

for the surfaces and more certainly because of difficulties in choosing suitable potential functions for the simulations. However, molecular dynamic simulations of the hen egg white lysozyme–Fab D1.3 complex have been reported; both the crystal state and the complex in solution were studied (42). The findings are consistent with the observation by various experimentalists of reduced water mobility in a region extending several angstroms beyond the first hydration layer (64–67), as reported also from CMD simulations (70).

From the above comparison, it seems clear that there are considerable discrepancies in the degrees of slowing down between NMR experiments and CMD. This is especially true for the translational diffusion constant.

A way to resolve these discrepancies has been recently attempted by quasi-elastic and inelastic neutron scattering. Neutron scattering is a powerful and unique tool for studying the self-dynamics of interfacial water; actually the large incoherent scattering cross-section of the protons yields unambiguous results about the individual motions of water molecules (31). In fact, this technique is a method for studying the diffusive motion of atoms in solids and liquids (71). It gives access to the correlation function for the atomic motions which are explored over a space domain of a few angstroms and for times of the order of  $10^{-12}$  seconds. This space and time domain makes the comparison between neutron scattering and CMD better justified. The correlation function can be calculated by various models of the motions of the particles (e.g., Brownian motion, jump diffusion, diffusion in a confined space, rotational motion, etc.). Microscopic properties of the molecules, such as the residence time, the jump length, the self-diffusion coefficients, the hydrogen bond lifetime can be evaluated as well.

Another quantity that can be obtained is the vibrational density of states of mobile protons, in particular the translational and librational modes for water of hydration as compared with that of bulk water.

This method has been used with success for studying the self-dynamics of bulk water as a function of the temperature (72), as previously reported.

Previous studies about dynamics of water near interfaces by quasi-elastic neutron scattering involved the mobility of water on the surface of Nafion membranes (73,74), the diffusive motions and the density of states of water in silica gels (75) and the interfacial melting of ice in graphite and talc powders (76). It is interesting to note that quasi-elastic scattering like effects for extremely small wave vectors can be observed in the pulsed gradient spin-echo NMR experiments. The latter technique has been used for studying diffusion of water in both permeable (77) and connected structures where the effects of confinement can be clearly identified (78).

### **Model Surface Water Systems**

A complete study of the self-dynamics of water close to some well-defined hydrophilic surface as the Vycor surface has been performed by quasielastic and inelastic neutron scattering. It has been done for levels of hydration ranging from full hydration down to the lowest one (25%), corresponding to one monolayer coverage of water molecules. The effect of temperature has also been studied. We report here the main results (79).

The short-time diffusion (few picoseconds) of water molecules close to the Vycor surface has been described in terms of simple models for all the studied samples (80). At short times, the water molecules, close to some hydrophilic