

the trimers Gly-Gly-Gly and Gly-Leu-Gly shows, in particular, that the onset of water dynamics observed at low temperatures (i.e., around 200 K) is sharper for the case of Gly-Leu-Gly because of its hydrophobic chain (86,87). Indeed, in this case, a network of intermolecular hydrogen bonds is formed in a stable way avoiding translational diffusion at low temperatures. In the case of Gly-Gly-Gly, the transition is more gradual, because, prior to translational diffusion, one observes rotational motions at intermediate temperatures. It was also shown that this temperature dependence (sometimes called a *dynamic* or a *glass* transition of the protein) depends drastically on the interaction between water molecules within a first layer on the surface of the protein and on the local hydrophobicity of each site, as well as on its spatial extent.

CONCLUSION

From the more recent findings combining neutron techniques and molecular dynamics simulations, it is now possible to have a more precise picture of confined water. Water, in the vicinity of a hydrophilic surface, is in a state equivalent to bulk water at a lower temperature. As previously demonstrated, this depends on the degree of hydration of the sample. In particular, at room temperature, interfacial water shows a dynamic behavior similar to that of bulk water at a temperature 30 K lower. It behaves like bulk supercooled water.

It appears that the short-time dynamics of water molecules at or near a hydrophilic model surface and at a soluble protein surface is much slower as compared with that of bulk water. It is important to notice that the more significant slow dynamics of interfacial water is reflected in the long residence time for jump diffusion. This suggests that there may be a common underlying mechanism for the slowing down of the single-particle dynamics of interfacial water.

This is the consequence of the confined diffusion theory, which has been used to analyze the quasi-elastic neutron-scattering data. This simple theory gives information on the confinement volume and the slow dynamics of the single-particle motions. To understand the microscopic origin of the confinement and slowing down of motions of water molecules and the exact role played in this context, the theory of kinetic glass transition in dense, supercooled liquids (88,89) has been recently used. This theory leads to some description of the dynamics of confined water in terms of correlated jump diffusion (90) instead of jump diffusion (72). This description looks consistent with molecular dynamics simulations of supercooled water (91) and has been confirmed by high-resolution quasi-elastic neutron-scattering experiments of water from hydrated Vycor (92) and from hydrated C-phycoyanin protein (93).

This more sophisticated way shows a large distribution of residence times for water molecules in the cage formed by the neighboring molecules, which is a more realistic view than the sharp separation of water molecules into two classes, according to their mobility (59). Short-time dynamics results about hydrated myoglobin have been recently interpreted by using this same theory of kinetic glass transition in dense, supercooled liquids (83).

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