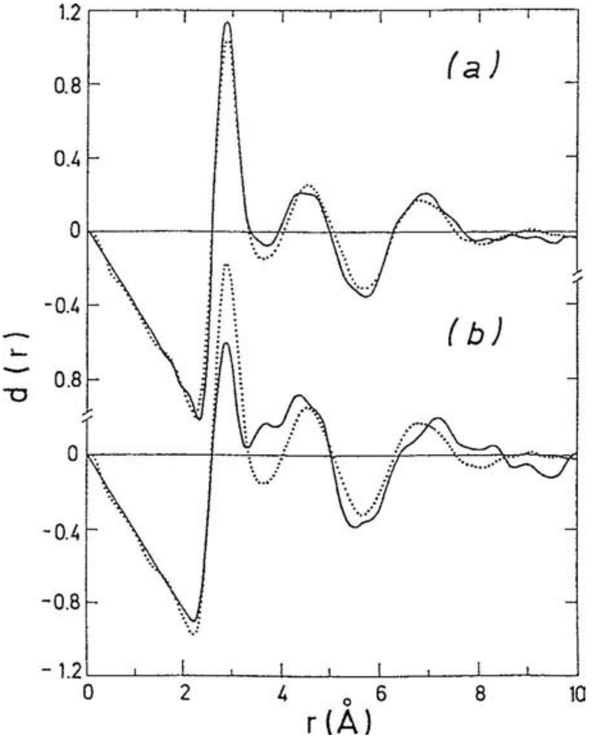

FIGURE 3 X-ray pair correlation function $d(r)$ of water contained in activated carbon, at room temperature, shown by solid lines for 188% (curve a) and 42% hydration (curve b). For comparison, the $d(r)$ of bulk water at the same temperature is also drawn (*dotted line*). *Source*: From Ref. 43.

appears that, at the lowest investigated water content, 42% hydration level, a distortion of the tetrahedral ordering is clearly observed (Fig. 3). Neutron-scattering experiments can be analyzed to describe the intermolecular correlations (Fig. 4). At the same lower level of hydration, the hydrogen bonding is modified and water molecules are more ordered. It is not possible to determine the thickness of the affected layer. However, a crude determination from the specific area indicates that for a hydration equal to 50%, the thickness does not exceed 5 Å. This value must be compared with the computer simulation data (32–37), which indicate that structural modifications do not extend beyond 10 Å from the solid surface. When partially hydrated samples are cooled down to 77 K, no crystallization peak is detected by differential thermal analysis. Both X-ray and neutron diffraction show that an amorphous form is obtained and its structure is different from those of low- and high-density amorphous ice already known (5). This phenomenon looks similar in both hydrophilic and hydrophobic model systems. However, to characterize more precisely the nature of the amorphous phase, the site-site partial correlation functions need to be experimentally obtained and compared with those deduced from molecular dynamics simulations.

Macromolecules-Water Interactions

The structure of water near polymeric membranes (52) has been studied by neutron diffraction. The structure of water confined in a hydrogel has been