogel

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Water behavior in hydrogels is one of the important factors governing their properties. To investigate water structure in a hydrogel, neutron diffraction measurements were performed on poly-N,N,-dimethylacrylamide (PDMAA) hydrogel swollen in D₂O in temperature range of 10 to 300 K. The neutron diffraction pattern of PDMAA hydrogel changed with temperature. At temperature above 273 K, there was a broad band in 2θ range of 18 to 45°. The broad band disappeared at around 260 K and the sharp peaks at around 21°, 23°, 24°, 32°, and 38° were observed at temperature below 260 K. The results show that the D₂O exists as water in the hydrogel at 273 to 300 K, and transformed to ice Ih below 260 K. By comparing the diffraction patterns of D₂O, we investigated the structure of the water and ice in detail. The results show that the average distance between water molecules in the hydrogel is larger than that of bulk water. This indicates that the water in the swollen hydrogel has lower density than that of bulk water. The changes of the Bragg peak profiles of ice formed in the hydrogel show that the high-density ice Ih consisting disordered water molecules exists in the hydrogel below 260 K. The present results suggest that the polymer network of hydrogels effects to water and ice structure. The structural changes of water and ice in a hydrogel might have important implications for the interpretation and development of gel materials and gel systems such as biomaterials and foods.